

Fuel Spray Modeling for Direct Injection Compression Ignition Engine Configurations

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ABSTRACT

This study presents a computationally efficient numerical model that accurately predicts complex spray distribution and spray penetration for a direct injection compression engine configuration. Experimental data obtained from available literature is used to construct a semi-empirical numerical model. A modified version of a multidimensional computer code KIVA-3V is used for the computations, with improved sub-models for varying mean droplet diameter, varying injection velocity and drop distortion and drag. Results show good agreement with the published in-cylinder experimental data for a Volkswagen 1.9 L turbo-charged direct injection under actual operating conditions.

INTRODUCTION

Today, our nation faces tremendous energy, economic and environmental challenges. Significant changes in the production and consumption of energy must take place to minimize adverse energy and environmental impacts. Currently, 93% of the energy consumed in the US comes from non-renewable fossil and nuclear fuel. Transportation accounts for 67% of the petroleum consumed and the transportation sector is 97% dependent on oil. In 2004, this country used 572 million gallons of petroleum based fuel every day. By 2020, U.S. oil imports are expected to grow to over 65% of domestic oil consumption with the Persian Gulf nations accounting for over 65% of the world oil exports. In 2020, the U.S. net annual expenditures for imported crude oil and petroleum products are projected to exceed \$130 billion in current dollars. Further, with a steady increase in the number of vehicles and miles traveled, air quality problems in our cities continue to worsen. It is now recognized that one of the "clean" products of complete combustion, CO₂, is a strong contributor to the greenhouse effect, and may ultimately be the most dangerous by-product. Global fuel conservation and a reduction of our reliance on foreign oil supplies as well as environmental concerns are compelling reasons to find cost-effective solutions to reduce our consumption of energy. Since the automobile forms an important

component of the U.S. economy, and is an integral part of our lives, it is essential to address the issues of increased fuel efficiency and reduced pollutant emissions. Such a solution would have a positive impact on the environmental issues and lessen our reliance on foreign oil supplies.

To accomplish these tasks, in 1993, industry and government outlined a ten-year program entitled the Partnership for a New Generation Vehicle (PNGV). The partnership pursued substantial advances in vehicle technology that led to marked improvements in fuel efficiency and emissions of standard vehicle designs. The primary goal was the attainment of three times the fuel efficiency (80 mpg) of today's six passenger family sedan without sacrificing cost, comfort or power. One of the most important improvements required to obtain these goals was to have an engine thermal efficiency in the range of 45-55 percent. The direct injection compression ignition engine was selected as the only engine that could approach this requirement in the near future.

Most of today's conventional automobile engines employ multi-port injection (MPI) in which fuel is injected into each intake. Load control is accomplished by engine throttling. In MPI engines, there are limits to fuel supply response and combustion control because the fuel mixes with the air before entering the spark-ignited (SI) engine. The thermal efficiency of current gasoline engines is only about 30 to 32 percent peak or about 23 percent on an in-use cycle.

Four-stroke, compression-ignition direct injection (CIDI) engines offer a potentially desirable alternative to conventional SI engines with thermal efficiencies that may approach 40 percent. The fundamental advantage of the diesel engine lies in the direct link between the mixture preparation and auto-ignition. The thermodynamic condition of the mixture necessary for auto-ignition can always be reached with a sufficient compression ratio. Ignition will take place in any region of the inhomogeneous mixture where sufficient conditions for combustion exist. With their non-homogeneous combustion process, direct-injection diesel (compression ignition) engines allow overall leaner combustion, resulting in higher baseline efficiency (about 40 percent peak), 20 to 35 percent better fuel economy, 10 to 20 percent lower CO₂ emissions, near-

zero evaporative emissions, and low cold-start emissions. Current designs of diesel engines, however, still produce unacceptable levels of nitrogen oxides (NO_x) and particulate emissions (mainly soot) at high engine loads. To accomplish the goal of using the diesel cycle in an alternative high-efficiency engine, research is required in the areas of fuel injection, in-cylinder fuel distribution, combustion, temperature distribution, and pollutant emission formulation.

The diesel engine represents one of the more complex combustion systems used today; consequently, understanding the physics and chemistry involved in diesel combustion is quite challenging. Specifically, the major complexity of diesel engines arises due to transient effects and the inhomogeneity of spray combustion. An overall description of diesel combustion requires an understanding of three major processes: spray dynamics and the interaction with the combustion chamber walls, ignition kinetics and post-ignition combustion. The proposed study will consist of a computational investigation to address these issues for spray combustion.

