Computational Fluid Dynamics Modeling of the Effects of Water Injection in a Diesel Engine

Rabun Z. Wallace
Georgia Southern University

Follow this and additional works at: https://digitalcommons.georgiasouthern.edu/etd

Part of the Automotive Engineering Commons, Computer-Aided Engineering and Design Commons, and the Heat Transfer, Combustion Commons

Recommended Citation
https://digitalcommons.georgiasouthern.edu/etd/1365
COMPUTATIONAL FLUID DYNAMICS MODELING OF THE EFFECTS OF WATER INJECTION IN A DIESEL ENGINE

by

RABUN WALLACE

(Under the Direction of Cheng Zhang)

ABSTRACT

Water injection has been used in internal combustion engines for many years. It has been used to cool combustion temperatures, reduce emissions, and in some instances clean carbon buildup from the cylinder. Research has shown that the water to fuel mass ratio is most effective between 20-30%, so the upper and lower limit were used for simulations in Converge CFD. To validate the CFD model, a case without water injection was compared to experimental data from Sandia National Laboratory. The predicted in-cylinder pressure and heat release rate showed good agreement with the experimental data. Cases were run with the injection of the water at 65 and 95 degrees BTDC to increase vaporization and reduce wall film. The water droplet size injected was the principal focus of the study as its effects on emissions had not been investigated. The water droplet sizes used were 0.196, 0.210, 0.240, 0.286 µm. The 0.196 µm droplet was chosen because it was equivalent to the fuel droplet diameter. The others were from literature research for tests done on the effect injected water droplet sizes had on the flame length and speed. It was found that the highest reduction in temperature and pressure was observed with the
water injected closer to TDC; however, this commonly resulted in larger emissions reductions. Also, increasing the water mass ratio generally reduced the temperature, pressure, and heat release rate more, which often further reduced the emissions. Maximum NOx reductions of 5.61\% using the 0.210 μm droplet size with 20\% water and 7.66\% using the 0.240 μm droplet size with 30\% water were observed. Droplet size comparison showed up to a 9.67\% variation in the NOx formation. Simulations were then run by changing the temperature of the water being injected ±20K from the original temperature of 368K. The decreased water temperature cases showed a larger variation between the results for the NOx formation in water injected at 65 and 95 degrees BTDC. Water was then injected at TDC which showed a 48.3\% reduction of NOx. However, all other emissions and combustion properties were negatively affected with the TDC injection timing.

INDEX WORDS: Computational Fluid Dynamics, Diesel Engine, Combustion, Water Injection, NOx, Emissions
COMPUTATIONAL FLUID DYNAMICS MODELING OF THE EFFECTS OF
WATER INJECTION IN A DIESEL ENGINE

by

RABUN WALLACE

B.S. Georgia Southern University, 2011

M.S., Georgia Southern University, 2015

A Dissertation Submitted to the Graduate Faculty of Georgia Southern University in

Partial Fulfillment of the Requirements for the Degree

MASTER OF APPLIED ENGINEERING

STATESBORO, GEORGIA
COMPUTATIONAL FLUID DYNAMICS MODELING OF THE EFFECTS OF WATER INJECTION IN A DIESEL ENGINE

by

RABUN WALLACE

Major Professor: Cheng Zhang
Committee: Aniruddha Mitra
Mosfequr Rahman

Electronic Version Approved:
Fall 2015
ACKNOWLEDGEMENTS

First, I would like to thank my Savior Jesus Christ for all I have been given and for blessing me with the opportunity to pursue my graduate degree. Also, I would like to thank my family for all of the love and support given to me during the completion of my education. Especially I would like to thank my parents, Steve and June Wallace, and my aunt and uncle, Jan and Lewis Faucett, for everything that they did for me through this time. As well, a special thanks to my sister and brother-in-law, brother and his family, grandmothers, and aunt for all of their support. Without them I would not have been able to make it through successfully. Also, I want to thank all of my friends who supported and encouraged me to pursue my degree. I want to thank the staff and professors in the Mechanical Engineering department of Georgia Southern University for their help and direction during the past couple of years while I completed my degree. Their knowledge and experience was a crucial component of my ability to learn advanced engineering concepts and prepare for my career as an engineer. In particular, I would like to thank Dr. Zhang for being my advisor and helping direct me through my research. As well, I would like to thank my thesis committee, Dr. Rahman and Dr. Mitra, for their help, encouragement, and support during my graduate collegiate career. They were instrumental in aiding me to learn important skills that were and will continue to be very beneficial to me. These are just a few people who have been a part of my experience in higher education and have aided me along the way. Each one of these people played a key role in helping me through and making my experience much easier and more enjoyable. Something this important takes many people to succeed and my experience was no exception. Thank you to all mentioned and all who are not directly specified but who had a role, no matter how small, in supporting me during this time.
NOMENCLATURE

°F – Degree Fahrenheit

ATDC – After Top Dead Center

BTDC – Before Top Dead Center

BSU – Bosch Smoke Unit

°C – Celsius

C14H30 – Decane

CAD – Computer Aided Drawing

CFD - Computational Fluid Dynamics

CO - Carbon Monoxide

CO2 - Carbon Dioxide

DI – Direct Injection

EGR – Exhaust Gas Recirculation

FEA – Finite Element Analysis

g/kgf – Gram Per Kilogram Fuel

H2O – Water

HO2 – Hydroperoxyl
HRR – Heat Release Rate

ICE - Internal Combustion Engine

J/deg - Joules Per Degree

K – Kelvin

kJ/Kmol*K – Kilojoule Per Kilomol * Kelvin

kPa – Kilopascal

m – Meter

m - Mole

m/s - Meter Per Second

mg – Milligram

mm – Millimeter

MPa – Megapascal

N – Nitrogen

N2 – Nitrogen Molecule

NO – Nitric Oxide

NO2 – Nitrous Dioxide

NOx - Nitrogen Oxides
O – Oxygen

O2 – Oxygen Molecule

OH – Hydroxide

P - Pressure

Pa – Pascal

ppm – Parts Per Million

Q - Heat Transfer

Q H - High Heat Transfer

Qnet - Net Heat Transfer

R - Gas Constant

rpm - Revolutions Per Minute

S – Entropy

SI - Spark Ignition

SOx – Sulfer Oxides

T - Temperature

TDC – Top Dead Center

U - Internal Energy
V - Volume

W - Work

Wnet - Net Work

\(\eta_{th}\) – Thermal Efficiency

\(\mu m\) – Micrometer
# TABLE OF CONTENTS

ACKNOWLEDGEMENTS ........................................................................................................... 6
NOMENCLATURE ......................................................................................................................... 7
LIST OF TABLES .......................................................................................................................... 12
LIST OF FIGURES ........................................................................................................................ 13

## CHAPTERS

1 **INTRODUCTION** ................................................................................................................. 22
   Motivation ................................................................................................................................. 22

2 **LITERATURE REVIEW** ....................................................................................................... 26
   Internal Combustion Engine .................................................................................................... 26
   Water Injection ......................................................................................................................... 32
   Computer Simulation ............................................................................................................. 37

3 **METHOD** .......................................................................................................................... 45

4 **RESULTS** ............................................................................................................................ 51
   Model Verification ................................................................................................................... 51
   Effects of Water Droplet Size ................................................................................................. 57
     *20% Water Injected at 65 Degrees BTDC* ........................................................................... 57
     *20% Water Injected at 95 Degrees BTDC* ........................................................................ 67
     *30% Water Injected at 65 Degrees BTDC* ........................................................................ 77
     *30% Water Injected at 95 Degrees BTDC* ........................................................................ 85
   Effects of Water Temperature Variation ............................................................................. 93
   Effects of Water Injection at TDC ......................................................................................... 103

5 **DISCUSSION** ..................................................................................................................... 111
   Comparison to Literary Research Results ............................................................................ 131

6 **CONCLUSION** .................................................................................................................... 134

**REFERENCES** ....................................................................................................................... 137

**APPENDICIES**

A **ANSYS Fluent Chemical Mechanisms** ................................................................................ 142
B **Converge CFD Chemical Mechanism** ............................................................................. 147
LIST OF TABLES

Table 1 : Zeldovich Mechanism and Supplementary Reactions for NOx Formation.................. 34
Table 2 : Boundary Conditions for the Experimental Sandia Engine..................................... 46
Table 3 : 20% Water Droplet Size Variation at 65 and 95 Degrees BTDC (Reduction = +)..... 113
Table 4 : 30% Water Droplet Size Variation at 65 and 95 Degrees BTDC (Reduction = +)..... 116
Table 5 : Water Temperature Variation Results and Percent Difference (Reduction = +)....... 119
LIST OF FIGURES

Figure 1: P-V and T-S Diagrams for Gasoline Engines.................................................................29

Figure 2: P-V and T-S Diagrams for Diesel Engines......................................................................31

Figure 3: Verification of Converge CFD Simulation for Water Injection Effects............................48

Figure 4: Validation of Converge CFD Simulation Model without Water........................................52

Figure 5: Results for Mesh Size Independence and Convergence Simulations............................53

Figure 6: Pressure Curve Results for Varied Cone Angle and Mesh Size.........................................54

Figure 7: Heat Release Rate Comparison for Simulation to Experimental Results..........................55

Figure 8: Soot Level Comparison for the Simulation to the Experimental Results.........................56

Figure 9: Effects of Water Particle Size on the Combustion Temperature Curve (20% Water Injected at 65 Degrees BTDC)
   A) Effects on Temperature...........................................................................................................57
   B) Effects on Peak Temperature.................................................................................................58
   C) Effects on Temperature During Pre-Combustion.....................................................................58

Figure 10: Effects of Water Particle Size on the Combustion Pressure Curve (20% Water Injected at 65 Degrees BTDC)
   A) Effects on Pressure................................................................................................................60
B) Effects on Peak Pressure.............................................................................................................60

Figure 11: Effects of Water Particle Size on the Combustion Heat Release Rate Curve (20% Water Injected at 65 Degrees BTDC)

A) Effects on Heat Release Rate.............................................................................................................61

B) Effects on Peak Heat Release Rate.............................................................................................................62

Figure 12: Effects of Water Particle Size on the NOx Formation Curve (20% Water Injected at 65 Degrees BTDC)

A) A) Effects on NOx Formation.............................................................................................................63

B) Effects on Peak NOx.............................................................................................................................63

Figure 13: Effects of Water Particle Size on the Soot Formation Curve (20% Water Injected at 65 Degrees BTDC)

A) Effects on Soot Formation.............................................................................................................................64

B) Effects on Expansion Stroke Soot.....................................................................................................................65

Figure 14: Effects of Water Particle Size on the CO Formation Curve (20% Water Injected at 65 Degrees BTDC)

A) Effects on CO Formation.............................................................................................................................66

B) Effects on Expansion Stroke CO.....................................................................................................................66

Figure 15: Effects of Water Particle Size on the Combustion Temperature Curve (20% Water Injected at 95 Degrees BTDC)
A) Effects on Temperature

B) Effects on Peak Temperature

C) Effects on Pre-Combustion Temperature

Figure 16: Effects of Water Particle Size on the Combustion Pressure Curve (20% Water Injected at 95 Degrees BTDC)

A) Effects on Pressure

B) Effects on Peak Pressure

Figure 17: Effects of Water Particle Size on the Combustion Heat Release Rate Curve (20% Water Injected at 95 Degrees BTDC)

A) Effects on Heat Release Rate

B) Effects on Peak Heat Release Rate

Figure 18: Effects of Water Particle Size on the Combustion NOx Formation Curve (20% Water Injected at 95 Degrees BTDC)

A) Effects on NOx Formation

B) Effects on Peak NOx Formation

Figure 19: Effects of Water Particle Size on the Combustion Soot Formation Curve (20% Water Injected at 95 Degrees BTDC)

A) Effects on Soot Formation
B) Effects on Expansion Stroke Soot

Figure 20: Effects of Water Particle Size on the Combustion CO Formation Curve (20% Water Injected at 95 Degrees BTDC)

A) Effects on CO Formation

B) Effects on Expansion Stroke CO

Figure 21: Effects of Water Particle Size on the Combustion Temperature Curve (30% Water Injected at 65 Degrees BTDC)

A) Effects on Temperature

B) Effects on Peak Temperature

C) Effects on Pre-Combustion Temperature

Figure 22: Effects of Water Particle Size on the Combustion Pressure Curve (30% Water Injected at 65 Degrees BTDC)

A) Effects on Pressure

B) Effects on Peak Pressure

Figure 23: Effects of Water Particle Size on the Combustion Heat Release Rate Curves (30% Water Injected at 65 Degrees BTDC)

A) Effects on Heat Release Rate

B) Effects on Peak Heat Release Rate
Figure 24: Effects of Water Particle Size on the Combustion NOx Formation Curve (30% Water Injected at 65 Degrees BTDC)

A) Effects on NOx Formation........................................................................................................82

B) Effects on Peak NOx.................................................................................................................82

Figure 25: Effects of Water Particle Size on the Combustion Soot Formation Curve (30% Water Injected at 65 Degrees BTDC)

A) Effects on Soot Formation........................................................................................................83

B) Effects on Peak Soot.................................................................................................................83

Figure 26: Effects of Water Particle Size on the Combustion CO Formation Curves (30% Water Injected at 65 Degrees BTDC)

A) Effects on CO Formation........................................................................................................84

B) Effects on Peak CO..................................................................................................................84

Figure 27: Effects of Water Particle Size on the Combustion Temperature Curve (30% Water Injected at 95 Degrees BTDC)

A) Effects on Temperature........................................................................................................86

B) Effects on Peak Temperature................................................................................................86

C) Effects on Pre-Combustion Temperature................................................................................87

Figure 28: Effects of Water Particle Size on the Combustion Pressure Curve (30% Water Injected at 95 Degrees BTDC)
A) Effects on Pressure ......................................................................................................................88

B) Effects on Peak Pressure ..............................................................................................................88

Figure 29: Effects of Water Particle Size on the Combustion Heat Release Rate Curve (30% Water Injected at 95 Degrees BTDC)

A) Effects on Heat Release Rate ...........................................................................................................89

B) Effects on Peak Heat Release Rate ....................................................................................................89

Figure 30: Effects of Water Particle Size on the Combustion NOx Formation (30% Water Injected at 95 Degrees BTDC)

A) Effects on NOx Formation .................................................................................................................90

B) Effects on Peak NOx ............................................................................................................................91

Figure 31: Effects of Water Particle Size on the Combustion Soot Formation (30% Water Injected at 95 Degrees BTDC)

A) Effects on Soot Formation ..................................................................................................................92

B) Effects on Expansion Stroke Soot ........................................................................................................92

Figure 32: Effects of Water Particle Size on the Combustion CO Formation (30% Water Injected at 95 Degrees BTDC)

A) Effects on CO Formation ...................................................................................................................93

B) Effects on Expansion Stroke CO ........................................................................................................93
Figure 33: Effects of the Water Temperature on the Combustion Temperature Curve

A) Effects on Temperature ................................................................. 95

B) Effects on Peak Temperature ........................................................... 96

C) Effects on Pre-Combustion Temperature .............................................. 96

Figure 34: Effects of the Water Temperature on the Combustion Pressure Curve

A) Effects on Pressure ................................................................. 97

B) Effects on Peak Pressure ............................................................. 97

Figure 35: Effects of the Water Temperature on the Combustion Heat Release Rate Curve

A) Effects on Heat Release Rate ................................................................. 98

B) Effects on Peak Heat Release Rate ................................................... 98

Figure 36: Effects of the Water Temperature on the Combustion NOx Formation

A) Effects on NOx Formation ................................................................. 99

B) Effects on Peak NOx ................................................................. 100

Figure 37: Effects of the Water Temperature on the Combustion Soot Formation

A) Effects on Soot Formation ................................................................. 101

B) Effects on Expansion Stroke Soot .................................................. 101

Figure 38: Effects of the Water Temperature on the Combustion CO Formation
A) Effects on CO Formation.................................................................102

B) Effects on Peak CO......................................................................102

Figure 39: Effects of TDC Water Injection Timing on the Combustion Temperature Curve

A) Effects on Temperature....................................................................103

B) Effects on Peak Temperature...............................................................104

C) Effects on Pre-Combustion Temperature...........................................104

Figure 40: Effects of TDC Water Injection Timing on the Combustion Pressure Curve

A) Effects on Pressure............................................................................105

B) Effects on Peak Pressure.................................................................105

Figure 41: Effects of TDC Water Injection Timing on the Combustion HRR Curve

A) Effects on Heat Release Rate..............................................................106

B) Effects on Peak Heat Release Rate....................................................106

Figure 42: Effects of TDC Water Injection Timing on the Combustion NOx Curve

A) Effects on NOx Formation.................................................................107

B) Effects on Peak NOx.........................................................................108

Figure 43: Effects of TDC Water Injection Timing on the Combustion Soot Curve

A) Effects on Soot Formation.................................................................108
B) Effects on Peak Soot

Figure 43: Effects of TDC Water Injection Timing on the Combustion Soot Curve

A) Effects on CO Formation

B) Effects on Peak CO

Figure 44: Comparison of Contours for Temperature at 13° ATDC for Best Cases

Figure 45: Comparison of Contours for Pressure at 9.5° ATDC for Best Cases

Figure 46: Comparison of Contours for NOx at 22° ATDC for Best Cases

Figure 47: Comparison of Contours for Soot at 9.5° ATDC for Best Cases

Figure 48: Temperature Contours for Water Injection at TDC

Figure 49: NOx Contours for Water Injection at TDC

Figure 50: n-Heptane Contours for Water Injection at TDC

Figure 51: H2O Contours for Water Injection at TDC
CHAPTER 1

INTRODUCTION

Motivation

Air pollution has been an issue of concern for all countries around the world for many years now. Pollution in the air has led to many different issues for the environment as well as humans and animals inhabiting it. Some issues commonly caused by pollution for humans are respiratory conditions, smog in cities and highly populated areas, and degradation of lawns and crops from acid rains. Pollution can also cause respiratory issues in pets or other animals in the wild. In addition, the increases in acid rains also have adverse effects on wild plant life and animal species. Acid runoff into bodies of water also may have adverse effects on aquatic plant and animal life. Another concern with pollutants in the air is its effect on the ozone and increase in greenhouse gases. This leads to increase in ultra-violet rays being allowed to penetrate to the earth’s surface and can even alter eco-systems in different locations to a degree.

Due to the increase in awareness and concern for emissions causing pollution of the air, water, and soil, restrictions on many aspects of the automotive industry have been implemented. The laws concerned with emissions and the automotive industry can be traced back to the 1960’s. The first regulations were designated to encourage research on their effects instead of limiting the output of them and had little effect on the pollutants coming from cars. Regulations have increased greatly throughout the years and now hold a large influence on the direction for the automotive industry. This has led to a need for engineers to be able to design engines that produce greater fuel efficiency as well as fuels which are cleaner burning as compared to
standard fossil fuels used over the last century of automotive history. Post combustion exhaust treatment processes and fuel additives, which enhance the reduction in emissions or modify the emissions into a less harmful property, have become quit prevalent in diesel powered automobiles. One means of reducing fuel emissions is to reduce the temperature of combustion which, particularly in diesel engines, is shown to reduce the formation of some emissions like NO\textsubscript{x} and SO\textsubscript{x} if properly implemented. One method that has been used for many years is the addition of water to the combustion process. Other materials commonly injected into injection are ethanol, methanol, and nitrous.

