Three Dimensional Modeling of Mixture Formation and Combustion in a Direct Injection Heavy-Duty Diesel Engine

A. R. Binesh, and S. Hossainpour

Abstract—Due to the stringent legislation for emission of diesel engines and also increasing demand on fuel consumption, the importance of detailed 3D simulation of fuel injection, mixing and combustion have been increased in the recent years. In the present work, FIRE code has been used to study the detailed modeling of spray and mixture formation in a Caterpillar heavy-duty diesel engine. The paper provides an overview of the submodels implemented, which account for liquid spray atomization, droplet secondary break-up, droplet collision, impingement, turbulent dispersion and evaporation. The simulation was performed from intake valve closing (IVC) to exhaust valve opening (EVO). The predicted in-cylinder pressure is validated by comparing with existing experimental data. A good agreement between the predicted and experimental values ensures the accuracy of the numerical predictions collected with the present work. Predictions of engine emissions were also performed and a good quantitative agreement between measured and predicted NOx and soot emission data were obtained with the use of the present Zeldowich mechanism and Hiroyasu model. In addition, the results reported in this paper illustrate that the numerical simulation can be one of the most powerful and beneficial tools for the internal combustion engine design, optimization and performance analysis.

Keywords—Diesel engine, Combustion, Pollution, CFD.

I. Introduction

DUE to the growing importance of future emission restrictions, manufacturers of internal combustion engines are forced continuously to improve the mixture formation and combustion processes in order to reduce engine raw emissions.

In this context, the numerical simulation and optimization of mixture formation and combustion processes is today becoming more and more important. One advantage of using simulation models is that in contrast to experiments, results can often be achieved faster and cheaper. Much more important is the fact that despite the higher uncertainty compared to experiments, the numerical simulation of mixture formation and combustion processes can give much more extensive information about complex in-cylinder processes than experiments could ever provide[1].

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Using numerical simulations, it is possible to calculate the temporal behavior of every variable of interest at any place inside the computational domain. This allows the obtainment of a detailed knowledge of the relevant processes and is a prerequisite for their improvement. Furthermore, numerical simulation can be used to investigate processes that take place at time and length scales or in places that are not accessible and thus cannot be investigated using experimental techniques. In the case of high-pressure diesel injection for example, the spray break-up near the nozzle is mainly influenced by the flow conditions inside the injection holes. However, because of the small hole diameters (less than 200 μm for passenger cars) and the high flow velocities (about 600 m/s and more), the three-dimensional turbulent and cavitating two-phase flow is not accessible by measurement techniques. One very costly and time-consuming possibility of getting some insight into these processes is to manufacture a glass nozzle in real-size geometry and to use laser-optical measurement techniques. Outside the nozzle in the very dense spray measurements of the three-dimensional spray structure (droplet sizes, velocities etc.) become even more complicated, because the dense spray does not allow any sufficient optical access of the inner spray core. In these and other similar cases numerical simulations can give valuable information and can help to improve and optimize the processes of interest [2].

Summarizing the situation today, it must be pointed out that the predictive quality of the models currently used in CFD codes has already reached a very high level, and that the use of CFD simulations for the research and development activities of engine manufacturers with respect to the design of new and enhanced mixture formation and combustion concepts is not only practical but already necessary. Today, the complex task of developing advanced mixture formation and combustion concepts can only be achieved with a combination of experimental and numerical studies [3].

II. Computational Model

A. Model Geometry and the Mesh

FIRE code is used to simulate the overall combustion processes of a Caterpillar diesel engine. The specifications and operating conditions of this engine are listed in Table I. Notice that the spray angle is 27.5 degrees from the head, which makes the spray droplets, impinge on the piston surface shortly after injection.

In addition to the assumption of cyclic symmetry, the bowl assessment work was concentrated on the mixing, combustion and pollutant formations. Therefore only a sector mesh was developed for carrying out the spray and combustion simulation. The computational mesh was created using AVL ESE Diesel Tool [4]. The final mesh consists of a hexahedral dominated mesh. The mesh for the bowl is shown in Fig. 1. Number of cells in the mesh was about 21425at TDC, respectively. The angle of the sector mesh was chosen in such a way that only one nozzle hole could be located in the sector.
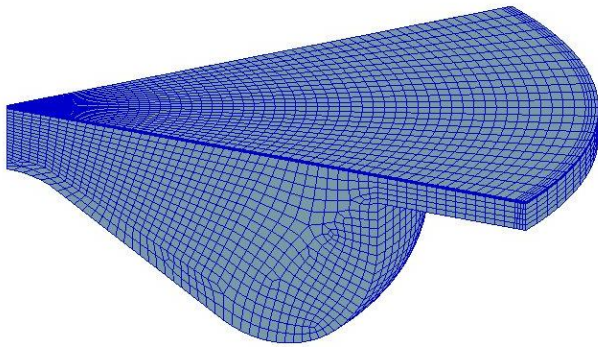

Fig. 1 Computational Mesh for the Caterpillar engine at TDC

B. *Boundary Conditions*

Fig. 2 shows the boundary conditions that used in computational domain for simulating Caterpillar diesel engine. Due to assumption of cyclic symmetry, periodic boundary condition is applied to two contiguous boundaries and moving wall boundary condition is applied to piston bowl as shown in Fig. 2.
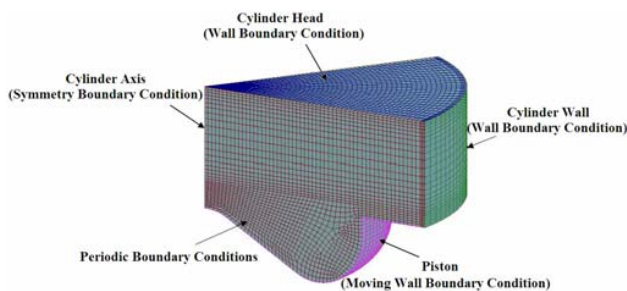