The current computational study activities will use the KIVA-3V¹ computer code. The spray modeling in KIVA-3V is based on a discrete particle technique in which computational particles are injected into the domain. Each computational particle contains a number of droplets of identical size, velocity and temperature. Probability distributions govern the assignment of droplet properties at injection using a Monte Carlo sampling technique.^{3,4} The particles and fluid interact by exchanging mass, momentum and energy.³ Modeling the droplet collisions and coalescence is included and an aerodynamic Taylor Analogy Breakup Model.⁵ The location, shape, rate of development, and mass flow distribution within each fuel jet are of paramount importance in controlling fuel air mixing, wall interactions, combustion rate and the resulting levels of emissions.

Ongoing studies by this investigator and others^{6,7} have found that the accurate modeling of the liquid spray must be obtained to study overall engine performance and pollutant emission formation. If the in-cylinder liquid and vaporous fuel distribution is incorrectly modeled, then the resulting combustion process and temperature distribution will be inaccurate and the pollutant emission predictions will be of little or no value.

The most recent version of the KIVA-3V code has been modified by this investigator with improved physical models. These include the effects of an improved spray model to provide the correct fuel spray penetration and distribution within the cylinder, a fuel spray-wall impingement model, an improved heat transfer model, a mixing-controlled hybrid turbulent combustion model⁸ and a soot formation model⁹. The code modifications were validated against available experimental data and good agreement was found for of a CIDI engine under actual operating conditions.

NUMERICAL DETAILS

The current computational analysis is carried out using the computer code KIVA-3V. KIVA-3V code is one of the recent versions of a series of codes that were developed over the last 25 years at Los Alamos National Laboratory. The code's primary application is the modeling of the complex combustion processes in internal combustion and gas turbine engines. Predecessors to KIVA-3V, i.e., KIVA-III, KIVA-II, and KIVA have been widely used by the automobile industry for a number of years and have been thoroughly tested under a wide range of operating conditions. The KIVA-3V computer code is a version of the KIVA series of codes that solves the compressible, turbulent, three-dimensional transient equations of multi-component gas mixtures with the flow dynamics of an evaporating liquid spray with the capability to handle moving valves. The conservation laws for vapor-gas mass, momentum and energy are solved by a Lagrange-Euler finite volume approach by using an explicit time marching technique. KIVA-3V uses an explicit quasi-second order upwind scheme for convection. This scheme is monotone and approaches second order accuracy when convecting smooth profiles. Typically, turbulence is modeled using a standard isotropic $k-\epsilon$ model. While this may work for a large class of flow fields, it has been found to be inadequate for the flows past intake valves where large vortical structures are formed. Improvements are found by using a Re-Normalization Group (RNG) theory $k-\epsilon$ that improves the accuracy of simulation for flows with large vortical structures such as flows past intake valves. Although accuracy is improved, computational effort is increased relative to the standard model.

COMPUTATIONAL MODEL

When the most complex models for the fuel spray are used, the computational effort increases by as much as an order of magnitude. Therefore a semi-empirical approach was taken here to accurately model the spray.

The following are the modifications were made to KIVA3V for the current application:

- A correlation was defined for Sauter Mean Radius (SMR) using the experimental data available and is used for calculating and automatically updating SMR for each iteration.
- A nozzle discharge coefficient was introduced into the KIVA3V code to account for viscous effects in the fuel injection process.
- Expressions for the varying fuel injection velocity which is updated at each iteration.
- The model was further improved an improved expression for the drop drag coefficient which varies depending on in-cylinder conditions

The droplet size distribution is one of the most important factors affecting the characteristics of spray combustion and subsequent pollutant emission formation in diesel

engines. There are at least six mean diameters to describe the physics of spray distribution. Among which is Sauter Mean Diameter (SMD), D_{32} which deals with atomization efficiency. It is thus used for the mass transfer and combustion problems since the surface area and the volume of droplet are of primary importance for evaporation and combustion.