Water has been long used as an additive in combustion for both diesel and gasoline engines. It lowers the temperature of combustion, reduces NO\textsubscript{x} emissions, lowers soot emissions, and reduces engine knock. It also helps to clean the carbon buildup off of the engine cylinder head and piston surfaces. It does have negative effects though in some cases as the water particles can attach to the cylinder walls and contaminate the oil causing reduced lubrication and increasing the oil breakdown process. Also, reducing the combustion temperature can reduce the power output and efficiency of the engine. By quenching the flame with too much water in the combustion, water can cause an engine to run poorly and even to stop running if the problem increases too much. Improper addition of water into the combustion process can lead to an increase of the exhaust emissions, like CO and CO\textsubscript{2}. Properly understanding the effects of adding water to internal combustion engines is important for the engineering profession as we are leaders in the forefront of energy and power generation. This technology is nothing new as it has been used for many years in high performance applications and more recently, within the last few decades, it has become available for average citizens to install on their personal vehicles. These are available in kits which can be purchased and either
installed by trained mechanics or by individuals at home if they have some mechanical experience and knowledge. Many kits that are sold to implement water injection in diesel engines use a mixture of water and methanol which is injected into the intake of the engine and drawn into the cylinder for increased power generation. Others, especially in gasoline or spark ignition engines, spray water into the carburetor or throttle body which is then drawn into the cylinder.

Water injection has been used for many years as stated previously to aid in power production, reduce emissions, cool combustion and engine temperatures, and help reduce knock in spark ignition engines. However, much of the work previously done was through experimentations and not as much work has been done on the simulation of combustion in a cylinder with the addition of water injection either directly into the cylinder or into the intake system gases. Simulations allow for a better understanding of the effect of water injection into a combustion system with a reduced cost for researchers. In addition, it allows for a better visual understanding of the effect water has on combustion. The size of the water particle being injected into the cylinder has not been previously researched. Most research has been done on the effects that water has on emissions, pressure in the cylinder, and temperature curve in the combustion. This was largely done through variance in the quantity by volume or mass percentage of water to fuel in the cylinder, the timing of the water injection into the cylinder, or the injection duration timing of the water. Using the results found by other researchers in the field on these different parameters and applying the new conditions of water droplet size effects will allow for a better understanding of the capabilities of water as an additive to diesel combustion for increased effects in lowering the negative emissions while still maintaining the highest power generation for the engine.
Simulations have become a very important part of the engineering profession and have helped to create a much more cost effective and time efficient means for designing products. Through this process engineers are also able to do a large amount of preliminary testing through simulating many different situations a product may undergo during standard usage. This can eliminate the need for some prototype experiments, which in turn reduces the cost for the products. This aids in advancing the science for many different fields, such as power generation and finding replacements or supplements to standard fossil fuels. However, the experimental results which have already been run are very important as a basis for simulating conditions. By applying the research found in these experimental lab tests to the simulations being run, other tests for advancing the science and increasing the understanding of combustion can be created. By altering different parameters such as water particle size, engineers could see how to enhance the properties of combustion. Since water can have positive as well as negative results, engineers need to better understand the properties of water injection into combustion to create a more stable system for its use. Simulations allow for engineers to better understand the process of combustion in an engine and provide ways to improve the technology in the internal combustion engine for the fuels that are showing promise for the future to replace or supplement standard fuels. As engineers we are assigned with improving the world and helping to reduce the impact that humans have on the environment. This is very important as it is the basis for ensuring the sustainability of power and transportation through increasing comprehension of the reactions that take place during combustion.
CHAPTER 2

LITERATURE REVIEW

Internal Combustion Engine

The internal combustion engine has been in existence for quite a long time. The first models did not use compression, instead just used a mixture of coal-gas and air for fuel. This model was created and used until the 1860s when Lenoir designed an engine with a compression stroke before the combustion process took place. This led to Otto’s concept of a four-stroke engine, prototyped in 1876, which was the beginning of the engine used today in automobiles (Heywood 1988). These spark ignition engines, commonly called Otto engine, led to the invention of two-stroke engines and compression engines, also known as diesel engines. Common configurations for spark ignition engines are vertical inline cylinders, common in 5 cylinder or smaller engines, and V shaped configurations where an equal number of cylinders are on each side of the V, which is used generally for 6 cylinder or larger engines. Diesel engines often have vertical inline cylinders; however, some more recent models have begun to use the V configuration for some automotive applications. Engines also come as small as one cylinder for both the spark ignition and diesel engines which are commonly used for small power and lawn care equipment.

To create power, the internal combustion engine uses the energy from the combustion of an air and fuel mixture. The expanding gases force a piston in the cylinder downward which turns a crank. The rotating crank can be attached to a flywheel or gear to power an external device. Air is drawn into the cylinders through an intake manifold then through the cylinder
head which has valves that open to allow gasses to enter the cylinder and close to contain the gases during the combustion process. The cylinder head also has exhaust valves which open to let the combusted gases exit the cylinder through an exhaust manifold or exhaust header. Fuel is injected into the cylinder by either mixing with the air as it is drawn into the cylinder or by injecting it directly into the cylinder. A four-stroke engine’s initial stroke is an intake stroke where the piston goes down in the cylinder and the vacuum created draws in air from the intake manifold. In the compression stroke the intake valve then closes and the piston is pushed back up to compress the air-fuel mixture. Compressed gases are then ignited and they expand pushing the piston back down which is known as the expansion stroke. In a spark ignition engine, the ignition of the fuel is accomplished by sending electrical current to a spark plug. Spark plugs have a gap between the electrode and ground so as the current crosses from the electrode to the ground it generates a spark which ignites the fuel and air mixture. Diesel engines do not have spark plugs but instead use a higher compression ratio so the air is compressed, and then fuel is injected into the chamber. Because compression causes temperature in the cylinder to rise drastically, the fuel automatically ignites once it is injected. This is also why the diesel engine is referred to as a compression engine. The final stroke, called the exhaust stroke is where the piston is pushed back up forcing the gases out of the cylinder through an exhaust valve (Rogowski 1953).

Internal combustion engines have multiple ways of introducing fuel into the combustion chamber to create power. With spark ignition gasoline engines, which are used in a large percent of civilian vehicles, the use of carburetors, throttle body fuel injection, and direct fuel injection are the most common types (Pundir, 2010). Diesel engines use direct injection to fuel the engines since the fuel and air are not premixed. Instead, fuel is injected when the air in the
cylinder is at maximum compression. Carburetors were used on most gasoline engine, up until the late 1980’s, held fuel in a reservoir. With respect to the throttle position, varying fuel amounts was intermixed into the air going down from the air intake system into the cylinders. Proper jet sizing, nozzles for feeding the fuel into the system, is critical for the engine’s fuel demands. Carburetors require some tuning and adjustment to maintain proper operation. The throttle body injection that followed the carburetor is a system that uses a devise, like the carburetor, which sits on top of the air intake system and injects fuel into the air that is flowing into the cylinders. It does not, however, hold fuel in a reservoir like a carburetor, but instead has a fuel line feeding fuel to the throttle body that houses an injector that feeds fuel to the engine.

The diesel engine has been using direct injection however since its origination. The original system was fueled by a pump which pushed fuel through lines to each cylinder. Each injector had a bleed off screw which was used to remove all air from the lines. The fuel was pressurized to the injector so it would consistently deliver proper fuel to the engine but there was also a leak off line that allows excess fuel to return to the tank so that pressure does not exceed specifications. The components in this system were all mechanical as electronic computers were not standard in the automotive industry until the 1990s.

Throttle body systems were the standard on most gasoline engines until the mid-1990’s when direct fuel injection became standard. This system used fuel rails which ran parallel to the cylinder head and had injectors that fuel each cylinder independently. The injection was controlled by the vehicle’s computer which dictated the timing and amount of fuel injected into the cylinder. At this point, diesel engines began using the computer controlled fuel injection systems as well for its controllability and performance. This system is used on modern flex fuel vehicles because the computer reads from sensors in the exhaust which tells it if the combustion
is running rich or lean in the air to fuel ratio and can adjust the quantity sprayed into the cylinder accordingly. This system was created and became the standard control system for engines and fuel delivery systems because of the increase in technology.

The thermodynamics of the Otto or spark ignition engine cycle can be shown by two different diagrams. One diagram commonly referred to as the P-V diagram is a relationship of the pressure and volume in a cylinder during the 4 stroke process. The area of the P-V diagram shows the work done by the engine. The second diagram, used for Otto engines, is a T-S diagram which shows the temperature and entropy for the 4 stroke processes. This is the diagram of the net heat energy. Figure 1 shows the P-V and the T-S diagrams of a gasoline engine side by side for comparison.

![P-V and T-S Diagrams for Gasoline Engines](image)

Figure 1: P-V and T-S Diagrams for Gasoline Engines

The P-V diagram shows that during the combustion process, 2-3, and the heat rejection process, 4-1, there is a constant volume, or isometric, process. In the T-S diagram, during the intake stroke, 1-2, and the expansion stroke, 3-4, we see that it is an adiabatic process, constant
entropy. From points 1-2 and points 3-4 in the P-V diagram it is an isentropic or constant entropy process, \( s = c \). In the T-S diagram, from 2-3 is a constant volume process, \( v = c \). As well, from point 4-1 is a constant volume process, \( v = c \). The first law of thermodynamics can be written as

\[
Q = \Delta U + W
\]

where \( Q \) is the heat transfer, \( U \) is the internal energy, and \( W \) is the work (Lindeburg, 2011). This equation can be used for solving for the work done by the engine. Also, from thermodynamics we can solve for the efficiency of the engine based on heat transfer from the high temperature reservoir. The equation for thermal efficiency is found by

\[
\eta_{th} = \frac{W_{net}}{Q_H} = \frac{Q_{net}}{Q_H}
\]

with \( W_{net} \) being the net work done, \( Q_{net} \) the net heat energy, and \( Q_H \) the high heat energy of the system (Lindeburg 2011). The ideal gas law shows the equation of

\[
pV = mRT
\]

where \( p \) is the pressure, \( V \) is the volume, \( m \) is the mass of the gas, \( R \) is the gas constant, and \( T \) is the temperature (Heywood 1988). Diesel engines use the same diagrams to show the process capabilities and the relation of the pressure to the volume as well as the temperature to entropy. However, the diagrams differ due to the variations in the processes of combustion. Below, in Figure 2, is shown the diagrams for diesel engines.
The difference in the P-V diagrams shows that from point 2 to point 3 the pressure, instead of being a constant volume process, has a constant pressure. This is because in a spark ignition engine the constant volume signifies when the fuel and air mixture is fully compressed and held constant as the spark ignites the air and fuel mixture. This leads to the expansion of the gases in the chamber. Diesel engines have increasing volume but constant pressure because when the air reaches peak compression the fuel is injected into the chamber, thus increases the volume of the cylinder contents. These are ideal cases as actual combustion is not completely constant so it makes more of a slight radius at both ends of the isentropic curves. The work is found by the area of the P-V diagram because it shows the relationship of the work into the system versus the work out. The T-S diagram shows the heat in versus the heat out of the engine.
Water Injection

Water injection has been used for many years in spark ignition and compression engines. It can have great effects on the combustion of the fuel in the cylinder. One of the reasons for injecting water into the combustion process is to add oxygen into the combustion. As well, it reduces the temperature of the combustion in the cylinder. Another effect is that the addition of water can reduce NO\textsubscript{x} emissions because of the lowered temperature of the combustion (Lawrence, Deepanraj, and Mathews 2010). In some studies it has been shown to increase the knock limit for the engine. Where water has been used in some applications, it has been shown to reduce the carbon build up which helps to keep the engine operating more efficiently. It has been known also to increase fuel efficiency in some cases.

There are three main ways that water could be injected into the cylinder to affect the combustion process. One way is to make an emulsion of the water and fuel to be injected into the cylinder as a mixture. The issue with this process is that it does not always fully mix well so the ratios of the fluids can vary throughout the tank. This is partly because the water particles sink to the bottom of the tank, due to the density variance between water and fuel, thereby causing separation over time. The fuel mixture injected into the cylinder has higher water percentage through the initial portion of the fuel volume and is thus water lean in the later portion of the fuel volume. To ensure the proper amount of water content, water is generally either injected directly into the cylinder or is injected into the intake manifold as a mist to be drawn into the cylinder. Water mist sprayed into the intake is the most common form of water injection into internal combustion engines. Other advantages with direct injection or intake injection are that the water quantity being injected into the combustion process can be controlled by an electronic controller to modify the volume quickly and that the water percentage will be
constant in each combustion revolution. Similarly, if water is injected separately, the type and geometry of the injector can be changed to alter the spray for optimum efficiency and performance of the system.

Often the use of water injection is done through a liquid mixture of water and methanol to increase power and can be purchased in kits by many different companies which supply all the needed hardware for installation with only minor modifications to the vehicle. In recent years this technology has become increasingly popular with diesel engines for the general public wanting to increase the power output of their engine without having to spend large amounts of money on extensive modifications. Additionally, water has been used for many years in highly modified diesel and gasoline competition engines for cooling combustion temperature and allowing for added fuel to be injected increasing the power output of the engine. The cooled temperature of the combustion also allowed an engine to be run at a higher load for a longer period of time without over heating or causing damage to internal components.

Many different papers have been written which covered the research done by different organizations on the water injection into both diesel and gasoline engines. These previous works also covered multiple forms of water addition including direct injection, injection into the intake, and emulsion with the water and the fuel. In a paper by Tanner, Brunner, and Weisser, they did research on water injection into large bore diesel engines by using KIVA to do simulations for a two stroke engine and did experimental tests on another 4 stroke engine (Tanner, Brunner, and Weisser, 2001). The basic model used for combustion was based on the global reaction of

\[ 2C_{14}H_{30} + 43O_2 \rightarrow 28CO_2 + 30H_2O \]
but the models for the creation of NOx were listed separately based off of the Zeldovich Model shown below.

\[ O + N_2 \leftrightarrow N + NO \]

\[ N + O_2 \leftrightarrow O + NO \]

\[ N + OH \leftrightarrow H + NO \]

They added other supplement reactions that were based off of the research by Weisser (Tanner, Brunner, and Weisser, 2001) on the reactions that had the most effect on its formation. This complete reaction model is shown in Table 1.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Forward Reaction</th>
<th>Backward Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td>b</td>
</tr>
<tr>
<td>Zeldovich:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O + N_2 \leftrightarrow N + NO</td>
<td>6.68E+12</td>
<td>0.4</td>
</tr>
<tr>
<td>N + O_2 \leftrightarrow O + NO</td>
<td>6.40E+09</td>
<td>1</td>
</tr>
<tr>
<td>N + OH \leftrightarrow H + NO</td>
<td>3.80E+13</td>
<td>0</td>
</tr>
<tr>
<td>Supplementary Reactions:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NO_2 + OH \leftrightarrow NO + HO_2</td>
<td>8.45E+12</td>
<td>0.02</td>
</tr>
<tr>
<td>NO + OH \leftrightarrow NO_2 + H</td>
<td>9.46E+09</td>
<td>0.81</td>
</tr>
<tr>
<td>N_2 + OH \leftrightarrow N_2O + H</td>
<td>5.73E+07</td>
<td>1.31</td>
</tr>
<tr>
<td>N_2 + O + M \leftrightarrow N_2O + M</td>
<td>5.21E+07</td>
<td>1.34</td>
</tr>
<tr>
<td>N_2 + O_2 \leftrightarrow N_2O + O</td>
<td>2.91E+10</td>
<td>0.91</td>
</tr>
<tr>
<td>NO + NO \leftrightarrow N_2O + O</td>
<td>1.26E+09</td>
<td>0.92</td>
</tr>
<tr>
<td>N_2 + HO_2 \leftrightarrow N_2O + OH</td>
<td>1.39E+10</td>
<td>0.48</td>
</tr>
</tbody>
</table>

Table 1: Zeldovich Mechanism and Supplementary Reactions for NOx Formation (Tanner, Brunner, and Weisser, 2001)

A modified version of the Arrhenius reaction rate formula was used to calculate the speed of the reaction. In it $T_A$ is activation temperature, A and $T^b$ are pre-exponential factors, and T is temperature.
The simulations were done to prove the effects of the water with direct injection of 50% and 100% of water to fuel by mass. Their tests also increased the fuel injected to account for the lost pressure in the cylinder and the power reduction, however, the results for the NOx reduction showed that it was able to reduce the levels by nearly 37% and 45% for the water levels of 50% and 100% respectively.

The Zeldovich mechanism has also been used as a basis for tests with added mechanisms done by Kannan and Udayakumar (Kannan and Udayakuma, 2014) to show the creation of NO2 from oxygenation of the NO and its return to NO shown below.

\[
NO + HO_2 \rightarrow NO_2 + OH
\]

\[
NO_2 + O \rightarrow NO + O_2
\]

They state that 89.5% of NO formed during combustion processes come from thermal formation and the formation from the NO2 model listed. Their cases are based on water and fuel emulsions containing 10% and 20% water. Different equivalence ratios were used to show its effect on NOx formation along with the water addition. Equivalence ratios are important to their study as it was discussed that the primary source of nitrogen is due to the air content because diesel as a fuel contains only small amounts of it in general. The injection of water proved to decrease the peak pressure of the combustion by approximately 2.5 bar for every 10% increase. This resulted in the NO reducing from nearly 1300 ppm without water to approximately 1050 ppm for 10% water and 800 ppm for 20% water. As well as showing a decrease in NOx created, it shows that water added to combustion can reduced the fuel consumption approximately 12% and increased
thermal efficiency nearly 2%. With the emulsified water a slight increase in cylinder pressures was seen as well as increases in the heat reaction and heat release rate due to the micro-explosion of fuel and water droplets. This was all done using the simulation of a single cylinder diesel engine. Further tests were done on the formation of NO\textsubscript{x} from water injection through the use of emulsion and injection into the intake. The engine modeled was a heavy duty diesel engine and was validated to the data attained from it. The simulations were done with the water levels of 0, 10, 20, and 30% for both styles of water addition. The increased water content increased the NO\textsubscript{x} reduction for all cases. However, at 30% water content in the emulsion, it was stated that there was some inconsistency in the reductions and the formations of NO\textsubscript{x} curtailed in some cases. As has been shown in most all cases researched, the highest effect of water injection is found during higher engine loads. Another interesting result found was that the addition of water lowered the exhaust particulates in the emulsion case but increased them in the intake injection cases. Also, injection of the water into the intake seemed to have less effect on the temperature of the bulk gas. The results for the simulations showed that the injection of water into the intake reduced the bulk gas temperature from approximately 1575 K with no water to 1475 K with the maximum water injection of 30%. Each 10% increase of water content lowered the temperature at constant intervals. There were no effects seen on the combustion delay. The NO showed a reduction of approximately 0.25 mg for each increase percentage of water giving the maximum reduction of 1 mg with 30% water. The base without water gave approximately 4.2 mg of NO. Their results for soot showed an increase of approximately 0.05 mg with each successive increase in water percentage. The simulation of the emulsified water showed increases in combustion delay up to nearly 20 degrees. The water lowered the maximum temperature of the combustion by 125 K with 30% water from 1575 K to 1450 K. The NO in the emulsion
simulations resulted in a larger decrease for each successive percent, a maximum reduction to 2.5 mg from 4.2 mg. Soot decreased from no water at 2.5 mg to nearly 1.8 mg for both the 20% and 30% water. The 30% water delayed the peak formation by around 10 degrees. It can be noted that the 30% water emulsion maintained more soot after the levels dropped during expansion than all of the other cases by nearly 0.05 mg.

Water was shown to have many benefits on the combustion of diesel but there are certain aspects of its combustion that are more important for achieving the desired positive results. The tests shown in the research paper (Kumar, Sharma, and Vibhanshu, 2013) were done with emulsions of diesel and water to test different injection angles for the most effect. In their research, it was found that the emulsified droplet size is extremely important to the benefits of adding water. It was also stated that the water percentages, as compared to the diesel fuel, is most effective when it remains under 40% but lower water content makes the mixture more stable.

Computer Simulation

The use of computer simulations has become an invaluable tool for engineers. There are many different programs that aid in the simulations. Programs such as ANSYS, Solidworks, Converge, and AVL Fire are used to run simulations on all different types of computer models. ANSYS, for example, has components of the software that allow for solving structural, thermal, and fluid problems which allows for the design process to circumvent some issues which would have been found after prototypes of parts were made. It can solve for many stresses, deformation, fluid flow, and even heat transfer or stress which can occur from possible boundary
conditions or external forces to which the part could be subjected. Being able to see these issues from computer models saves time as well as money for manufacturing and design processes. AVL Fire and ANSYS Fluent are two commonly used simulation programs that have components capable of solving for combustion. As engineers strive to find new ways to increase efficiency and reduce emissions for the future, the use of modern technology will prove invaluable.

By creating simulations of combustion, effects of the angle of the fuel injection, compression ratio, fuel composition, cylinder and piston configurations, air to fuel ratio, and forced air induction can be seen clearly. New modifications to the combustion process can also be tested to find out if they are able to aid in resolving issues in combustion or even just the most efficient ways operate current engines. All this can be done through simulations without having to modify actual engine components which can be very expensive or time consuming.

Simulation can give invaluable information to design and research engineers in understanding the combustion and ways to improve it. The air and fuel flow into and out of the cylinder are important to the engine’s performance and the combustion. The fluid dynamics within the cylinder are also important to the performance of the engine. The use of CFD allows for visual understanding of the effects of cylinder and piston geometry on fluid flow as well as the propagation of the flame through the cylinder upon ignition of the gases. By altering the injection angles or methods of the fuel and air we see by the use of simulating modes that a more complete combustion can be obtained.

ANSYS simulation software has an internal combustion engine tool that allows for combustion simulation with the use of ANSYS Fluent for modeling the flow of gases in the
engine cylinder. A model of the cylinder is created in a CAD program, like Solidworks, and attached to the ICE toolbox in ANSYS to allow for the simulation (ANSYS 2012). ANSYS has done extensive testing and created a program that is very effective for combustion modeling. As well, it allows for alteration of the spray for fuel injection and can be set to the desired crank angle.

Test done by Daimler Chrysler (Resh et al., 2002) in the design of their 5.7 liter Hemi engine used ANSYS to optimize the configuration of the valves and piston for fluid flow in the cylinder. Two tests were done, one of which used a slight dome topped piston and had a concave surface on the intake valve and a deep concave on the surface of the exhaust valve. This test showed the highest flow at the concaved surfaces of the two valves. The air flow speed was approximately 13 m/s at these points. In the second test the concaved surfaces of the intake and exhaust valves was increased. On the surface of the piston a large dome was placed in the center of the piston as opposed to the small sloping dome that was original configuration. This created high velocity flow along the edge of the center dome of the piston surface in a small pocket at an increased speed of approximately 15 m/s. By using simulation, the company was able to optimize the flow to have minimal interruptions to allow for the best combustion and exhaust of the gases. Simulations allowed a way to see the effects of the geometry changes and pressure points for the air.

As well as the flow of the air into the cylinder, tests have been done using simulation CAD software on the effects of the angle of injection into an internal combustion engine cylinder and the flow of combustion through the gases. At the University of Wisconsin-Madison test were done in 1999 on these issues in combustion (Fan, Li, Han, and Reitz 1999). The use of KIVA allowed for the better understanding of the process of combustion and ways to improve it.
The piston had a scalloped formation on the top surface. Testing of the injection angle into the cylinder showed where the fuel particles would disseminate throughout the whole cylinder more completely when the injection angle was 30 degrees, filling the area under the injector and the scalloped dome more completely. By increasing the angle to 45 degrees and then 60 degrees, it was seen that the fuel particle would flow more towards the top of the piston dome and collect nearer to the spark plug. The following tests were done on the combustion of the air and gasoline mixture in the cylinder. By doing the simulation of these tests, ignition of the fuels is shown at different crank angles. For increased injection angles, it was shown that the fuel would burn faster. At the lower angles the fuel that pooled on the piston surface created a higher fuel to air mixture that took longer to combust. Simulation allowed for a visualization of the pressure effects of increased injection angles. The highest pressure, approximately 2.8 MPa, was given by the 60 degree fuel injection. The use of the simulation software, KIVA, allowed for a better understanding of this effect on combustion and power generation.

S. Falfari and G. M. Bianchi at the University of Bologna tested the ability of KIVA3 to simulate the ignition of fuel gases in an internal combustion engine (Falfari and Bianchi 2007). Initially tests were done with a propane fueled single cylinder engine that had a transparent side for viewing the combustion. The speed of the flame growth was measured by recording images of the flame at set times. Then a simulation of the same combustion cylinder was done to compare the results and validate the software’s ability to simulate combustion. By applying the same boundary conditions, the simulations were run and results recorded. In comparing the data, it was shown that KIVA was able to closely simulate the combustion process of the engine. Images of the flame propagation for experimental and simulations were very similar with the software closely mimicking the speed of the flame travel and size of the flame. In comparing the
graphical results of the flame travel speed, we see that the computer simulation curve follows the results from the experiment with only a slight lag in the speed’s numerical value, with nearly a 4 m/s delay in all tests. The comparisons were done for all engine speeds, 300, 750, 1000, and 1250 rpm, and showed the software was equally accurate at all speeds.

For the injection of the fuel and water into the cylinder, there have been many concepts designed for using an injector that allows for duel fluid injection with two separate fuels from the same location. This allows for the original geometry of the head to be maintained as well as elevates the need to machine the head for the use of a second injector to accommodate the water injection. Murotani et al. (Murotani et al., 2007) used the concept that by injecting water into the air space around the fuel stream. When sprayed into the cylinder, this would create a better mixture of water and fuel droplets within the chamber and allow for the best effect on combustion. Tests were run experimentally, and then further tests were run by simulations with varying injection angles. Simulations were run using the KIVA software. The water was injected for the same duration as the fuel and simulations were run with the water injected before, at the same time, and after the fuel injection. The fuel mass injected was 62 mg and began at 8° before top dead center, BTDC. This simulation showed good reductions of NOx and only a slight reduction in the pressure after combustion began. With the injection of 60 mg of water the pressure decreased around 0.5 MPa from the baseline without water of 5.9 MPa.

Experimentally the NOx were 600 ppm without water. Then NOx was reduced to 500 ppm with 20 mg of water and then dropped to around 425 ppm with 40 mg. With 60 mg it was reduced to around 180 ppm and at 80 mg it gave around 100 ppm of NOx experimentally. Simulations gave a baseline of approximately 650 ppm of NOx and with 20 mg of water it reduced to around 300 ppm. With 40 mg of water the levels reduced to nearly 150 ppm and at 60 mg it dropped to
almost 100 ppm. The simulations showed the steepest reduction curve from 0 – 40 mg of water while the experimental results showed the steepest drop from 40-60 mg.

Another test done by Chadwell and Dingle (Chadwell and Dingle, 2008) used direct water injection into the cylinder with diesel fueling the engine and they were able to obtain a 42% reduction in NO emissions produced by the combustion process. The use of the water injection combined with exhaust gas recirculation, EGR, was able to reduce emissions by 82% over the test with just diesel used in the engine. Also, it obtained a faster torque increase with the direct water injection at 30 percent water content. In other research (Musculus et al., 2002), a 20 percent content of water injected into a large bore diesel engine showed a delay in ignition of 30-60 percent as well as a 20-60 percent longer flame lift off.

More tests reported in research (Şahin, et al., 2014) showed similar results as previous test discuss with reduction in NOx and smoke emissions. It also discussed that a 4 percent fuel increase was needed for water content up to 10 percent. They created a duel water and diesel fuel injector which used a plunger and needle that opened up separate passages for the diesel and water separately. The water passage had a check valve to help control the amount injected.

In one paper, (Bedford et al. 2000) a model for a duel fuel injector was modeled. Their concept used intermitted fuel and water injection from the same injector. This was done by having two systems that delivered each fuel and created a mixture when the liquids were injected into the cylinder. Water passages went through the center of the injector and was pressurized to force water intermittantly into the outer channels of fuel being injected. It was controlled to stop adding water when the desired amount was injected. The fuel used was n-heptane which is used as a surrogate for diesel because of its close similarity to diesel in properties for combustion.
The engine was run at 45% and 86% loads and with cases at 45% and 30% water injected. The simulations for the engine combustion were run using KIVA to model the different combustion processes. The NOx is modeled by the extended Zeldovich mechanism and soot is modeled with the Hiroyasu model which are both standards to use for simulation modeling. The results showed the spray of the water and fuel penetrated 35% further with this model. Two different injection process were used for the water. One had an equal timing and duration to the fuel injection. The second injection style used for water injected water injected the water for half of the duration of the fuel injection and occurred during the middle of the fuel injection. Thus fuel would be injected before the water began and continue past the end of the water injection. The results gave varying degrees of NOx reduction but many were found at the expense of reduced efficiency of the engine. The timing for the start of the injection was 2 degrees after top dead center, ATDC. The pressure showed a reduction of approximately 0.5 MPa during combustion. Simulation results for the heat release rate, HRR, trends showed at increase from 200 J/deg without water to nearly 500 J/deg with 45% water. The water caused it to delay 5 degrees before the slope began upward and gave a much steeper slope. The curves showed very similar levels after 20 degrees ATDC.

Tests done by Subramanian (Subramanian, 2011) showed that NO emissions were reduced from 1034 ppm to 643 ppm with the addition of water injection into a diesel engine. It was found that smoke emissions were lowered from 3.6 to 3.2 BSU, Bosch smoke unit, through the addition of water injected into the cylinder. All tests were done with 40 % water by volume as compared to the diesel injected. Emulsion was shown to have higher emission reductions at partial engine loads but at high loads the water injected into the cylinder gave the greater results listed above.
Other research has been shown on the effects of the timing of the water inject, commonly occurring during the middle of the diesel fuel injection in direct injection. However, one group researched the best spray timing for water to reduce issues of impingent droplets on the walls and piston (Bhagat et al., 2013). They ran tests at 60 degrees BTDC and 90 degrees BTDC in simulations using Converge CFD. This research showed that earlier injections decreased the water droplet’s inclination to adhere to the walls and create a water film. The droplets hitting the walls can also cause pitting over time from the impacts, which leads to seal failure for the piston rings. Also, the earlier injections allowed for better vaporization of the water droplets, which allowed for better mixture with the fuel in the chamber and thus enhanced the effectiveness of water injection while allowing reduced flame quenching.

There has been very little research discussing the size of the water droplets being injected into the chamber. One paper discussed the use of different size water and fuel droplets, with water droplet sizing being 0.210 μm, 0.240 μm, and 0.286 μm (Wang et al., 2013). The tests showed that by decreasing the droplet size, combined size of the water and fuel droplets increased the water percentage per droplet, yet allowed for flash vaporization with the higher percentages of water. An increase in the length of the blue flame was seen with an increased water content; however, the overall flame length was shortened. The discussion on the effects these sizes had on the flame length and flame propagation was specified but the paper did not discuss the effects on the temperature of the flame nor the emissions.
CHAPTER 3

METHOD

Data and information received from the literature led to the conclusion that a good way to increase the knowledge and science of using water injection to reduce the harmful emissions is to test the effects of the water droplet size being injected into the engine cylinder. To reduce the costs of the research and to allow for easier changes without having to make permanent changes to one of the engines in Georgia Southern Universities engine laboratory, simulation software was used for the research project. The simulation software which the university currently has that is capable of running engine combustion simulation is Converge CFD and ANSYS Fluent. The simulation’s engine model configuration was based on an data from an actual engine that experimentation results were accessible for to be able to validate the model. Sandia National Laboratories has done extensive testing on multiple engines under a variety of conditions and recorded the data. The data for multiple cases which were run on a Cummings single cylinder diesel engine, model N-14 (Musculus et al. 2002), are available to use for research purposes. This engine has a 0.1397 m bore and 0.1524 m stroke. It has a 2.34 liter displacement and operates at a 16:1 compression ratio. The mesh for the cylinder was created as a 1/8th section of the cylinder because of its symmetry. Symmetry of a chamber allows it to be divided into sections for simulations as the results within each section are equal. The model mesh was already created for the cylinder so it was only required to be imported into the software. For the first attempt ANSYS Fluent was used to run the combustion simulations. After the mesh was imported into the software, boundary conditions were set to mimic conditions in the experimental data, which were given with the experimental data results. Below shows the
conditions for the engine experimental case from Sandia National Laboratories which was used as a base line.

| Operational Parameters for the Sandia National Laboratory Engine Experimental Case |
|-----------------------------------------------|------------------|
| Speed                                         | 1200 rpm         |
| IMEP                                          | 4.5 bar          |
| SOI                                           | 5 BTDC           |
| DOI                                           | 10               |
| Injection quantity                            | 61 mg            |
| O2                                            | 21% by volume    |
| Injection Pressure                            | 1200 bar         |
| Intake Temperature                            | 47 °C            |
| Intake Pressure                               | 192 kPa          |
| BDC Temperature                               | 62 °C            |
| TDC Motored Temperature                       | 800 K            |

Table 2: Boundary Conditions for the Experimental Sandia Engine Research Case

The mesh used in ANSYS Fluent was a hexahedral 3D mesh and gave a total of 373,796 cells with 391,416 nodes. Other engine parameters engine from the experimental tests at Sandia National Laboratories are as follows: the intake valve closes 165 degrees of crank angle BTDC, the injector has a radius of 1.5 mm, and an injection angle of 152 degrees. The injector has a cone angle of 7.5 degrees, with a mean droplet diameter of 0.196 mm, and an estimated injection velocity of 200m/s. The chamber conditions were recorded to be 320.15 Kelvin with a gage pressure of 90,675 Pa and the oxygen mass fraction was 0.233. The injection for the diesel fuel begins at 5 degrees BTDC and has a duration of 10 degrees. During this time it injects $7.65e^{-6}$ kg of fuel at 368 Kelvin. The chamber conditions before compression are as listed: a piston temperature of 500 K, a cylinder wall temperature 420 K, and a cylinder head temperature 470 K. Conditions were set to match the experimental case then tests were run to be able to compare the results of the simulation to the experimental data. Alterations were then made to verify the accuracy of the data attained in the simulations by checking for mesh independency and
convergence of the simulation. This process was repeated until the results were proven to be accurate and matched the curves for temperature and pressure of the experimental case. At this point, the model was ready to do simulations with the modified conditions of the engine for the research purposes. Next, a supplementary injection for the water into the combustion process was added. The second injection for water was positioned at the same location as the fuel injector, based on research for duel fuel injectors. The water mass was set to 20% of the fuel injected and injection occurred at the same crank angle timing as the fuel injection. Cases were run and results were compared to literature for the expected consequences of the added water. These results were inaccurate, as the water did not reduce the temperature but instead increased it as pressure was increased. This was due to an added substance in the chamber that was not accounted for by the global chemical mechanism that was used.

\[ C_{10}H_{22} + 15.5O_2 = CO_2 + H_2O \]

Multiple chemical mechanisms were used and tested to account for the added water but all failed to create a satisfactory result, as shown in Appendix A. Due to this issue, the software was changed to use Converge CFD. Once again, the mesh was imported for the engine cylinder and the case was set up to mimic the experimental cases that were run at Sandia National Laboratory. The same data was used in Converge CFD from Table 2 as was used for ANSYS Fluent. In Converge CFD, to verify the most accurate results, a 29 chemical species and 52 reaction n-heptane reduced chemical mechanism, shown in Appendix B, was used that solved for the simulation results of the combustion. The mesh generated for use in Converge was a hexahedral 3D element, hexa8. The mesh had a total of 63,801 elements and 132,173 nodes. For further accuracy, to solve for NO\textsubscript{x} formation, the Extended Zeldovich Model was used. Also, for soot formation calculations, the Hiroyasu/NSC Soot Model was chosen. To better solve the
calculations, the Kelvin-Helmholtz, K/T, breakup model was selected. This was initially done with an injection that used 10% of water mass to fuel mass and was injected over a duration of 2 degrees of crank angle. This was used for a base low level to check for the capability of the software to account for the water effects on combustion in the chemical reactions. Also, it needs to be noted that the water was injected at the same starting time as the fuel injection, 5 degrees BTDC, and at the same temperature as the fuel which was 368 K. This process yielded successful results following the data that was found in literature by simultaneously decreasing the temperature and pressure curves of the combustion.

![Figure 3: Verification of Converge CFD Simulation for Water Injection Effects](image)

The next step after verifying that the case was operating correctly was to modify it to closer resemble the cases which were shown in literature research. Literature showed that levels from 20-30% were the most effective without being too low to have beneficial effect or too high which caused quenching of the flame during the combustion process. Thus a water content of 20% as compared to the fuel mass was initially used in the simulations. Also, based on cases from the literature, the same duration time was used for the water injection as was used for the
fuel injection. These changes were made and a case was run with these conditions. Another condition that is commonly modified in water injection cases is the water injection timing. Some cases showed that injecting the water at earlier intervals allowed for more effective results. Cases in the literature were run at 60 degrees and 90 degrees before the fuel injection. With this taken into account, cases were then run at 65 degrees BTDC and then at 95 degrees BTDC, which were 60 and 90 degrees before the fuel injections. These cases were all run with the particle of water being injected at the same size as the fuel being injected which was 0.196 mm. The results for cases run at all of the different timings were recorded. Due to the research seen in the different literature cases (Wang et al., 2013) (Bhagat et al., 2013) (Bedford et al. 2000) (Kumar, Sharma, and Vibhanshu, 2013) (Kannan and Udayakuma, 2009), the topic for this research project was chosen to test for different water particle sizes being injected into the chamber. Sizes used for the water injection particles, 0.210 μm, 0.240 μm, and 0.286 μm, were based off of literature research for water injection effects on flame properties. Cases were then run at 5 degrees BTDC with all of the different particle sizes and the results were recorded. Next the injection timing was altered to 65 BTDC degrees and the cases were run with each particle size as listed above. The results were recorded as was done before with the other simulations. The third sets of tests were run with each of the three particle size at 95 degrees BTDC. All results were again recorded to be compared. Data that was collected for the different injection timings and different particle sizes was then compared to one another to better understand the effects of the tests that had been completed. This was done by creating graphs in Microsoft Excel for the purpose of comparing the temperature, pressure, and emission curves for each of the tests. The data was analyzed to see the effects of different particle sizes being injected into the chamber and how they affected all aspects of combustion. In the figures showing the results
for the simulations, the crank angle of 0 degrees specifies when the piston is at top dead center, TDC. Next, as an added step to further understand the results for water injection into a diesel engine, the water’s initial temperature as it was being sprayed into the chamber was altered. The first step was to begin with the boundary conditions set as they had been for the first water injection case, run with having the water injected at 5 degrees BTDC and at 0.196 μm. The first case run was with the water temperature set to 348 K instead of 368 K. After completing this case, cases were run at 65 degrees and at 95 degrees BTDC. Once again, all data was recorded and saved. The next step was to alter the temperature of the water being injected once again to see further effects of it. The water temperature was changed to 388 K next and cases were run at the same injection timings of 5, 65, and 95 degrees BTDC as was done in the previous cases. All of the data was saved for comparing the results. Once again, the data was loaded into Excel to create charts for the temperature, pressure, and emissions of the combustion process within the chamber. The plots were compared to see how the alteration of water temperature being injected affected combustion. Also, contours of the combustion process for all of the altered cases were made to create a visual inspection of the different initial conditions for water being injected and its effect on the different properties of combustion. This was done for the cases that were run varied water particle sizes and water temperature alterations cases. The software used to complete the contours and further analyzation was Ensight 10.0.
CHAPTER 4

RESULTS

Model Verification

The first step in running the simulations for the research was to verify the results of the simulations mimicking the experimental case from Sandia National Laboratory. Initially, ANSYS Fluent was used to run the simulations in an attempt to match the engine’s experimental data. This was successful in attaining results that showed a good comparison to the experimental data, however, when the water injection was added the results were inaccurate to the literature’s expected results. The software was not able to solve for the effects of the added chemical mechanism correctly. Multiple chemical mechanisms, shown in Appendix A, were used for the combustion process in an attempt to resolve the problem but none succeeded in resolving it. The added water only increased the pressure because of being an added substance in the chamber during combustion instead of being accounted for chemically and recognizing its effects on combustion. From the literature it can be seen that added water reduces the pressure during combustion by reacting with the fuel and through microburst of the water particles. This lowers the temperature of the combustion which in turn lowers the pressure in the cylinder. Due to this issue, the software was changed to Converge CFD which is more dedicated to engine combustion than ANSYS Fluent. The same experimental data and conditions were used to set up the case in Converge for model verification without the water injection that was used for the case that was run in ANSYS Fluent. This case was then run to create a base which could be verified
to the experimental data and could be used for the research of added water directly injection into the chamber. The results are shown below in Figure 4 for the pressure curve.