A correlation is defined for SMD using the technique and experimental data provided by Elkotb¹⁰. In the work, based on dimensional analysis, the following expression was developed for SMD (D_{32}):

$$\frac{D_{32}}{d} = A Re^a We^b C_d^c \left(\rho_f / \rho_a\right)^f (l_n / d)^g \quad (1)$$

Where A, a, b, c, f and g are constants to be determined from the experimental results. In the current work, the experimental data was plotted and curve fit as shown in figure 1. The following correlation for the Sauter mean diameter was obtained:

$$\frac{D_{32}}{d} = 110.22 \left(Re^{-0.183} We^{-0.442} C_d^{-0.422} \left(\rho_f / \rho_a\right)^{-0.05} \right)^{0.422} \quad (2)$$

Eqn. (2) was modified to obtain an explicit equation for SMR:

$$SMR = 47.435 \nu^{0.155} \sigma^{0.374} C_d^{-0.357} \rho_f^{0.0351} \rho_a^{0.042} \Delta P^{-0.451} d^{0.472} \quad (3)$$

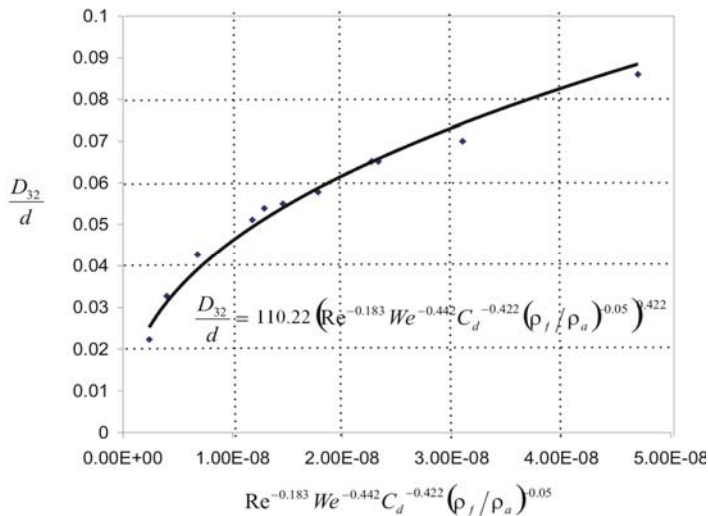


Figure 1 Curve Fitted Graph for Obtaining Correlation (Eq. 2)

where

SMR is Sauter mean radius, cm
 ν is the viscosity of the fuel, cm^2/sec
 σ is the surface tension of the fuel, dyne/cm

C_d is the coefficient of discharge.

ρ_f is the density of fuel, g/cm^3

ρ_a is the density of air, g/cm^3

ΔP is the difference in pressure, dyne/cm^2

d is the diameter of the nozzle, cm

Nozzle geometry affects the spray characteristics and therefore the atomization process and the engine performance. Thus, expressions for the coefficient of discharge, C_d , must be known.

The coefficient of discharge was defined as the ratio of actual flow rate to the theoretical flow rate. The general equation for discharge coefficient can be obtained by combining the Bernoulli's equation and the mass conservation equation:

$$C_d = \frac{\dot{m}}{A \sqrt{2\rho(P_i - P_b)}} \quad (3)$$

Where $\dot{m}$ is the mass flow rate, P_i is the upstream nozzle pressure and P_b is the orifice outlet pressure, ρ represents the density of the liquid and A the geometric cross section of the orifice. The discharge coefficient can be expressed in terms of Reynolds number. The Reynolds number is given by the following equation:

$$Re = \frac{D_0 U_0}{\nu} \quad (4)$$

Where D_0 is the outlet diameter, ν is the kinematic viscosity and U_0 is the velocity at the outlet orifice calculated from the experimental mass flow rate and the continuity equation:

$$U_0 = \frac{\dot{m}_0}{A_0 \rho} \quad (5)$$

An empirical relationship between C_d , the coefficient of discharge and Re , the Reynolds's number is defined as follows¹²:

For Cylindrical Nozzles:

$$C_d = 0.91 - 8.49 / Re^{0.5} \quad (6)$$

For Conical Nozzles:

$$C_d = 0.96 - 10.17 / Re^{0.5} \quad (7)$$

For the present research cylindrical nozzle was used. So, Eqn. (6) was used in Eqn. (3) for calculating SMR. In diesel combustion engines, the spray penetration strongly depends on velocity of the injected fuel. As the combustion proceeds, the in-cylinder pressure and

temperature increases and the velocity decreases. Thus updating the velocity was considered to be critical since the fuel is incompressible, the Bernoulli's equation was employed which was given by:

$$v_{inj} = \sqrt{\frac{2(\Delta P)k}{\rho_f}} \quad (8)$$

Where, v_{inj} is the velocity of the injected fuel (cm/sec), ΔP is the difference in pressure (dyne/cm²), k is the loss coefficient and ρ_f is the density of the fuel (gm/cm³). The above equation was introduced into the KIVA3V code and the velocity was updated for every cycle.

In engine sprays the fuel drops undergo high distortion as the fuel penetrates into the cylinder. The drop drag coefficient changes and is increased as the drop departs from the spherical shape. The KIVA3V employed the empirical equation obtained by Putnam¹³:

$$C_D = \frac{24}{Re} \left(1 + \frac{1}{6} Re^{2/3} \right) \quad (9)$$

The above equation was recommended for low temperatures and for Reynolds numbers less than 1000. Since the current research involves high temperatures and high velocities, the above equation was considered to be not the appropriate empirical formula. The drop drag coefficient equations suggested by Lambris and Combs¹⁴ takes the entire range of Reynolds numbers into account, and hence was determined as applicable correlation:

$$C_D = \begin{cases} 27 \times Re^{-0.84} & (\text{For } Re < 80) \\ 0.271 \times Re^{0.217} & (\text{For } 80 < Re < 10,000) \\ 2 & (\text{For } Re > 10,000) \end{cases} \quad (10)$$

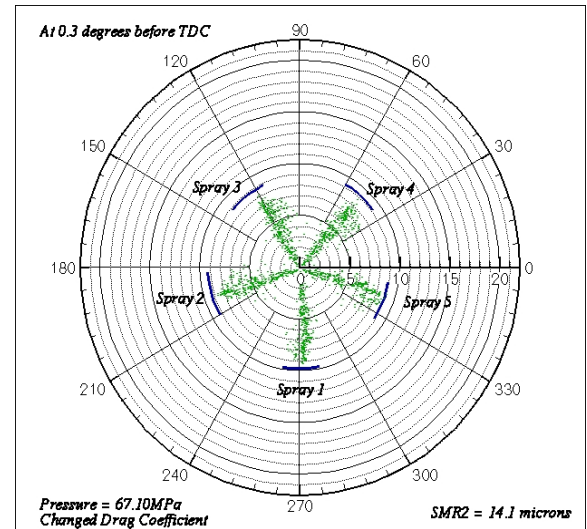
Where, Re is the Reynolds number. The above equation was incorporated into the KIVA3V code. The numerical results thus obtained presented good match when compared against the experimental data.

NUMERICAL RESULTS

To predict the in-cylinder fuel penetration and distribution a varying fuel injection velocity, varying fuel particle size model was created. The injection velocity was a function of the nozzle geometry, the nozzle discharge coefficient, the fuel injection pressure and the changing in cylinder pressure. The fuel particle size or Sauter mean radius (SMR) was calculated as a function of the fuel density, fuel viscosity, fuel surface tension, in-

cylinder gas density, fuel injection velocity, injection pressure, in-cylinder pressure, and the nozzle geometry. The numerical results were compared against the experimental in-cylinder fuel distribution for a transparent, quartz 1.9 L turbocharged direct injection (TDI) Volkswagen engine¹¹. Numerical simulations were carried out with the base mesh that was considered to be adequately refined for the current problem. As it is important to obtain a grid independent solution, the mesh was refined by a 25 % increase in resolution two times. Each 25% increase in resolution increase the computational effort by approximately 60%. With the refined grids there was no significant change in the solution and therefore a further study was performed to investigate the effects of the above parameters on fuel sprays. Consequently, the main focus of the work was to derive and to employ the empirical correlations for the above mentioned parameters and to get the correct important physics into the numerical model. Previously, SMR and injection velocity were input and then held constant. First, the expression for the SMR was derived from the available experimental data and employed to carry out the numerical simulations. The results obtained showed significant discrepancies when compared with the experimental results due to lack of initial penetration of the fuel particles. Next, the second parameter of importance, a varying injection velocity calculated with Bernoulli's equation and a varying discharge coefficient was applied. A significant error still existed when compared against the experimental data. Finally, the improved expressions for the droplet drag coefficient were incorporated.

Agreement was excellent as seen in figures 2 and 3. The blue line seen in figure 2 represents the experimental fuel penetration and distribution for each of the 5 fuel injector nozzles.