![Figure 4: Validation of Converge CFD Simulation Model without Water](image)

This simulation case showed good agreement with the experimental data, as can be seen. The time delay of combustion was shown to be nearly the same and the peak pressure of combustion only differed by 0.11 MPa as the experimental data peaked at 7.25MPa and the simulation peaked at 7.14MPa. The simulation model needed to still be verified further so cases were run with the mesh altered to check for mesh independence and to verify that the results converged. The initial case was set with the mesh size at 0.0025 meters. Next cases were run with the mesh at 0.0015 meters and 0.002 meters and then the results for the pressure curve were once again compared. This is shown below in Figure 5 and again shows very good comparison as the results barely change for any of the mesh sizes.
In the initial case with the 0.0025 meter mesh, the peak pressure was 7.14 MPa as previously stated. Altering the mesh size to 0.002 meters, the pressure peaked at 7.26 MPa which resulted in a 1.6% change. By further decreasing the mesh size to 0.0015 meters, the pressure peak was observed to be 7.44 MPa. This yielded a difference of only 2.5% from the first case that was run with the 0.0025 meter mesh size. The 0.002 meter mesh was chosen to use as the mesh size for all simulations, because of the small variations seen with each size, which showed mesh independence. Also, the cone angle used for the injector was initially set to 15 degrees. Further review showed that a cone angle of 7.5 degrees would be accurate to the experimental case. This was done and cases were run to compare the results. Looking closer at the comparison of the 0.002 meter mesh and experimental data results, it could be seen that the point of peak pressure in the simulation was a smoother curve than was obtained in the experimental case. This was due to multiple factors and the fact that simulations assume ideal conditions so they do not account for imperfections within the system. When the cone angle was
altered to match the experimental data, however, the peak pressure curve gave a sharper peak point and decline in the pressure in the chamber. This is shown below in Figure 6.

![Pressure Curve Results for Varied Cone Angle and Mesh Size](image)

Figure 6: Pressure Curve Results for Varied Cone Angle and Mesh Size

Also, general heat release rate trends can be compared for the experimental data and simulations to better analyze the simulation results. With the results from the experiment, the curve holds at 0 until near TDC then the value has a slight drop before it begins to rise and peaks after 5.75 degrees of crank angle at 642 J/deg. It then drops back down where it holds fairly steady around 5 J/deg. The simulation holds the same initial 0 value but instead of a slight drop it has a small rise and has a large peak in the curve where the maximum attained value is found. Its peak is equal to 1683 J/deg and is found at 6 degrees ATDC. It dropped back to 0 J/deg as the expansion stroke occurred. The two peaks are found only 0.25 degrees of crank angle apart from each other which shows good agreement for the timing of the peak. The values, however, vary greatly in the simulation results with it peaking at 2.6 times the value of the experimental data. Heat release rate is difficult to accurately simulate so the general trend of the graph has a greater importance in showing the capability of the system than the actual number attained.
These show good agreement with the only large difference being peak value. Figure 7 below shows the graphs for both of the heat release rate curves.

![Heat Release Rate Comparison for Simulation to Experimental Results](image)

The next step was to compare the emissions for the simulation and the experiment cases. In Figure 8 the comparison of the soot emissions are shown. The experimental data begins at 6 degrees ATDC and goes through 20 degrees ATDC. It can be seen that the soot increases sharply to 0.307 g/kgf around 8 degrees of crank angle then drops back down and starts to flatten out around 0.02 g/kgf. The simulation show a gentler slope which peaks at 9 degrees of crank angle near 0.053 g/kgf. Though the peak values differ greatly, the timing of the peak soot generation shows good agreement to one another being only different by 1 degree of crank angle.
With the model verified and convergence found, next a water injection was added to the system. The first case was set up and run with a water injection of 10% water to fuel by mass and began at the same crank angle as the fuel to check for the capability of the system to solve for the chemical reaction of the water added into the combustion. Water was injected for 2 degrees of crank angle. This simulation showed that the system was capable of solving for the chemical effects of the water so the injection was adjusted to the designated conditions picked from reviewing literature. The first water injection condition was set to 20% water by mass and injected at 5 degrees BTDC for a total duration of 10 degrees, which is the same as the fuel injection. The particle diameter was set to 0.196 μm, which was the same specification used for the injected fuel, and a case was run. The other water particle sizes that were based off of literature values were then set up in separate cases and all were run to check for the effect of the particle diameter on the combustion. The diameters were set to 0.210, 0.240, and 0.286 μm. After reviewing the results for these cases it was found that water injection occurring for the
same amount of time, at the same location, and at the same beginning injection time as the fuel allowed for the water to quench the flames, thus causing the engine to not achieve combustion.

Effects of Water Droplet Size

20% Water Injected at 65 Degrees BTDC

From the literature review section, it was shown that injecting the water earlier into the chamber could aid in reducing the negative effects of adding water while maintaining much of the desired emission reduction. Next cases were run with the injection timing set to 65 degrees BTDC for all of the different particle injection sizes listed before. The temperature effect of the added water into the combustion is very important as it has a direct effect on the emissions that are emitted. This graph is shown below in Figure 9. Graph A shows the temperature curves of the different water droplet sizes whereas graph B shows the maximum temperature of the combustion for the different water droplet sizes. These two together allow for a good understanding of the results of the different particle sizes.

A) Effects on Temperature
B) Effects on Peak Temperature

Figure 9: Effects of Water Particle Size on the Combustion Temperature Curve (20% Water Injected at 65 Degrees BTDC)

Looking at the graph for the temperature curves it can be seen that larger particles create a smaller delay in combustion as compared to the baseline case without water injection. As the particle size increases it causes the maximum temperature of combustion to increase. However,
in the case with the 0.286 μm water droplet injection the temperature peak begins to decrease again slightly. This is verified by graph B. In the case with the 0.240 μm droplet, it was shown that the temperature peak in the chamber was approximately the same as the original case without water injected, which was 1175 K. The highest effect for lowering the temperature is from the case with the 0.196 μm droplet which gave a decrease of approximately 8 K, down to 1167 K. Injection of water into the cylinder is shown through literature to lower the temperature of the chamber during compression. Injections of different droplet sizes did show a reduction of up to 5 K with the most effect being shown by the smallest droplet size of 0.196μm. Each increase in the droplet size showed a reduced effect on the in-cylinder temperature previous to combustion. The amount of temperature reduction was small for multiple reasons. One was that the temperature of the water was rather hot at 368 K, so it was nearly the same temperature of the chamber upon injection. Early injection of the water used in this research allowed for the water and air temperature to increase simultaneously during the compression stroke, which had a reduced effect on the cylinder temperature. Additionally, it gives more time for further vaporization of the water droplets before the fuel is injected and combustion occurs. Vaporization of the water reduces the effects from the micro burst of the water droplets because there is less percentage of water in the fuel/water combined droplets. This also has a direct correlation to the pressure curves based off of the ideal gas law from thermodynamics $PV=\text{mRT}$ where $P$ is pressure, $V$ is volume, $\text{m}$ is moles, $R$ is the gas constant, and $T$ is the temperature. In the formula $R$ and $\text{m}$ are constants for the fuel. Thus, if temperature increases on the right side of the equation, then the pressure or volume has to change on the left side of the equation in order to account for the temperature change and to remain equal. This is shown in the correlation of the graphs for the pressure curves and peak pressure values in Figure 10.
Figure 10: Effects of Water Particle Size on the Combustion Pressure Curve (20% Water Injected at 65 Degrees BTDC)

Results show the same trends as the temperature curves and the injection of the 0.196μm water particle which reduces the peak pressure to 7.215 MPa for the lowest value found. As was seen in the temperature graphs, the injection with the 0.240 μm water particle maintained nearly
the same peak pressure as the case with no water at approximately 7.275 MPa. The reductions in the pressure curves from literature showed to be up to 0.5 MPa, but the water injected was at a larger percentage and was injected during the time of the fuel injection. This research had less effect through the early injection timings, which maintained closer values to the baseline for the engine’s efficiency. This is further examined in the Discussion section of this paper. To better understand the effect of the water injection, it is important to look at the comparison of the trends in the heat release rate from the combustion process without water and with each water droplet size. The heat release rate is very closely related to the temperature of the system as it is a product of the energy released from the combustion of the fuels in the chamber. With that being noted, it is to be expected that the release of heat from the burning of fuels in the cylinder will have similar trends to the temperature curves for the same cases.

A) Effects on Heat Release Rate
B) Effects on Peak Heat Release Rate

Figure 11: Effects of Water Particle Size on the Combustion Heat Release Rate Curve (20% Water Injected at 65 Degrees BTDC)

The heat release rate graph shows that the first two water particle sizes created a slower peak in the heat release value. This is due to the fact that combustion delay was affected the most in these cases and it had the highest peak with the 0.240 μm water particle. Without water injection, the measured heat release rate peaked at 1683.78 J/deg. By injecting the 0.196 μm water particle it was decreased to 1275.69 J/deg which is a 24.2% decrease. The least affected case was with the 0.240 μm injected water particles, as it was decreased by 4.4% to 1609.04 J/deg. A trend that was shown is that the smaller two particle sizes, 0.196 and 0.210 μm, had very similar delay in the heat release rate curve’s initial rise point and was very near the same point as the rise found without water injection. The larger two particle sizes, 0.240 and 0.286 μm, had a slightly longer delay but were very similar to each other, approximately a degree of crank angle after the smaller sizes.
To truly understand the full effects of the water and its possible benefits, emissions need to be reviewed by comparing them with regards to the different droplet sizes. One of the most important emissions that should be analyzed from diesel combustion is the amount of NOx formed during combustion. This is also one of the most highly effected emissions by the addition of water, resulting in a temperature change in the combustion process. To see these effects for the different water particle sizes that are injected, both the NOx formation curves and peak NOx graphs are shown in Figure 12 below.

Figure 12: Effects of Water Particle Size on the NOx Formation Curve (20% Water Injected at 65 Degrees BTDC)
In review of the graph for the NOx formation with 20% water injected into the cylinder, it can be seen that the NOx forms at the point of combustion and remains steady throughout the rest of the engine stroke. All of the cases for the different water particle droplet sizes are plotted together and it is noted the water injection did not have an effect on the formation timing but instead just on the amount created over all. The first case of 0.196 μm created just slightly less NOx as compared to the case without water. When the droplet sizes of the water were increased to 0.210 μm, the lowest amount of NOx formation of any droplet size was found to be approximately 1.62 x 10^{-6} kg, which was a 5.8% decrease from no water injection. The increase in the droplet size after that case showed an increase in the amount of NOx formed, as compared to the lowest amount formed. In the case using the largest water droplet size, 0.286 μm, the amount of NOx formed during combustion closely paralleled the case with no water injected at 1.72 x 10^{-6} kg. As was seen in the pressure curve, earlier injection timing reduced the effects on the amount of NOx formation from the water injection, but this allowed for closer results as compared to the case without water injection in the properties for combustion. Though literature showed larger reductions, in those cases, the engine efficiency suffered.

A) Effects on Soot Formation
B) Effects on Expansion Stroke Soot

Figure 13: Effects of Water Particle Size on the Soot Formation Curve (20% Water Injected at 65 Degrees BTDC)

Results for soot formed in the combustion process for each case followed the same trends as was shown in the results for the NOx formation, decreasing up to the 0.210 μm water droplet case and then increasing with each success size afterwards, as seen in Figure 13. The lowest level attained was $1.86 \times 10^{-7}$ kg in the 0.210 μm water droplet case, which gave a 34.5% drop over the baseline level of $2.84 \times 10^{-7}$ kg. Soot levels increased as the water droplet increased in size, to a maximum level found in the 0.286 μm water droplet case, $2.44 \times 10^{-7}$ kg. In addition, during the expansion stroke, the levels of soot maintained are reduced as compared to the baseline. The lowest level found for soot during the expansion stroke is $5.36 \times 10^{-8}$ kg with the 0.196 μm water droplet. Water injection lowered the soot levels over the case without water in all simulations.
One other emission that is important to review is CO formation through combustion. By adding water injection, the same general trends were followed as for results seen in the other emissions. By adding water to the combustion process, the CO was lowered in all cases over the

A) Effects on CO Formation

B) Effects on Expansion Stroke CO

Figure 14: Effects of Water Particle Size on the CO Formation Curve (20% Water Injected at 65 Degrees BTDC)
baseline level of $3.87 \times 10^{-5}$ kg at peak and $2.09 \times 10^{-6}$ kg in the expansion stroke. CO was shown to peak at 7 degrees of crank angle ATDC for all cases, and was shown to sharply peak then drop back down quickly to a level where it held steady throughout the rest of the cycle until exhausted from the cylinder. Injecting water was the most effective for lowering the peak level of CO generated with the 0.210 μm water droplet size, which decreased the CO to $3.62 \times 10^{-5}$ kg giving it a 6.5% reduction. The CO level drops off to $2.5 \times 10^{-6}$ kg after it peaks. Even by using the 0.286 μm droplet size, which gave the highest CO formation levels of the water injection cases, the CO formation was lowered 2.8% to $3.76 \times 10^{-5}$ kg at peak and $2.19 \times 10^{-6}$ kg in the expansion stroke.

An interesting factor that can be noted is that the higher the peak value, the lower the final value attained at the exhaust level. The levels were all increased over the baseline in the expansion stroke with the highest formation found when the 0.210μm droplet size was used. This attained an increase of 22.81% to $2.57 \times 10^{-6}$ kg.

20% Water Injected at 95 Degrees BTDC

Next the timing for the injection of the water was adjusted to 90 degrees before the fuel injection and cases were run with each droplet size again. This meant the water was injected at 95 degrees of crank angle BTDC. Cases were set up and run, and then the data was compiled to analyze the effects of the droplet size changes at earlier injection timings.
A) Effects on Temperature

B) Effects on Peak Temperature
C) Effects on Pre-Combustion Temperature

Figure 15: Effects of Water Particle Size on the Combustion Temperature Curve (20% Water Injected at 95 Degrees BTDC)

Results for the water injection at 95 degrees BTDC showed the same general trends as the 65 degree BTDC injection timing. The maximum temperatures of combustion were lowered in the smallest droplet size water injection but as the droplet size increased, the maximum temperature of combustion increased. With the largest size droplet of 0.286 μm, the temperature was once again reduced, to the lowest maximum temperature. However, all temperatures were higher than at the later injection timing for the same particle size. The 0.196 μm droplet had a slightly lower maximum temperature of combustion, 1175.29 K, than the baseline without water. The case with the 0.286 μm droplet resulted in a maximum temperature of 1174.36 K. However, the 0.210 and 0.240 μm droplet sizes actually increased the temperature over the baseline to 1177.24 K and 1178.51 K respectively. The highest combustion delay was found with the 0.196 μm droplet. As the droplet size increased, the amount of delay decreased. As was seen with the 65 degree BTDC injections, each decrease in the injection droplet size created a slight larger
reduction in the in-cylinder temperature before combustion. Once again though, only a small reduction was seen due to the water temperature and timing during injection. The results showed approximately a 3 K reduction before combustion with the 0.196μm droplet size. This is again due to the increased vaporization of the water droplets at the earlier injection timing. Injecting water at 95 degrees BTDC shows further vaporization of the water droplets from the small pre-combustion temperature variations shown, as opposed to the 65 degree injection timing run before.

Pressure is the next constraint to review as was done previously. The earlier injection shows the same effect on pressure as was discussed with temperature. Pressures were decreased by using the smallest droplet size of 0.196 μm to 7.26 MPa, from the baseline of 7.28 MPa. Pressures were then increased over the baseline to 7.29 and 7.30 MPa when using the next two larger droplet sizes. The largest droplet of 0.286 μm decreased the pressure further to 7.27 MPa. This earlier injection timing for the water showed even less effects on the pressure, which should, in turn, maintain the engine efficiency, as opposed to the cases in literature. In addition, it can be seen that the larger droplets had less delay in the combustion in the cylinder. The results are shown below in Figure 16.
Heat release rate can then be reviewed, and as expected, shows the same trends as the pressure and temperature with the 0.196 and 0.286 μm droplets lowering the peak levels. Also,
the 0.210 and 0.240 μm droplet sizes increased the peak levels, as compared to the baseline.

Figure 17 below shows the results of the HRR.

Figure 17: Effects of Water Particle Size on the Combustion Heat Release Rate Curve (20% Water Injected at 95 Degrees BTDC)
HRR was decreased the most with the 0.210 μm water droplet size to 1402.93 J/deg and increased to the highest level with the 0.196 μm water droplet size to 1691.52 J/deg. This is as compared to the baseline of 1683.78 J/deg without water injection. Also, the two smaller sizes show a slight delay in the peak generation, whereas the larger two sizes show very little effect on the delay. With regard to the other components of the combustion process, it can be seen that the earlier injection of water has a smaller variation from the baseline than the later injection.

The next step is to review the emissions for the different water injection particle sizes. These results are very similar to the cases run at the 65 degree BTDC water injection. The only tangible variation in results for the different particle sizes is the amount of NOx formed. At an earlier injection however, the results showed an increase in the production of NOx for the 0.196 μm and 0.240 μm droplet sizes, producing 1.75*10^{-6} kg and 1.73*10^{-6} kg respectively. The 0.286 μm droplet size reduced NOx the most down to 1.68*10^{-6} kg. Literature showed higher reductions in emissions as previously stated, but in this research, the earlier injection timing and lower water percentage used maintained combustion efficiency better. More in depth comparisons are done to the literature in the Discussion.

A) Effects on NOx Formation
B) Effects on Peak NOx Formation

Figure 18: Effects of Water Particle Size on the Combustion NOx Formation Curve (20% Water Injected at 95 Degrees BTDC)

Again, it was seen that the only effect water had on the curve was the amount of soot formed, shown in Figure 19. All droplet sizes reduced the amount of soot over the baseline, where formation increased with each size droplet as compared to each other. The lowest level generated was $2.21 \times 10^{-7}$ kg at peak then, it dropped down to $5.30 \times 10^{-8}$ kg where it remained through the expansion stroke. The amount of soot formed was increased, in both peak and expansion levels, as the water droplet sizes were increased, with the highest at $2.73 \times 10^{-7}$ kg and dropping off to $5.88 \times 10^{-8}$ kg.
The CO that formed in combustion initially peaked then dropped down to a lower level where it remained through the expansion stroke. The peak level was the lowest in the case with the 0.210 μm droplet at 3.69*10^{-5} kg. As discussed before, the level in the expansion stroke is...
inversely proportional to the peak level formed. The lowest level at the expansion stroke was
with the 0.240 μm droplet case at $2.13 \times 10^{-6}$ kg.

A) Effects on CO Formation

B) Effects on Expansion Stroke CO

Figure 20: Effects of Water Particle Size on the Combustion CO Formation Curve (20% Water
Injected at 95 Degrees BTDC)
30% Water Injected at 65 Degrees BTDC

After running all of the different cases at 20% water to fuel by mass, the water percentage was increased to 30%. Then all of the different droplet sizes were run again at all three injection timings, 5, 65, and 95 degrees BTDC. The results were then plotted to fully analyze the effects of the water addition with the higher content used.