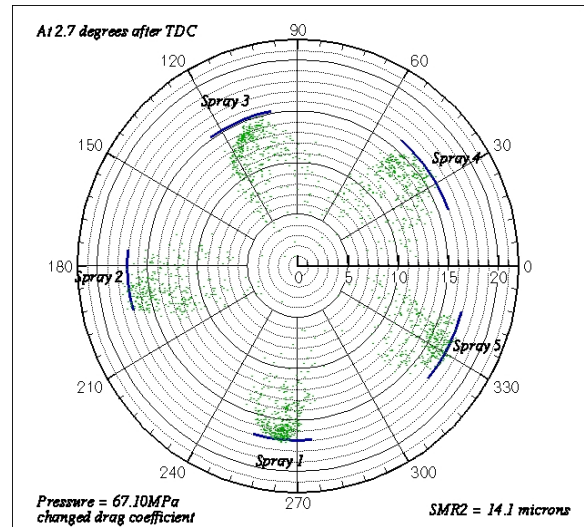
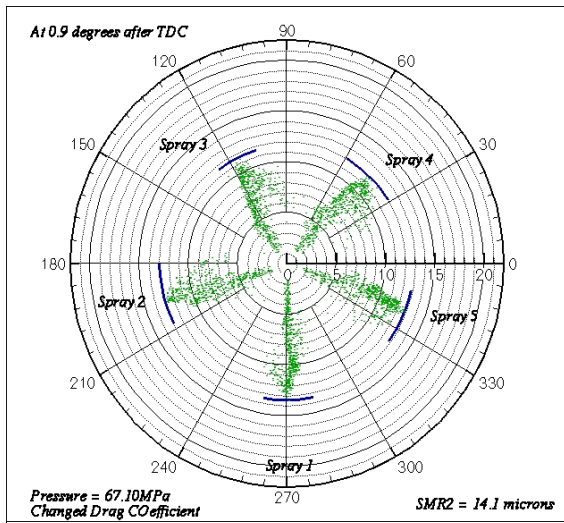
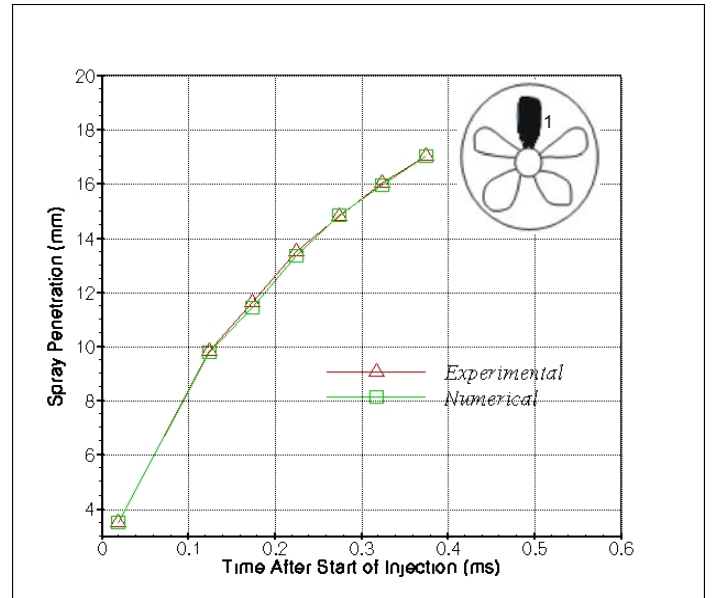
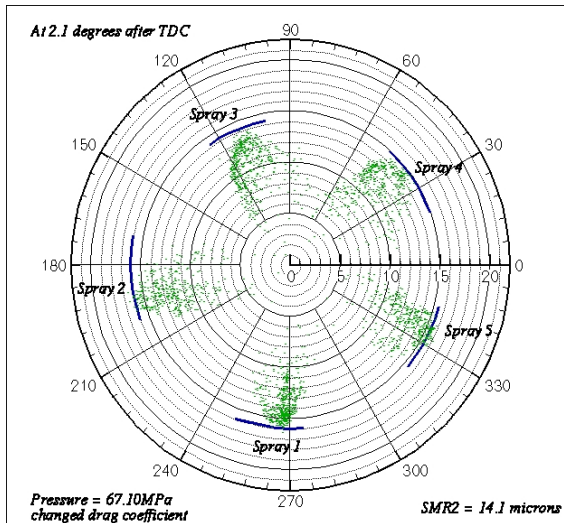
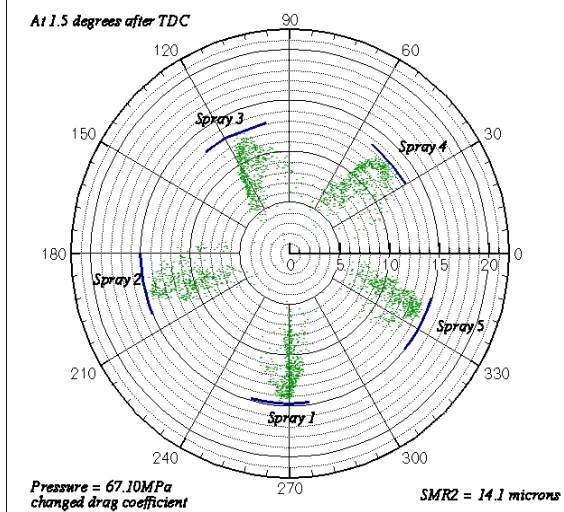


Figure 2 Experimental versus computational fuel distribution.



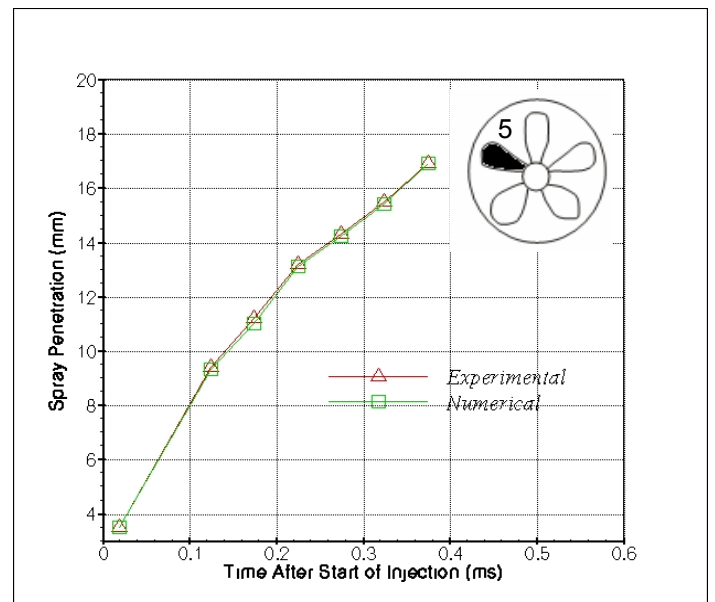
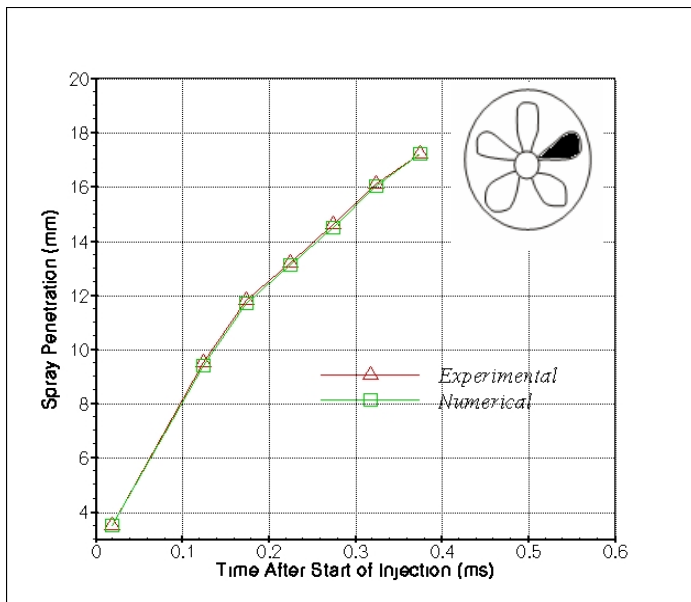


Figure 3 Fuel Penetration Versus Time for each fuel injector.