A) Effects on Temperature

B) Effects on Peak Temperature
C) Effects on Pre-Combustion Temperature

Figure 21: Effects of Water Particle Size on the Combustion Temperature Curve (30% Water Injected at 65 Degrees BTDC)

Looking at the temperature effects of the different water particle sizes, it can be seen that the smallest injection droplet size, 0.196 μm, had the highest effect and reduced the maximum temperature of combustion the most down to 1168.91 K, shown in Figure 21, which was a 6.7 K drop from the baseline. Maximum temperatures of the combustion increased up to the 0.240 μm droplet then decreased slightly with the larger droplet size of 0.286 μm. The closest temperature found to the original case without any water was 1174.59 K, which is a less than a 0.01% change. Additionally, looking at the pre-combustion temperature, it is seen that the smallest droplet size had the largest effect, with a reduction of nearly 10 K. This reduction was twice that seen at the same injection timing using 20% water by mass. The reduction was still low but the water temperature being nearly the same as the cylinder when injected, and it being injected so early, caused the effect to be rather small. The increased vaporization once again held effective for maintaining the in cylinder temperature before combustion.
Pressure curves, like the temperature curves, show a delay in the combustion of the fuels by adding water. The delay can be seen to be up to 2 degrees of crank angle. The least amount of delay is found with the largest particle size spray of 0.286 μm. Peak pressures are lowered the most in the case with the 0.196 μm and increased by each successive particle size except for the largest particle size of 0.286 μm, which drops somewhat from the previous size. This gave the
lowest peak pressure which was 7.173 MPa. Without water injection, the baseline peak pressure of combustion was found to be 7.278 MPa. In the 0.240 μm case, an increased peak pressure over the baseline to 7.284 MPa. Even with the increased water percentage, the reductions of the peak pressure during combustion were still small as compared to literature. This was mostly due to the timing of the injection which allowed for less negative effects on the combustion. Further comparisons are made in the Discussion for this result.

A) Effects on Heat Release Rate

B) Effects on Peak Heat Release Rate

Figure 23: Effects of Water Particle Size on the Combustion Heat Release Rate Curves (30% Water Injected at 65 Degrees BTDC)
Heat release rate is the last component of combustion that will be reviewed. The graphs of the curves for the different cases show that water delayed the peak heat release rate for all cases. However, interestingly, the smallest three droplet sizes delay the peaks essentially the same amount, but the largest droplet size actually has less effect on the delay. All cases are shown to have a reduced heat release rate at the peak except for the 0.210 μm size water droplet case. The lowest rate seen is with the smallest droplet at 0.196 μm at 1436.31 J/deg. The highest is shown to be 1725.80 J/deg. These are in respect to the base level of 1683.78 J/deg without water.

The next step, as discussed before, is to review the results shown by the addition of water on the emissions of the combustion process at this higher water percentage. The NOx graphs show that the increased percentage does not affect the timing for the NOx creation, just the amount formed. All droplet sizes decreased the amount of NOx formed, but as the droplet size increased, the amount of NOx was reduced until the last case, with the 0.286 μm droplet size, which did not decrease the amount as much as the other sizes. The greatest reduction was found to be 1.59x10^-6 kg in the 0.240 μm case. Though literature found reductions of 35% or greater, the efficiency and combustion were negatively affected. This research showed the timing of the injection reduced the negative combustion effects while still maintaining up to 7.66% reductions in NOx using the increased water percentage. The Discussion section analyzes this more for further research opportunities.
Additionally, water injection did not affect in the timing soot began to form, but instead, reduced the amount of soot formed during combustion. Also, as shown with NOx, as the size of the droplet increased the soot level decreased, except for with the largest droplet size of 0.286 μm which had the least overall reduction. This is shown in Figure 25 below. The highest peak
reduction was with the 0.240 μm water droplet size injection at 1.14x10^{-7} kg, which equaled 60% as compared to the baseline of 2.84x10^{-7} kg. However, levels in the expansion stroke show the most reduction with the 0.286 μm droplet, giving a value of 5.19*10^{-8} kg.

A) Effects on Soot Formation

![Graph showing effects of water particle size on soot formation curve.]

B) Effects on Peak Soot

Figure 25: Effects of Water Particle Size on the Combustion Soot Formation Curve (30% Water Injected at 65 Degrees BTDC)

Once again, the graph for the curves shows little effect on the formation timing for CO but instead affects the amount formed. The size of the droplet has the same effect on the peak
CO, as was shown by the other emissions, with the increased sizes having more of a reduction until the 0.286 μm size. However, the lowest amount, once the CO levels off after the peak, is with the largest droplet size at 2.6x10⁻⁶ kg which is an increase over the base line of 2.09x10⁻⁶ kg.

A) Effects on CO Formation

B) Effects on Peak CO

Figure 26: Effects of Water Particle Size on the Combustion CO Formation Curves (30% Water Injected at 65 Degrees BTDC)
30% Water Injected at 95 Degrees BTDC

Next the injection timing was moved back to 95 degrees BTDC, as was done with the 20% water by mass. The temperature curves show that water injected at the earlier time still creates a delay on the combustion, but is less than shown by the 65 degrees BTDC injection. The levels reduced to the lowest maximum temperature of combustion in the 0.210 μm case, at 1164.93 K, then increased in each subsequent case to the highest peak of 1173.68 K, with the 0.286 μm droplet. The baseline was 1175.61 K, shown in Figure 27 below. As was shown with the lower water to fuel mass ratio, the increased time for the water to vaporize further reduced the effect seen on the in-cylinder temperature before combustion. It is also instrumental in explaining the reduced effect on the peak temperature of combustion as compared to literature, because of the decreased micro burst and flame quenching. Once again, the water reduced the pre-combustion temperature and the largest effect was found with the smallest droplet size of 0.196μm giving nearly a 7 K decrease. The amount of reduction once again was approximately twice the reduction found with 20% water for the same injection timing. Even with the increased water percentage, the effect was still small because of the early injection timing and the hot temperature of the water. The Discussion section better compares the literature results to the research results in this project.
A) Effects on Temperature

B) Effects on Peak Temperature
C) Effects on Pre-Combustion Temperature

Figure 27: Effects of Water Particle Size on the Combustion Temperature Curve (30% Water Injected at 95 Degrees BTDC)

The pressure curves once again follow the same general trends as the temperature with a slight delay in the combustion. Also, increasing the water droplet sizes showed larger reductions in peak pressure through the 0.210 μm droplet size, but then began to have less reduction as the droplet size continued to increase. All water injection cases decreased the overall peak pressure from the baseline of 7.28 MPa. The least effect was shown to reduce the peak pressure to 7.263 MPa. This was seen in both the 0.240 μm case and the 0.286 μm case, which had equal amounts of reduction. The lowest pressure was in the 0.210 μm case at 7.23 MPa. These results are shown in Figure 28 below.
A) Effects on Pressure

B) Effects on Peak Pressure

Figure 28: Effects of Water Particle Size on the Combustion Pressure Curve (30% Water Injected at 95 Degrees BTDC)

Heat release rate again shows some slight delay in the peak levels, but is less of a delay as compared to the later injection timing for the water, as shown previously. Peak levels are reduced in all water injection cases. As the size of the droplet size increased, the peak heat
release rate increased up to the largest droplet size, which had the highest overall reduction. The least effect was shown in the 0.240 μm case at 1613.95 J/deg and the highest effect was shown in the 0.286 μm case with a reduction of 22% down to 1314.31 J/deg. The base level without water injection was 1683.78 J/deg. Results are shown in Figure 29 below.

Figure 29: Effects of Water Particle Size on the Combustion Heat Release Rate Curve (30% Water Injected at 95 Degrees BTDC)
NOx, as the review of emissions is taken into consideration, shows only peak values being affected by the water injection. The lowest value is found in the case with the 0.196 μm droplet at 1.66x10^-6 kg, giving a reduction of 0.06x10^-6 kg from the baseline, 1.72x10^-6 kg. The size of the water particle being injected then showed an increase over the baseline for the next two sizes before being slightly reduced by the 0.286 μm droplet. The highest increase in the heat release rate is 1.76x10^-6 kg for the 0.210 μm droplet size case. NOx results in the literature did show higher reductions, but combustion suffered, having negative consequences from the water injection. The benefits of earlier water injection timings are reviewed further in the Discussion section.

A) Effects on NOx Formation
B) Effects on Peak NOx

Figure 30: Effects of Water Particle Size on the Combustion NOx Formation (30% Water Injected at 95 Degrees BTDC)

Soot once again showed the same tendency of water addition affecting the peak and expansion stroke levels, not the timing for soot formation. The soot levels show reduction for all water injection cases but the peak values vary without a general trend. The lowest peak value is with the 0.196 μm droplet at 2.21x10^{-7} kg. However, the lowest value, once the soot is reduced during the expansion stroke, is with the 0.240 μm water droplet case, at 5.40x10^{-8} kg. The standard level without water peaks at 2.84x10^{-7} kg and then is reduced during the expansion stroke to 6.31x10^{-8} kg. Results for soot are shown in Figure 31.
A) Effects on Soot Formation

B) Effects on Expansion Stroke Soot

Figure 31: Effects of Water Particle Size on the Combustion Soot Formation (30% Water Injected at 95 Degrees BTDC)

Additionally, CO levels only show effect in the peak and expansion stroke levels by adding water to the combustion. Peak levels showed a general increase in comparison to each other with an increase of the droplet size, except for the 0.240 μm droplet size, which is slightly lower than the 0.210 μm case. The most reduced peak value, as compared to the standard without water, is 3.73x10⁻⁵ kg in the 0.196 μm case. Conversely, at the expansion stroke level all are increased over the baseline of 2.09x10⁻⁶ kg. At expansion stroke levels, the largest droplet
size of 0.286 μm produced the least increase over the no water injection, which was 2.25x10⁻⁶ kg. These results are from Figure 32 below.

A) Effects on CO Formation

B) Effects on Expansion Stroke CO

Figure 32: Effects of Water Particle Size on the Combustion CO Formation (30% Water Injected at 95 Degrees BTDC)

Effects of Water Temperature Variation

To further understand the effects of water injection, tests were run with the water particles being injected at the same size as the fuel particles, 0.196 μm, with the temperature of
the water was varied to see if any effect was shown on the emissions or the combustion process. Water was injected at the 5, 65, and 95 degrees BTDC timings, as was done previously, to see if the effects of water temperature variation have any different effect while using the earlier injection timings. The temperature used initially was 368 K, which was the same as the fuel being injected. First the temperature was changed to 388 K to see if an increase in the temperature had an effect, then the temperature was reduced to 348 K and the simulations were once again run at all of the injection timings. The results are compiled together for the different injection timing and the different temperatures, in Figures 32 through 37 below.

The injections at 5 degrees BTDC once again caused quenching of the flame and therefore did not achieve combustion in the cylinder. Because of that issue, the earlier injections were the ones used for this research. Reviewing the temperature curves, it can be seen that the injection timing had the largest effect on the delay in the combustion but water’s temperature had very slight effect. At both timings, the 348 K temperature delayed the combustion more than the hotter temperature of 388 K. There was also an effect on the maximum temperature of combustion attained during combustion due to the temperature change in the water being injected. In the cases run, it was shown that the 65 degree BTDC injection increased temperature in the peak over the baseline, while both of the cases with the water injected at 95 degrees BTDC decreased the maximum temperature of combustion. In respect to the temperature of the water being injected, the higher temperature water, 388 K, was shown to have less of an effect on the combustion temperature than the lowered temperature water, 348 K. The baseline case gave a peak pressure of 1175.61 K. By increasing the water temperature 20 K, an increase to 1177.4 K and decrease to 1173.01 K was attained respectively at 65 degrees and 95 degrees BTDC. At 348 K, the temperature was increased to 1180.9 K at 65 degrees BTDC and decreased to 1171.99
K at 95 degrees BTDC. As was seen with the injection of 20% at the different injection timings of 65 and 95 degrees BTDC, the reductions were approximately 5 K and 3 K respectively. Once again, this showed injection timing allowed for further water droplet vaporization which negated much of the temperature reduction in the cylinder. However, the temperature of the water did have a slight effect. At both injection timings, the warmer 388 K water showed a slightly larger reduction with the injection at 65 degrees having more effect, around 0.5 K. This effect was very small, but did show a small capability to possibly further enhance the benefits of water injection. Once again, the earlier injection had lower effects as compared to the literature but the multiple factors causing this are considered more in the Discussion section.

A) Effects on Temperature
Figure 33: Effects of the Water Temperature on the Combustion Temperature Curve

The pressure curves followed the same trends as was seen by the temperature curves with the hotter water injection, of 388 K, having slightly less of a delay in combustion than the colder temperature of 348 K. Without water, the pressure peaked at 7.278 MPa. With the water temperature increased to 388 K, the pressure increased to 7.29 MPa during the 65 degree BTDC injection timing case and decreased to 7.263 MPa in the 95 degree BTDC injection case. When
the water was lowered to 348 K, the 65 degree BTDC injection yielded a peak pressure of 7.312 MPa and a peak pressure of 7.258 MPa for the 95 degree injection timing BTDC.

A) Effects on Pressure

B) Effects on Peak Pressure

Figure 34: Effects of the Water Temperature on the Combustion Pressure Curve

Following the results for pressure and temperature, heat release rate was shown to delay further with the water at the colder temperature. However, the later injection timing of 65 degrees BTDC showed more variation for the temperature of the water being injected than did
the 95 degree BTDC injection timing. The case without water showed a peak heat release rate of 1683.78 J/deg. The increased water temperature of 388 K gave a peak heat release rate of 1666.27 J/deg at 65 degree BTDC injection timing and a rate of 1210.84 J/deg at 95 degree BTDC injection timing. By decreasing the temperature a peak rate of 1674.46 J/deg at the 65 degrees BTDC injection and 1577.72 J/deg at the 95 degree BTDC injection was given.

A) Effects on Heat Release Rate

B) Effects on Peak Heat Release Rate

Figure 35: Effects of the Water Temperature on the Combustion Heat Release Rate Curve
Regarding emissions, the injection of water reduced the NOx levels in all cases, except the 95 degree BTDC injection with the 348 K water, which increased the NOx to $1.81 \times 10^{-6}$ kg over the baseline case of $1.72 \times 10^{-6}$ kg without water. The 348 K water at 65 degrees BTDC gave a NOx level of $1.64 \times 10^{-6}$ kg. The increased water temperature of 388 K gave $1.67 \times 10^{-6}$ kg and $1.69 \times 10^{-6}$ kg of NOx at the 65 and 95 degree BTDC injection cases respectively. Once again, the lower temperature water injected into the chamber had a larger effect on the emissions than the increased water temperature. The Discussion section of this paper further investigates the reasons, such as the injection timing and warmer water temperature, why the reviewed literature found more reductions.

A) Effects on NOx Formation
B) Effects on Peak NOx

Figure 36: Effects of the Water Temperature on the Combustion NOx Formation

For soot created in combustion, the baseline case without water peaked at $2.84 \times 10^{-7}$ kg then reduced to $6.31 \times 10^{-8}$ kg. The addition of water decreased the soot output in all cases over the baseline. The hotter water of 388 K decreased the soot levels less for the respective injection timing. At the 65 degree BTDC injection timing, the 388 K water lowered the peak soot to $1.54 \times 10^{-7}$ kg and dropped to $5.21 \times 10^{-8}$ kg. At the 65 degree BTDC injection timing, the 348 K water lowered the peak soot to $1.35 \times 10^{-7}$ kg and dropped to $5.26 \times 10^{-8}$ kg. The earlier 388 K water injection of 95 degrees BTDC yielded a result of $2.45 \times 10^{-7}$ kg, which dropped to $5.5 \times 10^{-8}$ kg. With the 348 K water injection, the soot peaked at $2.3 \times 10^{-7}$ kg and dropped to $5.27 \times 10^{-8}$ kg.
CO levels were also reduced at the peak but increased at expansion stroke levels in all water injection cases over the baseline without any water. The baseline had a peak of $3.87 \times 10^{-5}$ kg and an expansion stroke level of $2.09 \times 10^{-6}$ kg. The 65 degree BTDC case at 388 K reduced the CO levels to a peak of $3.54 \times 10^{-5}$ kg but increased expansion stroke level to $2.72 \times 10^{-6}$ kg.
The earlier injection at 95 degrees BTDC and with 388 K water gave reduced levels of $3.76 \times 10^{-5}$ kg and $2.19 \times 10^{-6}$ kg for the CO at the peak and expansion stroke level respectively. The colder water, 348 K, reduced CO to $3.52 \times 10^{-5}$ kg at peak and increased it to $2.87 \times 10^{-6}$ kg at the expansion stroke level when injected at 65 degrees BTDC. For the 95 degree BTDC injection, CO was reduced at the peak to $2.22 \times 10^{-6}$ kg and increased to $3.72 \times 10^{-5}$ kg at the expansion level.

A) Effects on CO Formation

B) Effects on Peak CO

Figure 38: Effects of the Water Temperature on the Combustion CO Formation
Effects of Water Injection at TDC

A last case was run with the injection of water which started at 0 degrees of crank angle, TDC, and lasted for 5 degrees of crank angle. This was done to closer match conditions for boundary conditions in much of the literature that injected the water during the fuel injection. The intent was to show higher reductions in emissions similar to their results and thus further verify the results in this research. The 0.196 μm water droplet size was used, which matched the fuel droplet size. Also, the water temperature of 368 K was used to be more comparable to the cases that had already been run.

The injection of water at TDC showed a greater effect on the combustion temperature than was seen in the cases with the water injected earlier. The maximum temperature of combustion was 1121.69 K, giving a reduction over the baseline, 1175.61 K, of 5.6%. Also, there was a greater delay in the combustion. The earlier water injections had much less effect on the temperature curve as was previously discussed. There is not a decrease in the pre-combustion temperature of the cylinder because the water was not injected until combustion was already starting to occur. The results for the TDC water injection are shown in Figure 39 below.

A) Effects on Temperature
Next the pressure curve for the TDC injection was analyzed. Peak pressure of combustion was similarly reduced more with this later injection timing. It attained a maximum value of 6.76 MPa which gave a reduction of 7.1% from the baseline of 7.28 MPa. Additionally, the pressure curves show a greater delay in combustion. The reduction of 0.52 MPa closely matches the reductions found in literature of 0.5 MPa (Kannan and Udayakuma, 2009)(Bedford,
et al., 2000). Bedford et al. used a 2.0 liter engine with a bore of 13.0 cm and had a compression ratio of 17.25:1. In the paper by Kannan and Udayakuma, the 661 cc engine modeled had a bore size of 87.5 mm with a compression ratio of 17.5:1. These were smaller than the engine used in this research, 2.34 liter, but the model used by Bedford et al. was similar in size. Both also used a higher compression ratio than the 16:1 ratio used by the Sandia National Laboratory engine.

The results are shown in Figure 40 below.

![Graph of Effects of TDC Water Injection Timing on the Combustion Pressure Curve](image)

A) Effects on Pressure

B) Effects on Peak Pressure

Figure 40: Effects of TDC Water Injection Timing on the Combustion Pressure Curve
The heat release rate curve is also plotted to better see the results for water injection at TDC. Once again, there is a much higher reduction in the results for heat release rate at this timing. The maximum rate was reduced to 523.85 J/deg from the baseline of 1683.78, a 68.9% reduction. The heat release rate curve does not peak sharply as seen with the earlier injections of water, but instead it rises some and then varies around the peak value for approximately 2 degrees of crank angle before dropping back down. This is shown in Figure 41 below.

![Diagram of Heat Release Rate Curve](image)

A) Effects on Heat Release Rate

![Diagram of Peak Heat Release Rate](image)

B) Effects on Peak Heat Release Rate

Figure 41: Effects of TDC Water Injection Timing on the Combustion HRR Curve
Also, to fully understand the effects of the water injection timing, emissions need to be analyzed. As done previously, the NO\textsubscript{x} formation curve will be analyzed first, as it is the most common emission considered to be effected by water addition to combustion. NO\textsubscript{x} is reduced 48.3\% by injection of the water at TDC, to 9.76\times10^{-7} kg. This reduction was over the baseline of 1.72\times10^{-6} kg. Literature showed similar reductions as found in this case (Chadwell and Dingle, 2008)(Kannan and Udayakuma, 2009)(Subramanian, 2011). The other research showed 38-42\% reductions of NO\textsubscript{x} with 20\% water injection into the combustion process. The Discussion section expands on this significance. Figure 42 shows the results for the NO\textsubscript{x} formation.