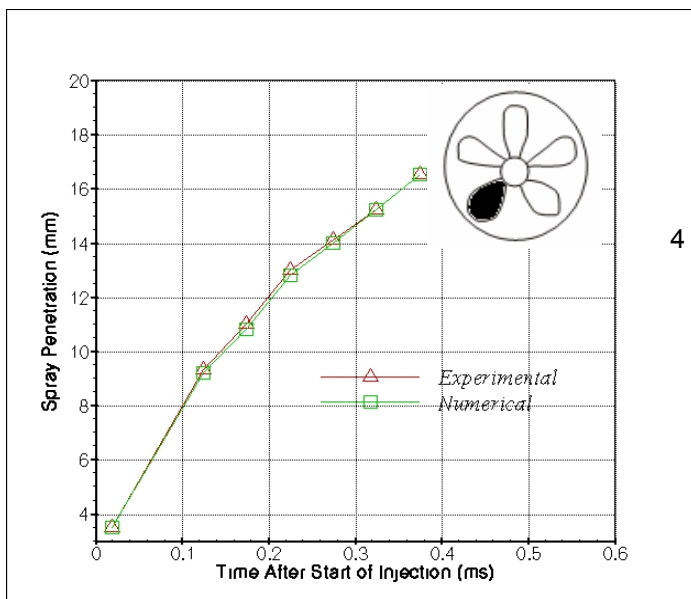
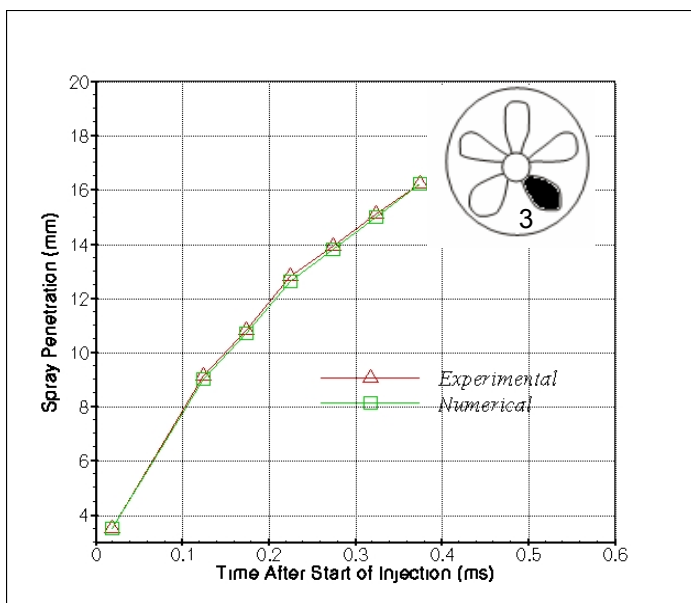
CONCLUSION

The aim of this work was to develop a computationally efficient numerical model which can accurately predict complex spray distribution and spray penetration. The fuel spray model was defined and the numerical model was developed. It was clearly seen that the transient characteristics of the fuel droplet distribution have to be considered because of rapid variation during the injection period due to the varying in-cylinder pressure. Hence, the important parameters of spray characteristics which highly influence the engine performance are Sauter mean radius (SMR), injection velocity and drag coefficient, and nozzle discharge coefficient.

Sauter Mean Diameter:

The Sauter mean radius was found to depend strongly on the injection pressure values. It was observed from numerical simulations that as the injection pressure increases the Sauter mean diameter decreases. This may be attributed to the increase of the available atomization energy affecting the initial disturbance and entrainment. For example, decrease of injection pressure from 90MPa to 67MPa caused the SMR to decrease by 17%. The effect of density of air from the equation derived indicates that the SMR increases with increase in air density. This was believed to be due to the agglomeration of the droplets due to the small penetration of the spray in the denser medium. It can also be observed from the equation that as the nozzle diameter increases the SMR also increases due to increase of the flow area. The numerical results showed under penetration at the starting phase of injection and matched later.

Varying Injection:



The decrease in velocity has a great impact on the spray penetration. It was noticed numerically that as the combustion commences in the diesel engine the in-cylinder pressure increases and the velocity of the liquid fuel particle decreases. The numerical results showed over penetration.

Drag Coefficient:

The drag coefficient was a function of the Reynolds number. When the new expressions for the drag coefficient were applied, it appeared numerically that as the diameter of the particle increases the fuel penetration decreases. It may be attributed by the following relation,

$$penetration = \frac{DragForce}{Mass} \Rightarrow \propto \frac{1}{D^2}$$

The results obtained showed excellent agreement with the available experimental data. A diesel spray was thus modeled, by applying the appropriate initial droplet conditions and the proper physics to the complex processes.

The numerical simulations were carried out only for the part load conditions. It is recommended to carry out the simulations for wide range of operating conditions and to compare them with the experimental data.

The present work concentrated on the fuel spray modeling in the modern diesel engines. It is recommended to work further on the fuel combustion process and pollutant emission formation.

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