![Effects on NOx Formation](image_url)
B) Effects on Peak NOx

Figure 42: Effects of TDC Water Injection Timing on the Combustion NOx Curve

Soot results for injection at TDC varied from the results at the earlier injection timings. The peak formation during combustion was reduced as seen before, but during the expansion stroke, the soot level was increased over the baseline. The peak reduction equaled 47.2% but more soot was retained during the expansion stroke with an increase of 21.4%. The later injection timing allowed for more quenching of the flame which resulted in higher soot content during the expansion stroke. The results are shown in Figure 43.

A) Effects on Soot Formation
B) Effects on Peak Soot

Figure 43: Effects of TDC Water Injection Timing on the Combustion Soot Curve

The formation of CO was also greatly decreased in the peak of combustion but was increased during the expansion stroke. The peak formation was reduced 26.1% to $2.86 \times 10^{-5}$ kg, over the baseline of $3.87 \times 10^{-5}$ kg. However, the expansion stroke CO was increased by 98.1% to $4.14 \times 10^{-6}$ kg. The baseline expansion stroke CO was $2.09 \times 10^{-6}$ kg. Figure 44 shows these results.
B) Effects on Peak CO

Figure 43: Effects of TDC Water Injection Timing on the Combustion Soot Curve
CHAPTER 5

DISCUSSION

The injection of water requires thorough investigation of both the properties of combustion as well as the emissions for all of the different cases run. It is important to consider both effects to find the best conditions for injecting water to reduce emissions, yet retaining the power and efficiency of the engine. To maintain the efficiency of an engine, the properties of combustion are desired to be as close to the original values found in the case without water injection as possible. A slight increase in temperature, pressure, and heat release rate would prove to be more beneficial than a decrease for maintaining the efficiency of the engine. This is due in part to the fact that efficiency is the result of maintaining as much power in the output as is input into the system. For an engine, this is by converting the most amount of energy possible from the fuel during its combustion. Many factors attribute to the loss in energy, such as friction, but the temperature and pressure are both determinates of the amount of energy released from the fuel by its combustion. However, the most amount of reduction for emissions possible is desired, therefore becoming more ecologically friendly and cleaner for the environment by reducing the pollutant levels in the air. The emissions created by the combustion of diesel fuel are also largely effected by the temperature in the cylinder. Temperature of a chemical reaction, like the formation of NOx from the presence of molecules in the fuel and air, can increase or reduce the rate in which the formations occur. In many cases, the higher the temperature of a reaction is, the faster the reaction occurs. This gives rise to the issue that as the temperature in the chamber decreases, reductions in the emissions are likely. However, with the in-cylinder
temperature reduction there will also likely be a decrease in efficiency. Looking back at the figures in the results section, Chapter 4, it can be seen that in most cases, emissions and the properties of combustion are inversely effected by the addition of water to the combustion. To see if the change in the water particle size or temperature of the water injected can help in maintaining the efficiency while reducing the emissions, the results for each simulation case that were run needed to be compared to one another to see which results are the best results. To achieve this, peak values for temperature, pressure, and heat release rate as well as the NOx, peak soot, expansion stroke level soot, peak CO, and expansion stroke level CO are plotted together in a table. The results for the 20% water by mass, with both the 65 degree BTDC and 95 degree BTDC injection timings, were all plotted in Table 3. The highest levels of reduction in each of the emissions were highlighted green, while the lowest levels of reduction for each were highlighted red. For the properties of the combustion, the least amount of reduction or highest increase in each of these properties was highlighted green, while the highest reduction in them was highlighted red. This allows for improved ease in seeing the case with the best results for all of the different conditions. The tables are made with a positive difference in the percent of change from the baseline, without water injection, for the each property signifying a reduction. Therefore, the negative values in the percent difference specify an increase over the baseline. In the table, combustion properties are represented by: T – temperature, P – pressure, and HRR – heat release rate. Symbols for the emissions are shown by: NOx – nitrous oxides and CO – carbon monoxide. Max. stands for the maximum level attained during the combustion process. Ex. is used to represent the level found during the expansion stroke.
Water injection proved to be beneficial in most cases for emissions reduction except in the formation of CO. At the peak levels during the fuel combustion, it was seen that the CO was

### Table 3: 20% Water Droplet Size Variation at 65 and 95 Degrees BTDC (Reduction = +)

<table>
<thead>
<tr>
<th>Timing : Size</th>
<th>No Water</th>
<th>65° btdc : 0.196 μm</th>
<th>% Diff.</th>
<th>65° btdc : 0.210 μm</th>
<th>% Diff.</th>
<th>65° btdc : 0.240 μm</th>
<th>% Diff.</th>
<th>65° btdc : 0.286 μm</th>
<th>% Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>T (K)</td>
<td>1175.61</td>
<td>1166.80</td>
<td>0.75%</td>
<td>1171.18</td>
<td>0.38%</td>
<td>1175.69</td>
<td>-0.01%</td>
<td>1173.47</td>
<td>0.18%</td>
</tr>
<tr>
<td>P (Mpa)</td>
<td>7.278</td>
<td>7.217</td>
<td>0.83%</td>
<td>7.242</td>
<td>0.49%</td>
<td>7.276</td>
<td>0.02%</td>
<td>7.257</td>
<td>0.29%</td>
</tr>
<tr>
<td>HRR (J/deg)</td>
<td>1683.78</td>
<td>1275.69</td>
<td>24.24%</td>
<td>1320.17</td>
<td>21.59%</td>
<td>1609.04</td>
<td>4.44%</td>
<td>1334.89</td>
<td>20.72%</td>
</tr>
<tr>
<td>NOx (kg)</td>
<td>1.72E-06</td>
<td>1.71E-06</td>
<td>0.76%</td>
<td>1.62E-06</td>
<td>5.61%</td>
<td>1.66E-06</td>
<td>3.51%</td>
<td>1.72E-06</td>
<td>0.22%</td>
</tr>
<tr>
<td>Max Soot (kg)</td>
<td>2.84E-07</td>
<td>2.00E-07</td>
<td>29.52%</td>
<td>1.86E-07</td>
<td>34.40%</td>
<td>2.00E-07</td>
<td>29.51%</td>
<td>2.44E-07</td>
<td>14.10%</td>
</tr>
<tr>
<td>Ex. Soot (kg)</td>
<td>6.31E-08</td>
<td>5.36E-08</td>
<td>15.08%</td>
<td>5.47E-08</td>
<td>13.28%</td>
<td>5.43E-08</td>
<td>13.94%</td>
<td>5.54E-08</td>
<td>12.25%</td>
</tr>
<tr>
<td>Max CO (kg)</td>
<td>3.87E-05</td>
<td>3.66E-05</td>
<td>5.62%</td>
<td>3.62E-05</td>
<td>6.67%</td>
<td>3.69E-05</td>
<td>4.64%</td>
<td>3.76E-05</td>
<td>2.90%</td>
</tr>
<tr>
<td>Ex. CO (kg)</td>
<td>2.09E-06</td>
<td>2.50E-06</td>
<td>-19.90%</td>
<td>2.57E-06</td>
<td>22.81%</td>
<td>2.46E-06</td>
<td>-17.80%</td>
<td>2.19E-06</td>
<td>-5.06%</td>
</tr>
</tbody>
</table>

(A) Water Injected at 65 Degrees BTDC

<table>
<thead>
<tr>
<th>Timing : Size</th>
<th>No Water</th>
<th>95° btdc : 0.196 μm</th>
<th>% Diff.</th>
<th>95° btdc : 0.210 μm</th>
<th>% Diff.</th>
<th>95° btdc : 0.240 μm</th>
<th>% Diff.</th>
<th>95° btdc : 0.286 μm</th>
<th>% Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>T (K)</td>
<td>1175.61</td>
<td>1175.29</td>
<td>0.03%</td>
<td>1178.47</td>
<td>-0.24%</td>
<td>1178.51</td>
<td>-0.25%</td>
<td>1174.36</td>
<td>0.11%</td>
</tr>
<tr>
<td>P (Mpa)</td>
<td>7.278</td>
<td>7.263</td>
<td>0.20%</td>
<td>7.286</td>
<td>-0.11%</td>
<td>7.301</td>
<td>-0.32%</td>
<td>7.267</td>
<td>0.15%</td>
</tr>
<tr>
<td>HRR (J/deg)</td>
<td>1683.78</td>
<td>1691.52</td>
<td>-0.46%</td>
<td>1402.93</td>
<td>16.68%</td>
<td>1689.84</td>
<td>-0.36%</td>
<td>1613.56</td>
<td>4.17%</td>
</tr>
<tr>
<td>NOx (kg)</td>
<td>1.72E-06</td>
<td>1.75E-06</td>
<td>-1.89%</td>
<td>1.72E-06</td>
<td>0.29%</td>
<td>1.73E-06</td>
<td>-0.71%</td>
<td>1.68E-06</td>
<td>2.33%</td>
</tr>
<tr>
<td>Max Soot (kg)</td>
<td>2.84E-07</td>
<td>2.21E-07</td>
<td>22.33%</td>
<td>2.26E-07</td>
<td>20.41%</td>
<td>2.52E-07</td>
<td>11.36%</td>
<td>2.73E-07</td>
<td>3.86%</td>
</tr>
<tr>
<td>Ex. Soot (kg)</td>
<td>6.31E-08</td>
<td>5.30E-08</td>
<td>16.06%</td>
<td>5.44E-08</td>
<td>13.83%</td>
<td>5.46E-08</td>
<td>13.48%</td>
<td>5.88E-08</td>
<td>6.75%</td>
</tr>
<tr>
<td>Max CO (kg)</td>
<td>3.87E-05</td>
<td>3.73E-05</td>
<td>3.67%</td>
<td>3.69E-05</td>
<td>4.85%</td>
<td>3.82E-05</td>
<td>1.49%</td>
<td>3.77E-05</td>
<td>2.67%</td>
</tr>
<tr>
<td>Ex. CO (kg)</td>
<td>2.09E-06</td>
<td>2.28E-06</td>
<td>-8.98%</td>
<td>2.27E-06</td>
<td>-8.52%</td>
<td>2.13E-06</td>
<td>-2.03%</td>
<td>2.25E-06</td>
<td>-7.83%</td>
</tr>
</tbody>
</table>

(B) Water Injected at 95 Degrees BTDC
lowered, but when the levels dropped off during the expansion stroke, the levels of CO decrease from the peak. It was shown that as the peak levels of the CO were lowered with the injection of water, there was a reduced drop in the CO during the expansion stroke. This resulted in an increase at the final levels, during the expansion stroke, over the baseline level. The least negative effects on combustion and on the final CO levels were found when the water was injected at 95 degrees BTDC. The best case for the properties of the combustion was shown with the 95 degree BTDC injection and with the 0.240 μm water droplet size. This same case also had the lowest increase in the final CO levels. The best result for all of the emissions, except for the expansion stroke level soot and CO, were found in the case with the 65 degree BTDC injection timing and 0.210 μm water droplet. The lowest expansion stroke level soot, as well as the highest heat release rate, was found in the 0.196 μm droplet case at 95 degrees BTDC. For the injection of 20% water by mass, it can be seen that water injection can be very useful in reducing the levels of NOx and soot but it comes with an increase in the levels of CO at the expansion stroke. The droplet size does show effect on the different results. The temperature and pressure peaks during combustion are just 1% or slightly greater but the droplet size along with the injection timing gave a variate of up to 25% for the heat release rate. For emissions, the modifications of the water droplet size shows a variation of 7.5% for NOx, 9.31% for expansion stroke soot, and 20.78% for expansion stroke CO. This is very interesting considering the small percentage of water used. The combination of injection timing and droplet size does allow for increased effectiveness of water injection. The best case for the 20% water by mass was with the 65 degree BTDC injection timing and the 0.240 μm water droplet size. Though for many emissions, this shows the second best reduction level. This case only had a 0.01% increase in the temperature at peak as well as only a 0.02% reduction in the peak pressure of the combustion.
Also, this case reduced the effect on the heat release rate to by 4.44% as compared to others which had over a 24% reduction. CO at the expansion stroke level was increased 17% but other cases had up to a 22.81% increase over the baseline. In the other cases where CO was less affected, the emissions were barely reduced from the baseline without water, and in some cases the NOx was even increased 2.01%. Due to this analysis of the results, the optimum case was selected for the best balance of emission reduction verses the least amount of effect or reduction in the combustion processes and properties to maintain the most power possible. This case allowed for a 3.51% reduction in NOx and a 13.94% reduction in expansion stroke level soot, along with having the minimal effects on the properties of the combustion process as discussed before.

Next, the water mass was increased to 30% of the fuel mass, which was regarded in the literature on water injection as the highest water content still capable of being effective without being too high of a percent and having unnecessarily high negative effects on the combustion. The same conditions were used in making the table to show the results for the increased mass of water being injected at all four size particles which were used before, 0.196, 0.210, 0.240, and 0.286 μm. Once the simulations were run with the water being injected at 65 degrees BTDC, the injection timing was moved back to 95 degrees BTDC and the simulations for each size particle were run. Table 4 below shows the results for all of the simulations with the best and worst results for each component of the simulation being marked accordingly.
When the water mass was increased to 30% of the fuel mass, the results were very interesting. In the 20% mass simulations, the best results for the combustion components, least
effect upon the temperature, pressure, and heat release rate, was with the 95 degree BTDC injection timing. However, the results for the emissions were better with the different particle sizes injected at 65 degree BTDC. With the increased water percentage, the 95 degrees BTDC injection timing did not have the lowest effect on the combustion properties. The 65 degrees BTDC injection timing with the 0.210 μm droplet size had the least negative effect on the heat release rate of a 2.5% increase. In the case with the water injected at 65 degrees BTDC and with the 0.240 μm droplet, the least amount of effect on the temperature peak was seen at just a 0.09% decrease over the baseline. Also, the pressure peak was the least effected, as compared to the baseline, with a 0.09% increase. This same case had the best result for the NOx levels with a 7.66% reduction, the peak soot at a 59.81% reduction, and the peak CO with a 13.85% reduction. This case also had the second largest decrease in the expansion stroke level soot with a 15.63%. The largest decrease, however, was one droplet size with the 0.286μm, 17.82%. The heat release rate was shown to decrease 5.88% in this case. The expansion stroke level CO in the case with the 0.240 μm droplet, however, was shown to increase 48.86% over the baseline level. In all cases with the 65 degree BTDC injection, the water caused the expansion stroke level soot to increase by more than 46% over the case without water, except for the largest droplet size of 0.286μm which only increased it 24.21%. With the increased water percentage, the effect of the droplet size can be seen to increase in most areas. The effect on the temperature and pressure are increased but still remain just under a 1.5% variation over all cases and timings. The heat release rate showed a slightly lower deviation in the result across all cases with 30% water mass injected, than with the 20% water injections, varying 24.44%. In emissions, variations with the different droplet sizes and injection timings allowed for a 9.67% change in NOx, 8.0% variation in the expansion stroke soot, and a 41.03% variation for expansion stroke CO. It can be seen that
the water droplet size has the most effect on the variations in CO and NO\textsubscript{x} with the increased percentage of water by mass. Since NO\textsubscript{x} is the most commonly considered emission for reduction by water injection, it can be interesting to note the results vary nearly 10%, which is substantial when looking at such small percentages of water. The best case for the 30% water by mass to use would be the case with the 95 degree BTDC injection timing and the 0.196 μm droplet size. Though this case did not have the best overall reduction in the emission levels, nor maintained the closest levels to the baseline for the combustion components, the overall combination was the best. In this case, the temperature peak reduced 0.57\%, the pressure peak reduced 0.3\%, and the heat release rate reduced 8.06\% which showed that the fuel combustion for power generation was well maintained. In regards to the emissions, the NO\textsubscript{x} was reduced 3.51\%, the expansion stroke level soot was reduced 9.81\%, and the expansion stroke CO was only increased 15.11\%. The increased water mass more of a negative effect on the expansion stroke level CO, especially in the 65 degree BTDC injection cases, which over shadowed the positive effects on the other emissions in many cases.

The last case was based on a change in the temperature of the water injected instead of changes in the droplet size. This was done because variations in the water temperature could commonly occur depending on the environments the engine was subjected to as well as the conditions of the fuel injection system. With the same injection timings of 65 degrees and 95 degrees BTDC, the droplet size was held at 0.196 μm which was the same as the fuel injection particle size. The original water temperature was 365 K, but an increase of 20 K was used to run simulations at the same injection times used previously, 5, 65, and 95 degrees BTDC. Once these were completed the temperature was reduced by 20 K to 348 K and the simulations for each of the injection timings were run again. The results for all of the components of
combustion and emissions were plotted in Table 5 to show the results as was done in Table 4.

Once again, the most beneficial and least beneficial results for each were marked.

<table>
<thead>
<tr>
<th>Timing :</th>
<th>Temp</th>
<th>No Water</th>
<th>65° btdc :</th>
<th>% Diff.</th>
<th>95° btdc :</th>
<th>% Diff</th>
<th>65° btdc :</th>
<th>% Diff</th>
<th>95° btdc :</th>
<th>% Diff</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>388 K</td>
<td></td>
<td>388 K</td>
<td></td>
<td>348 K</td>
<td></td>
<td>348 K</td>
<td></td>
</tr>
<tr>
<td>T (K)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1175.61</td>
<td>1177.4</td>
<td>-0.15%</td>
<td>1173.01</td>
<td>0.22%</td>
<td>1180.90</td>
<td>-0.45%</td>
<td>1171.99</td>
<td>0.31%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P (Mpa)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.278</td>
<td>7.290</td>
<td>-0.16%</td>
<td>7.263</td>
<td>0.20%</td>
<td>7.312</td>
<td>-0.47%</td>
<td>7.258</td>
<td>0.27%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HRR (J/deg)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1683.78</td>
<td>1666.27</td>
<td>1.04%</td>
<td>1210.84</td>
<td>28.09%</td>
<td>1674.46</td>
<td>0.55%</td>
<td>1577.72</td>
<td>6.30%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NOx (kg)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.72E-06</td>
<td>1.67E-06</td>
<td>3.01%</td>
<td>1.69E-06</td>
<td>2.04%</td>
<td>1.64E-06</td>
<td>4.74%</td>
<td>1.81E-06</td>
<td>-5.35%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Max Soot</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.84E-07</td>
<td>1.54E-07</td>
<td>45.78%</td>
<td>2.45E-07</td>
<td>13.68%</td>
<td>1.35E-07</td>
<td>52.56%</td>
<td>2.30E-07</td>
<td>19.12%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ex. Soot (kg)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.31E-08</td>
<td>5.21E-08</td>
<td>17.51%</td>
<td>5.51E-08</td>
<td>12.63%</td>
<td>5.26E-08</td>
<td>16.69%</td>
<td>5.27E-08</td>
<td>16.46%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Max CO (kg)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.87E-05</td>
<td>3.54E-05</td>
<td>8.56%</td>
<td>3.76E-05</td>
<td>2.89%</td>
<td>3.52E-05</td>
<td>9.22%</td>
<td>3.72E-05</td>
<td>3.90%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ex. CO (kg)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.09E-06</td>
<td>2.72E-06</td>
<td>-30.41%</td>
<td>2.19E-06</td>
<td>-4.69%</td>
<td>2.87E-06</td>
<td>-37.20%</td>
<td>2.22E-06</td>
<td>-6.14%</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5 : Water Temperature Variation Results and Percent Difference (Reduction = +)

It was shown previously in the figures for the result curves, that the lower temperature water had a larger effect on the combustion than the increased temperature of the water. The water temperature variation could have an effect on the micro explosions of the water droplets causing an intensified explosion of the droplet during vaporization. This would explain the lower variation shown by the higher temperature water as well because the energy in the vaporization would be reduced. For the temperature change in the water injection, the best results for all but two of the conditions were shown to occur in the case with the 348 K water injected at 65 degrees BTDC. In this case, the temperature peak increased 0.45%, the pressure peak increased 0.47% and the heat release rate decreased only 0.55%. The emissions gave the best reductions of 4.74% for NOx, peak soot decreased 52.56%, and the peak CO decreased
9.22%. The expansion stroke level CO, however, increased the most in this case, 37.2% over the baseline. The expansion level soot decreased the most in the case with the 388 K water at 65 degrees BTDC to 17.51% below the baseline. The expansion stroke level CO decreased by 4.69% in the case with the 95 degree BTDC injection of 388 K water. The differences in all cases show the water temperature increase and decrease gave a 0.76% variation in temperature and a 0.74% variation in pressure peaks. The heat release rate, however, has an increased variation, as compared to the droplet size cases, with a variation of 27.04%. For emissions, a variation is seen of 10.09% in NO\textsubscript{x}, 4.88% in expansion stroke soot, and 32.51% in expansion stroke CO. The temperature variation of the water along with different injection timings showed a higher effect on the heat release rate which is expected. The effects on the NO\textsubscript{x} show nearly the same amount of variation as was shown for 30% water injection with different droplet sizes. This could be useful to combine the two for greater emission reduction while still maintaining low consequences for the combustion. In comparison, the best overall result for the water temperature change was found in the case with the 348 K water injected at 65 degrees BTDC described before. This case had the best results for all of the conditions except for CO at the expansion stroke. It was increased the most in this case, but in the other cases the negative effects on the heat release rate or other emissions were greatly increased. Thus, the other cases either negated water injection’s effectiveness in reducing the emissions levels or decreased the components of combustion, thus causing probable power and efficiency losses.

Further analysis can be done to verify which condition proves to be the most effective by comparing the results for different contours to the baseline contours. The contours for the temperature within the cylinder begin with comparing the results to the case without water. The average combustion temperature peaked at a timing of 13 degrees after TDC, so this timing was
chosen as the comparison point for all of the cases. The best case as listed for 20% water by mass, 30% water by mass, and temperature variation in the water being injected were set with contours at the same timing as the baseline. The temperature range for the contours was also set the same for each case to see the true difference in each result. The contours for the temperature are shown in Figure 38 below for the visual comparison of the results.

![Temperature Contours](image)

(A) No Water  
(B) 20% Water at 65°BTDC & 240μm  
(C) 30% Water at 95°BTDC & 196 μm  
(D) Water Temp. at 348 K & 65°BTDC

Figure 44: Comparison of Temperature Contours at 13° ATDC for Best Cases

The variation in the results for the contours is interesting. As compared to the baseline, it is seen that all cases seem to have at least some reduction over the temperature peak zone. In the case without water, the maximum temperature area curves over the dish wall of the piston and continues towards the cylinder wall. In each case with water, there is a reduction in the area of the maximum temperature that extends towards the walls. Interestingly though, in the case with the smallest particle, 0.196μm, injected at 30% of the fuel mass at 95 degrees BTDC timing, the temperature peak area that occurs around the injection point of the fuel is shown to be longer in length. The water particles being injected into the chamber are going to pool in the same areas as the fuel particles so their presence will affect the combustion. This is proven by the slight
drops in pressure and temperature as well as the drop in the heat release rate that were shown by the variances in the values for temperature, which ranged in these cases from +0.57% to -0.45% from the baseline. These are very small variations from the baseline which is a positive result as it shows little change in the temperature contour, so the power of the engine should be relatively well maintained for all cases.

Next the pressure curves are shown for each case. The peak pressure occurs at 9.5 degrees of crank angle so this timing is used. Also, as done for the temperature, the same pressure values were used to equalize the conditions for the contours. The contours are set for the peak pressure timing, of 9.5 degrees after TDC, when it occurred in the case without water.

![Pressure Contours](image)

(A) No Water  
(B) 20% Water at 65° BTDC & 240μm  
(C) 30% Water at 95° BTDC & 196 μm  
(D) Water Temp. at 348 K & 65° BTDC

Figure 45: Comparison of Pressure Contours at 9.5° ATDC for Best Cases

The pressure is more affected than the temperature results contours. For the case without water, the lowest pressure area is seen in the middle of the chamber and the pressure increased towards the walls. Interestingly though, in the case with 30% water injected, the lowest pressure is shown in the corner of the dish on the piston and the pressure increases towards the outer wall. With the contours showing 30% water, the opposite of the baseline is shown with the lowest
pressure out by the wall and increasing towards the center of the chamber. The last case with only a temperature change in the water shows a very similar result to the baseline with the low pressure in the center of the chamber and increasing towards the cylinder wall. The 30% water case also shows less dark red areas thus signifying a decrease in the pressure in that case.

The emissions are the next components of combustion to be compared, so as to check for the effects of the water in the different contours. First the NOx will be compared. The NOx reached its peak point at 22.0 degrees ATDC where, in the baseline, its magnitude remained steady throughout the rest of the simulation. This timing was then used for the peak value’s initial point to compare the different cases once again. Figure 40 show the results below.

![NOx Contours at 22° ATDC for Best Cases](image)

The contours for the NOx are rather intriguing as they seem to defy the results of the cases shown in the formation graphs. In all of the cases being compared in the contours, the NOx levels were reduced 3 to 5% from the baseline levels. However, in the contours which all occur at 22.0 degrees of crank angle, it appears that the NOx in the cylinder is increased for all cases except for the 30% water injection, which seems to have nearly the same or slightly less NOx than the baseline case without water. There are two possible reasons why this result is seemingly
occurring. The appearance of the increase in the NOx is due to the fact that the peak levels are reached sooner, 20-21 degrees of crank angle instead of 22 degrees, and thus are beginning to disperse around the cylinder as the piston begins going down in the expansion stroke. The second reasoning is possibly due to the water being injected into the cylinder and undergoing micro burst causing a further dispersion of the molecules reacting to create NOx within the cylinder and thus the formations occurring at a wider range of area around the chamber.

As found in the contour for the temperature, the peak soot level in the baseline case occurred at 9.5 degrees of crank angle, so this timing was used for all contours. The contours were shown for all cases at this same timing to see the true effects of the water on soot formation. All cases use the same scale to show the comparisons more accurately.

![Soot Contours](image)

Figure 47: Comparison of Soot Contours at 9.5° ATDC for Best Cases

The soot formation contours are very similar for all of the different cases. Each case shows formation of soot coming from the fuel injector and gathering in the corner of the dish in the piston, then extending towards the cylinder wall across its top surface. The difference in the cases with water injected into the chamber is that there is an increased gap between the peak soot
zones coming from the injector and in the bowl of the piston in each successive case. As with the previous contours, the gap is a probable result from the delay in the combustion by water’s presence in the combustion process.

All of the results for the simulations that were run and the contours for the best resulting cases in both groups, the 20% and 30% water by mass, were reviewed to find the overall best case. Once again, the best case was chosen with the least amount of effect on the combustion while still reducing emissions effectively. The best case meeting this criterion was with 20% water mass injection and the 0.240 μm particle size, being injected 65 degrees BTDC. This case had very little change in the properties of the combustion with the maximum temperature of the combustion being increased 0.01% and the peak pressure only being reduced 0.02%. The heat release rate was only reduced 4.44% showing very little effect to it either. As well as very little effect to the combustion, the NOx level was dropped 3.51% and the soot at the end of the expansion stroke was lowered 13.94% over the baseline without water injection. The only negative side to this case was the increase in the exhaust level CO at the end of the expansion stroke of 17.8%. The other cases that had less of an increase or a reduction in the CO levels showed little to no positive effects on the other emissions. This case only had a 0.5 degree combustion delay over the case without water, once again showing little variation in the combustion process while still achieving reductions in the emissions.

The cases run with the temperature of the water injection having variations of ±20 K, from the baseline of 368 K, were very interesting as well. It was shown that the temperature changes did have an effect on the combustion process as well as the emissions. The first cases were run with the temperature increased from 368 K to 388 K. The results showed that at the 65 degrees BTDC injection timing, the temperature and pressure of combustion were increased and
the emissions were reduced. When the injection was moved back to 95 degrees BTDC, the temperature and pressure were decreased and the emissions were lowered but not as much as at the later injection timing. The temperature was then decreased by the same amount to 348 K. In these results, once again the same trends were shown with the temperature and pressure being increased at 65 degrees BTDC and then decreased at 95 degrees BTDC. The emissions were lowered also in both timings as before. Once again the timing showed to be very important to how much effect the water had on the different properties. However, when the temperature of the water was decreased, the variation between the amounts of effect on the different properties at the different injection timings was increased. This is likely from the extra energy that is involved in raising the reduced water temperature up to the temperature of combustion. The temperature did not alter the effect of the water being injected but instead it maximized the effect on combustion when injected at the different timings. This allows for future research possibilities to find the most effective temperature. Also, it can be used to see the effect of temperature variation from the different climates, and seasons within those climates, to find the method to achieve the best results. Possible insulation of the fuel injection system could retain a more constant and lower fuel temperature which would be closer to the ambient temperature, thereby by reducing convection of the heat that is put off by the engine as it operates.

The case run with the water injected at TDC for 5 degrees of duration was done to further analyze the effect of water addition. Literature often used the same timing and duration for the water injection as was used in the fuel injection, but in this research that condition cause quenching of the flame and thus did not achieve combustion. The water was injected at TDC to show that the effects for the water injection timing during the fuel injection timing are much higher. In this case, the combustion was very negatively affected by the water injection. The
maximum temperature of combustion was reduced 5.6%, the pressure peak was reduced 7.1%, and the heat release rate peak was reduced 68.9%. These results signify very probably losses in power and efficiency of the engine. The result for the expansion level soot was an increase of 26.1%. Expansion stroke level CO was increased 98.1% over the baseline, as a result of the later injection timing. The only benefit from this injection timing at TDC was a reduction in NO\textsubscript{x} formation by 48.3%. These results were much closer to the results found in the literature for water addition, through injection or emulsion, because the water was added during the fuel injection timing. Though this does reduce NO\textsubscript{x} much more, all of the other properties of combustion and other emissions suffer greatly. The earlier injections used previously still maintain reductions in NO\textsubscript{x} but they also were beneficial for soot reductions. They did not increase the CO nearly as much as the later water injection nor did it have such a negative effect on the combustion process.

Contours were also made for the case with water injection at TDC. Looking at the contours for this case, it can be seen that the water injected during the fuel injection does show an increased effect on the temperature in the cylinder. As was done before, the levels of temperatures in the contours were set to be the same for better comparison to previous cases. The contours begin 4 degrees of crank angle after the fuel and water injections end, 9 degrees ATDC. They run to 19 degrees of crank angle ATDC so that the temperature effects throughout the combustion process can be seen. With the later water injection, the area of the peak temperature was reduced and the peak spot coming from the injection of the fuel injector was eliminated. The location of the peak area was still shown to be in the bowl of the piston but the area going over the top of the piston to the sidewall was reduced. During the expansion, the peak temperature area increased in size and rolled further over top of the piston. By 19 degrees
ATDC, the peak temperature area started to decrease in size. Also, it could be noted that the temperature in the rest of the cylinder was lowered slightly at 19 degrees ATDC. This is shown in Figure 48 below.

![Temperature Contours for Water Injection at TDC](image)

Emissions were effected more from the water injection at TDC in addition to the effects on the combustion. NO\textsubscript{x} was reduced by nearly 50% at peak formation. The contours once again show the progression of the formation during combustion. At 9 degrees ATDC, NO\textsubscript{x} was starting to form due to combustion of the fuel. With the contour levels set to the same values as before, the formation occurred around the bowl of the piston and extended over towards the top towards the wall of the cylinder. At 9 degrees BTDC, the formation area was small and is not at peak levels yet. As the expansion progressed, the peak area of formation increased in size and density. However, the peak area does not extend all the way to the bottom of the piston bowl until 17 degrees ATDC. At that point the formation increased in size and the peak area was more concentrated around the bowl than over the top of the piston. 21 Degrees ATDC the peak area was shown to be more concentrated around the side of the bowl on the piston. The water
injected at the later timing not only affected the amount formed but the location and timing. All contours for NO$_x$ are shown in Figure 49 below.

![NO$_x$ Contours for Water Injection at TDC](image)

**Figure 49: NO$_x$ Contours for Water Injection at TDC**

The effect of water injection at TDC on the fuel was also interesting. At 5 degrees ATDC, the end of the fuel injection, the fuel droplets were the most concentrated at the fuel injection stream. 2 degrees later, 7 degrees ATDC, the fuel had begun to concentrate not only in the stream from the injection but also gathered around the side of the piston bowl. During combustion, the fuel droplets were converted to other properties. Thus, the peak fuel concentration around the piston bowl was reduced in size as combustion occurred. This was shown at 9 and 11 degrees ATDC. Peak fuel area in the piston bowl showed an outline similar in shape to the peak area found in the temperature contours. As expansion continued, the thickness of the outline decreased while the size of the shape increased. It was also shown that the concentration of fuel coming from the injector was decreased as the fuel was combusted. The size of the area remained similar in size however. Shown in Figure 51 below are the contours for the fuel droplets.
Water droplets also concentrate around the side of the piston bowl as they are injected into the cylinder. The contours for the water are shown for 2 degrees after the fuel injection stops, 7 degrees ATDC, and continue through 19 degrees ATDC to show the effects throughout combustion. At 7 degrees ATDC, the water is concentrated around the side of the piston bowl. During combustion of the fuel, water is formed in addition to the water that was injected. The peak area for the water was substantially increased at 11 degrees ATDC as the fuel combustion occurred. Peak water was shown to have a similar shape to the peak area for the temperature contour. This is expected as combustion converted the fuel to different properties which included water. Also, the peak water area began to extend over the top of the piston towards the side wall of the cylinder. Water in the contour increased in area at 15 degrees ATDC but the peak concentration area was decreased. Also, it showed a slight increase in water formation along the injection stream. The same trend continued to 17 degrees ATDC. Water formation area and the highest concentration area decreased in size. Additionally, the water found in the injection stream increased slightly. Figure 51 shows the contour results for the water.
Future research will be done to further investigate why the simulations run with the water injection at 5 degree BTDC were not able achieve combustion. However, the case run with the injection at TDC does show that earlier injection timings for the water can prove to be a far more beneficial way to attain emission reductions while still maintaining the power and efficiency of the engine. Other injection time, close to the fuel injection, would very interesting to research to find the best condition for water injection.

Comparison to Literary Research Results

In the literature, Kannan and Udayakumar (Kannan and Udayakuma, 2014) found that in experimental water injection into the intake of a diesel engine of 20% water by mass, the NO was lowered by 38%. Their simulations of an engine with water levels up to 30% gave a maximum reduction of 1 mg, which accounted for a 24% reduction, at the highest water content. In the simulations run in this experiment with 20% water, the NOₓ reduction maximum was 5.61% while at 30% the maximum reduction was found to be 7.66%. The reduction shown by
the simulations in this research gave nearly a third the reduction of the NO\textsubscript{x} for 30% water by mass. The difference from the literature results and this research likely is caused by the water being injected at different injection times and locations. The earlier injection times used allow for further vaporization of the droplets during the compression stroke. This increases the temperature of the water along with the air in the chamber simultaneously because of it being injected so early, when the cylinder is at almost the same temperature as the water. The further vaporization of the water also means reduced micro explosion of the water and n-heptane combined droplets because of the reduced water mass per droplet. In their research, the experimental case gave much higher reduction in the results for NO\textsubscript{x} formation, which can be difficult to accurately calculate the levels in simulations. The general trends in results are the intent of simulations to be able to investigate the effect on emission from modifications to different boundary conditions. Their paper also stated that the effects on the combustion delay for the added water were very small which was found in this research as well.

Chadwell and Dingle (Chadwell and Dingle, 2008) found a 42% reduction in NO with a combination of 20% water injection and EGR but it caused up to a 60% delay in the combustion. The combination of EGR and water injection during the fuel injection did attain high emission reduction but it greatly adversely affected the combustion process.

Subramanian (Subramanian, 2011) showed that NO emissions were reduced from 1034 ppm to 643 ppm, 38%, with an injection of 40% water during the fuel injection timing. This higher reduction is result of the higher water percent as well as the later injection timing. The earlier timing as used in this research does not yield as much NO\textsubscript{x} reduction as the later injection timing commonly used but the effects on the combustion properties of temperature, pressure, and heat release rate are reduced.
One paper (Bedford et al. 2000) found that with 45% water injected at 2 degrees ATDC the pressure of the combustion was lowered by 0.5 MPa. By injecting the water earlier as was done in this paper, it was found that at 20% water the maximum pressure effect was seen to be only a reduction of 0.061 MPa and at 30% the maximum was 0.10 MPa. This is more likely to maintain a higher efficiency for the engine by upholding the combustion properties closer to the baseline. The reduced pressure effects can be attributed to the increased vaporization of the water droplets during the compression stroke. This is consistent across all of the properties of the combustion and the emissions that were studied in this research.

Further investigation into the capabilities of injecting the water at earlier injection timings and with water particles from 0.210 to 0.240 μm, which was found to be the most effective size at 65 degrees BTDC, could allow for increased effectiveness on emissions without causing the combustion process to be compromised. Also, the earlier injection timing of 95 degrees BTDC showed the most effect with the largest droplet size of 0.286μm. That droplet size was the largest used, so this warrants further research at sizes over 0.286μm in the future to see if larger sizes would increase the effects even more. Also, the smallest sizes of 0.210 and 0.196 μm showed to be effective with 20% and 30% of water mass respectively. Further investigation is needed to see the cause of this but the smaller sizes appear to have less consistent benefits than the largest size droplet used.
CHAPTER 6

CONCLUSION

Engines and combustion research is very important to the field of engineering as increased demands on transportation and power generation continue to grow. This subject applies to nearly every person in the United States through personal vehicles, agriculture, electricity production, consumer goods delivery, and recreational experiences. As engineers, there is a calling to better the world and to create the most efficient products available. In the American Society of Mechanical Engineers, there is a code of honor that puts the safety of the people and environment as top priorities in any task that an engineer undertakes. This includes reducing the human footprint on the environment as well as protecting people from harmful emissions put in the air. As engines take a part in the lives of most every person around the world in some way, they require particular consideration.

Water injection has been used in engines for many years as an additive to combustion to reduce temperatures and can also reduce emissions from the burning of the hydrocarbon fuels. It is most often used in an emulsion with methanol or another substance which can be used as a power additive to internal combustion engines. By reducing the temperatures of the combustion benefits can be seen in high performance engines under heavy loads. This process has begun to become popular in kits that can be purchased and installed as an aftermarket component on modern vehicles, largely targeting the diesel engine and truck consumers, as a way to add horsepower and reduce emissions. These systems most often are designed to be installed and to inject the H$_2$O emulsion into the intake runners. Direct injection allows for a more controlled
system for water addition. By running simulations on the particle size of the water droplets being injected into the chamber, the droplets and thus their benefits can be altered to achieve the best result on emissions while maintaining the most amount of power generation. While reducing emissions is very important, it must not come at the cost of power reduction. Power reduction would cause detrimental effect to an engine by subjecting it to a higher work load in order to complete a simple task, which may negate the benefits from the water injection.

This research proved to be very interesting and enlightening for the effects of water injection into a diesel engine. The data from the Sandia National Laboratory allowed for an excellent way to verify the simulation cases to experimental data. The use of Converge CFD allowed for this research to be done more economically than would be possible by experimental research. This still increases the knowledge of the field of combustion research, giving a better understanding of how to attain the most benefits from injecting water. The results showed that in most cases, the smaller particle size, 0.196 μm, tends to have the most effect on the properties of combustion, but as the size increased, the droplets had more effect on the emissions levels. However, once the largest droplet size, 0.286 μm, was reached, the droplet had a higher effect on the combustion again. Maintaining a droplet size near 0.210-0.240 μm proved the most effective over all for injection of water while trying to achieve the best emissions reduction and holding the fuel combustion properties as constant as possible. The concern that arose, however, was in the effect the droplets had on the increase in CO levels at the end of the expansion stroke.

There are many different future research topics that could be run based off of the results from this project to further enhance the knowledge of wet combustion. One topic for further research would be to do more testing on the effects water has on the increase of CO levels and to attempt to find the best way to reduce its increase as water was added. Also, another topic to
look further investigate would be to do more research on the effects of the temperature of the water. This was shown to have increased effects on the emissions and combustion as the temperature was reduced. More extensive temperature variances could prove helpful in attaining the best results from the water injection, with appropriate control of the water being injected. Also, different temperatures with different droplet sizes, within the 0.210 - 0.240 μm range, needs to be tested to see if the effects can be better focused for the most beneficial droplet size to use. As well, since there is an increase in the need for a green renewable fuel to power engines, running these similar type tests on bio-fueled engines could be very informative and beneficial as bio-diesel is becoming increasingly common across the United States and the world. A last topic that would be very beneficial for researching water injection in the future is to test droplet size effect on spark ignition engines to see if the droplets still maintain the same effects or if the change in the system would cause variations to the water’s performance at the different droplet sizes or different water temperatures.

This project allowed for a great opportunity to enhance engineering in the field of engine development and combustion. It also was used to see the application of technology through computer simulations which reduced the cost of the project, thus increasing knowledge to lead in future research for the combustion of fossil fuels. The information obtained through this research allocates many opportunities for advancements in automotive engineering for the future.
REFERENCES


http://www.grc.nasa.gov/WWW/K-12/airplane/otto.html


APPENDIX A

ANSYS Fluent Chemical Mechanisms

188 Species Reaction Elements and Species

ELEMENTS

h c o n ar

END

SPECIES

h h2 o o2 oh h2o n2 co hco co2 ch3 ch4 ho2 h2o2 ch2o ch3o
c2h6 c2h4 c2h5 ch2 ch c2h c2h2 c2h3 ch3oh ch2oh ch2co hcco
c2h4oh sc2h4oh ch3co ch2cho ch3cho c3h4-a c3h4-p c3h6 c4h6 nc3h7
ic3h7 ic4h7 ic4h8ic4h7 c4h8-2 c4h8-1 pc4h9 ch3coch3 ch3coch2 ch2h5cho
c2h5coch5h9 c5h10-1 c5h10-2 bc5h11 ac5h10 bc5h10ic5h9 c5h11-1 c5h11-2
c2h5o ch3o2 c2h5o2 ch3o2h c2h5o2h c2h3o1-2 ch3co2 c2h4o2h
o2c2h4oh ch3co3 ch3co3h c2h3co ch3h5o c3h6ooh1-2 nc3h7o
c3h7o2h nc3h7o2 ic4h8oh c4h7o c4hoooh1-3o2 c4hoooh1-3 c4hoo1-3
pc4h9o pc4h9o2h pc4h9o2 ch3coch2o2 ch3coch2o2h ch3coch2o c5h11o2-1
c5h11o2h-1 c5h11o-1 c5h10oooh1-3 c5h10oooh1-4 c5h10oooh1-3o2 c5h10o1-4
c3h5-a c3h5-t ch3h c3h2 c2h2(s) nc4ket13 nc5ket13 nc3h5cho te3h6cho
ic4h7oh ic3h6co ic3h5co tc3h6oh ic3h5oh nc3h7cho nc3h7co ch2ch2coch3
c2h5coch2 c2h5coch3 ch3chcoch3 c2h3coch3 ch3chco c3h6cho-3 c3h6cho-2
c2h5cho c3hccho ch2h5coch2h pc2h4coch3 ic3h6choch2
nc3h7coch3 nc3h7coch2 nc4h9cho nc4h9co ac3h5cho c2h3chcho hoch2o
hocho c6h13-1 c6h13-2 c6h12-1 c6h11 nc7h16 c7h15-1 c7h15-2 c7h15-3
c7h15-4 c7h14-1 c7h14-2 c7h14-3 c7h13 c7h15o2-1 c7h15o2-2 c7h15o2-3
nc7h15o2-4 c7h15o2h-2 c7h15o-2 c7h15o-3 c7h15o-4 c7h14oooh1-3
nc7h14oooh2-3 nc7h14oooh2-4 nc7h14oooh2-5 nc7h14oooh2-1 nc7h14oooh2-2 nc7h14oooh2-3
nc7h14ooh3-5 c7h14ooh3-6 c7h14ooh4-2 c7h14ooh4-3 c7h14ooh1-3o2
c7h14ooh2-3o2 c7h14ooh2-4o2 c7h14ooh2-5o2 c7h14ooh3-5o2 c7h14ooh3-6o2
c7h14ooh4-4o2 c7h14o1-2 c7h14o1-3 c7h14o1-4 c7h14o2-3 c7h14o2-4
c7h14o2-5 c7h14o3-4 c7h14o3-5 nc7ket13 nc7ket23 nc7ket24 nc7ket25
nc7ket35 nc7ket36 nc7ket42 nc5h11cho nc5h11co

END
Zeldovich Extended Mechanism

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Forward Reaction</th>
<th>Backward Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td>B</td>
</tr>
<tr>
<td>Zeldovich:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O + N₂ ↔ N + NO</td>
<td>6.68E+12</td>
<td>0.4</td>
</tr>
<tr>
<td>N + O₂ ↔ O + NO</td>
<td>6.40E+09</td>
<td>1</td>
</tr>
<tr>
<td>N + OH ↔ H + NO</td>
<td>3.80E+13</td>
<td>0</td>
</tr>
<tr>
<td>Supplementary Reactions:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NO₂ + OH ↔ NO + HO₂</td>
<td>8.45E+12</td>
<td>0.02</td>
</tr>
<tr>
<td>NO + OH ↔ NO₂ + H</td>
<td>9.46E+09</td>
<td>0.81</td>
</tr>
<tr>
<td>N₂ + OH ↔ N₂O + H</td>
<td>5.73E+07</td>
<td>1.31</td>
</tr>
<tr>
<td>N₂ + O + M ↔ N₂O + M</td>
<td>5.21E+07</td>
<td>1.34</td>
</tr>
<tr>
<td>N₂ + O₂ ↔ N₂O + O</td>
<td>2.91E+10</td>
<td>0.91</td>
</tr>
<tr>
<td>NO + NO ↔ N₂O + O</td>
<td>1.26E+09</td>
<td>0.92</td>
</tr>
<tr>
<td>N₂ + HO₂ ↔ N₂O + OH</td>
<td>1.39E+10</td>
<td>0.48</td>
</tr>
</tbody>
</table>
29 Species Mechanism

elements
h c o n
end

species
nc7h16  o2  n2  co2  h2o  co  h2  oh  h2o2  ho2  h  o
ch3o  ch2o  hco  ch2  ch3  ch4  c2h3  c2h4  c2h5  c3h4  c3h5  c3h6  c3h7

c7h15-2  c7h15o2  c7ket12  c5h11co
end

reactions
nc7h16 + h = c7h15-2 + h2  4.380e+07  2.0  4760.0
nc7h16 + oh = c7h15-2 + h2o  9.700e+09  1.3  1690.0
nc7h16 + ho2 = c7h15-2 + h2o2  1.650e+13  0.0  16950.0
nc7h16 + o2 = c7h15-2 + ho2  2.000e+15  0.0  47380.0

c7h15-2 + o2 = c7h15o2  1.560e+12  0.0  0.0

c7h15o2 + o2 = c7ket12 + oh  4.500E+14  0.0 18232.712

c7ket12 = c5h11co + ch2o + oh  9.530e+14  0.0  4.110e+4

c5h11co = c2h4 + c3h7 + co  9.84E+15  0.0  4.02E+04

c7h15-2 = c2h5 + c2h4 + c3h6  7.045E+14  0.0  3.46E+04

c3h7 = c2h4 + ch3  9.600e+13  0.0  30950.0

c3h7 = c3h6 + h  1.250e+14  0.0  36900.0

c3h6 + ch3 = c3h5 + ch4  9.000e+12  0.0  8480.0

c3h5 + o2 = c3h4 + ho2  6.000e+11  0.0  10000.0

c3h4 + oh = c2h3 + ch2o  1.000e+12  0.0  0.0

c3h4 + oh = c2h4 + hco  1.000e+12  0.0  0.0
<table>
<thead>
<tr>
<th>Reaction</th>
<th>Rate</th>
<th>dE</th>
<th>E'</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{CH}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{O} + \text{OH}$</td>
<td>5.000e+13</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>$\text{CH}_3 + \text{OH} \rightarrow \text{CH}_2 + \text{H}_2\text{O}$</td>
<td>7.500e+06</td>
<td>2.00</td>
<td>5000.0</td>
</tr>
<tr>
<td>$\text{CH}_2 + \text{OH} \rightarrow \text{CH}_2\text{O} + \text{H}$</td>
<td>2.500e+13</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>$\text{CH}_2 + \text{O}_2 \rightarrow \text{HCO} + \text{OH}$</td>
<td>4.300e+10</td>
<td>0.00</td>
<td>-500.0</td>
</tr>
<tr>
<td>$\text{CH}_2 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2$</td>
<td>6.900e+11</td>
<td>0.00</td>
<td>5000.0</td>
</tr>
<tr>
<td>$\text{CH}_2 + \text{O}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$</td>
<td>2.000e+10</td>
<td>0.00</td>
<td>-1000.0</td>
</tr>
<tr>
<td>$\text{CH}_2 + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{O}$</td>
<td>5.000e+13</td>
<td>0.00</td>
<td>9000.0</td>
</tr>
<tr>
<td>$\text{CH}_2 + \text{O}_2 \rightarrow \text{CO} + \text{OH} + \text{H}$</td>
<td>1.600e+12</td>
<td>0.00</td>
<td>1000.0</td>
</tr>
<tr>
<td>$\text{CH}_3\text{O} + \text{CO} \rightarrow \text{CH}_3 + \text{CO}_2$</td>
<td>1.570e+14</td>
<td>0.00</td>
<td>11800.0</td>
</tr>
<tr>
<td>$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$</td>
<td>8.987e+07</td>
<td>1.38</td>
<td>5232.877</td>
</tr>
<tr>
<td>$\text{O} + \text{OH} \rightarrow \text{O}_2 + \text{H}_2\text{O}$</td>
<td>4.000e+14</td>
<td>-0.50</td>
<td>0.0</td>
</tr>
<tr>
<td>$\text{H} + \text{HO}_2 \rightarrow \text{OH} + \text{OH}$</td>
<td>4.000e+14</td>
<td>-0.50</td>
<td>0.0</td>
</tr>
<tr>
<td>$\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$</td>
<td>3.600e+17</td>
<td>-0.72</td>
<td>0.0</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}/21.0/ \text{CO}_2/5.0/ \text{H}_2/3.3/ \text{CO}/2.0/ \text{H}_2\text{O}_2 + \text{M} \rightarrow \text{OH} + \text{OH} + \text{M}$</td>
<td>1.000e+16</td>
<td>0.00</td>
<td>45500.0</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}/21.0/ \text{CO}_2/5.0/ \text{H}_2/3.3/ \text{CO}/2.0/ \text{H}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H}$</td>
<td>1.170e+09</td>
<td>1.30</td>
<td>3626.0</td>
</tr>
<tr>
<td>$\text{HO}_2 + \text{H} \rightarrow \text{H}_2\text{O} + \text{H}$</td>
<td>3.000e+12</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>$\text{CH}_2\text{O} + \text{OH} \rightarrow \text{HCO} + \text{H}_2\text{O}$</td>
<td>5.563e+10</td>
<td>1.095</td>
<td>-76.517</td>
</tr>
<tr>
<td>$\text{CH}_2\text{O} + \text{HO}_2 \rightarrow \text{HCO} + \text{H}_2\text{O}_2$</td>
<td>3.000e+12</td>
<td>0.00</td>
<td>8000.0</td>
</tr>
<tr>
<td>$\text{HCO} + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$</td>
<td>3.300e+13</td>
<td>-0.40</td>
<td>0.0</td>
</tr>
<tr>
<td>$\text{HCO} + \text{M} \rightarrow \text{H} + \text{CO} + \text{M}$</td>
<td>1.591E+18</td>
<td>0.95</td>
<td>56712.329</td>
</tr>
<tr>
<td>$\text{CH}_3 + \text{CH}_3\text{O} \rightarrow \text{CH}_4 + \text{CH}_2\text{O}$</td>
<td>4.300e+14</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{CH}_2\text{O} + \text{C}_2\text{H}_3$</td>
<td>6.000e+13</td>
<td>0.0</td>
<td>960.0</td>
</tr>
<tr>
<td>$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{C}_2\text{H}_3 + \text{H}_2\text{O}$</td>
<td>8.020e+13</td>
<td>0.00</td>
<td>5955.0</td>
</tr>
</tbody>
</table>
c2h3 + o2 = ch2o + hco  \quad 4.000e+12  \quad 0.00  \quad -250.
c2h3 + hco = c2h4 + co  \quad 6.034e+13  \quad 0.0  \quad 0.
c2h5 + o2 = c2h4 + ho2  \quad 2.000e+10  \quad 0.0  \quad -2200.
ch4 + o2 = ch3 + ho2  \quad 7.900e+13  \quad 0.00  \quad 56000.
oh + ho2 = h2o + o2  \quad 7.50E+12  \quad 0.0  \quad 0.
ch3 + o2 = ch2o + oh  \quad 3.80E+11  \quad 0.0  \quad 9000.
ch4 + h = ch3 + h2  \quad 6.600e+08  \quad 1.60  \quad 10840.
ch4 + oh = ch3 + h2o  \quad 1.600e+06  \quad 2.10  \quad 2460.
ch4 + o = ch3 + oh  \quad 1.020e+09  \quad 1.50  \quad 8604.
ch4 + ho2 = ch3 + h2o2  \quad 9.000e+11  \quad 0.00  \quad 18700.
ch4 + ch2 = ch3 + ch3  \quad 4.000e+12  \quad 0.00  \quad -570.
c3h6 = c2h3 + ch3  \quad 3.150e+15  \quad 0.0  \quad 85500.0
end
APPENDIX B

Converge CFD Chemical Mechanism

elements

h c o n
end

species

nc7h16 o2 n2 co2 h2o co h2 oh h2o2 ho2 h o
ch3o ch2o hco ch2 ch3 ch4 c2h3 c2h4 c2h5 c3h4 c3h5 c3h6 c3h7
c7h15-2 c7h15o2 c7ket12 c5h11co
end

reactions

nc7h16 + h = c7h15-2 + h2 4.380e+07 2.0 4760.0
nc7h16 + oh = c7h15-2 + h2o 9.700e+09 1.3 1690.0
nc7h16 + ho2 = c7h15-2 + h2o2 1.650e+13 0.0 16950.0
nc7h16 + o2 = c7h15-2 + ho2 2.000e+15 0.0 47380.0
c7h15-2 + o2 = c7h15o2 1.560e+12 0.0 0.0
c7h15o2 + o2 = c7ket12 + oh 9.000E+14 0.0 18232.712
c7ket12 = c5h11co + ch2o + oh 9.530e+14 0.0 4.110e+4
c5h11co = c2h4 + c3h7 + co 9.84E+15 0.0 4.02E+04
c7h15-2 = c2h5 + c2h4 + c3h6 7.045E+14 0.0 3.46E+04
c3h7 = c2h4 + ch3 9.600e+13 0.0 30950.0
c3h7 = c3h6 + h 1.250e+14 0.0 36900.0
c3h6 + ch3 = c3h5 + ch4 9.000e+12 0.0 8480.0
c3h5 + o2 = c3h4 + ho2 6.000e+11 0.0 10000.0
\begin{align*}
c_3h_4 + oh &= c_2h_3 + ch_2o & 1.000e+12 & 0.0 & 0.0 \\
c_3h_4 + oh &= c_2h_4 + hco & 1.000e+12 & 0.0 & 0.0 \\
ch_3 + ho_2 &= ch_3o + oh & 5.000e+13 & 0.00 & 0. \\
ch_3 + oh &= ch_2 + h_2o & 7.500e+06 & 2.00 & 5000. \\
ch_2 + oh &= ch_2o + h & 2.500e+13 & 0.00 & 0. \\
ch_2 + o_2 &= hco + oh & 4.300e+10 & 0.00 & -500. \\
ch_2 + o_2 &= co + h_2o & 2.000e+10 & 0.00 & -1000. \\
ch_2 + o_2 &= ch_2o + o & 5.000e+13 & 0.00 & 9000. \\
ch_2 + o_2 &= co_2 + h + h & 1.600e+12 & 0.00 & 1000. \\
ch_2 + o_2 &= co + oh + h & 8.600e+10 & 0.00 & -500. \\
ch_3o + co &= ch_3 + co_2 & 1.570e+14 & 0.00 & 11800. \\
co + oh &= co_2 + h & 8.987e+07 & 1.38 & 5232.877 \\
o + oh &= o_2 + h & 4.000e+14 & -0.50 & 0. \\
h + ho_2 &= oh + oh & 1.700e+14 & 0.0 & 875. \\
oh + oh &= o + h_2o & 6.000e+08 & 1.30 & 0. \\
h + o_2 + m &= ho_2 + m & 3.600e+17 & -0.72 & 0.
\end{align*}

h_2o/21./ co_2/5.0/ h_2/3.3/ co/2.0/

h_2o_2 + m &= oh + oh + m & 1.000e+16 & 0.00 & 45500.

h_2o/21./ co_2/5.0/ h_2/3.3/ co/2.0/

h_2 + oh &= h_2o + h & 1.170e+09 & 1.30 & 3626.

ho_2 + ho_2 &= h_2o_2 + o_2 & 3.000e+12 & 0.00 & 0. \\
ch_2o + oh &= hco + h_2o & 5.563e+10 & 1.095 & -76.517 \\
ch_2o + ho_2 &= hco + h_2o_2 & 3.000e+12 & 0.00 & 8000. \\
hco + o_2 &= ho_2 + co & 3.300e+13 & -0.40 & 0. \\
hco + m &= h + co + m & 1.591E+18 & 0.95 & 56712.329 \\
ch_3 + ch_3o &= ch_4 + ch_2o & 4.300e+14 & 0.00 & 0. \

\begin{align*}
\text{c2h4} + \text{oh} & = \text{ch2o} + \text{ch3} & 6.000e+13 & 0.0 & 960.0 \\
\text{c2h4} + \text{oh} & = \text{c2h3} + \text{h2o} & 8.020e+13 & 0.00 & 5955.0 \\
\text{c2h3} + \text{o2} & = \text{ch2o} + \text{hco} & 4.000e+12 & 0.00 & -250.0 \\
\text{c2h3} + \text{hco} & = \text{c2h4} + \text{co} & 6.034e+13 & 0.0 & 0.0 \\
\text{c2h5} + \text{o2} & = \text{c2h4} + \text{ho2} & 2.000e+10 & 0.0 & -2200.0 \\
\text{ch4} + \text{o2} & = \text{ch3} + \text{ho2} & 7.900e+13 & 0.00 & 56000.0 \\
\text{oh} + \text{ho2} & = \text{h2o} + \text{o2} & 7.50E+12 & 0.0 & 0.0 \\
\text{ch3} + \text{o2} & = \text{ch2o} + \text{oh} & 3.80E+11 & 0.0 & 9000.0 \\
\text{ch4} + \text{h} & = \text{ch3} + \text{h2} & 6.600e+08 & 1.60 & 10840.0 \\
\text{ch4} + \text{oh} & = \text{ch3} + \text{h2o} & 1.600e+06 & 2.10 & 2460.0 \\
\text{ch4} + \text{o} & = \text{ch3} + \text{oh} & 1.020e+09 & 1.50 & 8604.0 \\
\text{ch4} + \text{ho2} & = \text{ch3} + \text{h2o2} & 9.000e+11 & 0.00 & 18700.0 \\
\text{ch4} + \text{ch2} & = \text{ch3} + \text{ch3} & 4.000e+12 & 0.00 & -570.0 \\
\text{c3h6} & = \text{c2h3} + \text{ch3} & 3.150e+15 & 0.0 & 85500.0 \\
\end{align*}