Fig. 2 Boundary conditions used in computational domain at -40 ATDC

TABLE I
CATERPILLAR ENGINE SPECIFICATIONS AND CONDITIONS

Engine	Caterpillar 3401
Cylinder bore x stroke (mm)	137.19 x 165.1
Compression Ratio	15:1
Displacement	2.44 Liters
Connected Rod Length (mm)	261.62
Combustion chamber geometry	Mexican Hat
Engine speed (rpm)	1600

Injection system	Common Rail
Maximum Injection pressure (Mpa)	90
Number of nozzle holes	6
Nozzle hole diameter (mm)	0.259
Fuel injected (g/cycle)	0.1622
Injection duration (CA)	21.5
Start of injection (CA)	-9 ATDC
Intake Valve Closing (IVC)	-147 ATDC
Exhaust Valve Opening (EVO)	+136 ATDC

III. MODEL FORMULATION

Especially in Diesel engines there is a strong interaction of mixture formation and combustion since both processes occur simultaneously. The most important phenomena are the liquid core atomization, the collision and secondary break-up of fuel droplets, their momentum, energy and mass exchange with the gas phase and the droplet-wall-interaction. Simultaneously, numerous complex chemical reactions occur, which initiate the auto ignition, the burnout of the premixed phase and the subsequent turbulent non-premixed combustion. It is a demanding task for the numerical simulation tools to adequately describe all the above phenomena, which are physically divers, but strongly interactive.

The numerical simulation of flow and mixture formation is based on an Eulerian description of the gas-phase and on a Lagrangian description of the droplet-phase. The interaction between both phases is described by source terms for the momentum, heat and mass exchange. This methodology has widely been used for spray modeling and is also implemented in the CFD code FIRE.

The turbulent gas flow is described by a numerical solution of the complete ensemble averaged equations of the conservation of mass, momentum, energy and species mass fraction in an unstructured numerical mesh. Turbulence is modeled using a standard $k - \varepsilon$ model.

A. *Spray Submodels*

Spray model used in this study is WAVE breakup model suggested by Reitz and could be summarized as follows [5]:

Liquid breakup is modeled by postulating the new drops are formed (with drop radius, r) from a parent drop or blob (with radius, a) with Stripping:

$$r_{new} = B_0.\Lambda \qquad (1)$$

where $B_0 = 0.61$ is a constant, the value of which is fixed. The rate of change of drop radius in a parent parcel due to drop breakup is described by using the rate expression:

$$\frac{dr}{dt} = -\frac{r - r_{new}}{\tau_{bu}}, \quad \tau_{bu} = 3.788.B_1 \frac{r}{\Lambda.\Omega} \qquad (2)$$

The spray-wall interaction model used in the simulations is based on the spray-wall impingement model described in [6].

This model assumes that a droplet, which hits the wall is affected by rebound or reflection based on the Weber number. The Dukowicz model was applied for treating the heat-up and evaporation of the droplet, which is described in [7]. This model assumes a uniform droplet temperature. In addition, the rate of droplet temperature change is determined by the heat balance, which states that the heat convection from the gas to the droplet either heats up the droplet or supplies heat for vaporization.

With higher droplet densities and relative velocities droplet collisions occur. High droplet densities are restricted to the spray kernel. High relative velocities can especially be seen at the tip of the spray, where preceding droplets are decelerated by the gas. Depending on the droplet collision conditions various effects like elastic droplet bouncing, droplet coalescence and droplet atomization are observed. In the CFD-code FIRE these collision mechanisms are described by the model of O'Rourke [8].

B. Ignition and Combustion Models

The Shell auto-ignition model was used for modeling of the autoignition [9]. In this generic mechanism, 6 generic species for hydrocarbon fuel, oxidizer, total radical pool, branching agent, intermediate species and products were involved. In addition the important stages of autoignition such as initiation, propagation, branching and termination were presented by generalized reactions, described in [9].

The combustion model used in this study is of the turbulent mixing controlled variety, as described by Magnussen and Hjertager[10]. This model assumes that in premixed turbulent flames, the reactions (fuel and oxygen) are contained in the same eddies and are separated from eddies containing hot combustion products. The chemical reactions usually have time scales that are very short compared to the characteristics of the turbulent transport processes. Thus, it can be assumed that the rate of combustion is determined by the rate of intermixing on a molecular scale of the eddies containing reactants and those containing hot products, in other words by the rate of dissipation of these eddies.

C. NOx and Soot Formation Models

The reaction mechanism of NOx formation is expressed in terms of the extended Zeldovich mechanism.

$$N_2 + O \leftrightarrow NO + N \tag{3}$$

$$N + O_2 \leftrightarrow NO + O \tag{4}$$

$$N + OH \leftrightarrow NO + H \tag{5}$$

From the fact that in most stoichiometric and fuel-lean flames, the occurring OH concentration is very small, the third reaction of the Zeldovich mechanism can be neglected. For the formation of thermal NO, the partial equilibrium approach can be used and the equilibrium of the first two reactions result in one global reaction as follows:

$$N_2 + O_2 \longleftrightarrow 2NO \tag{6}$$

The chemical species appearing in this global reaction are used in the given single-step fuel conversion equation via:

$$\frac{d[NO]}{dt} = 2k_f[N_2][O_2] \tag{7}$$

where only the forward reaction is considered and the reaction rate kf is given as:

$$k_f = \frac{A}{\sqrt{T}} \exp\left(\frac{-E_a}{RT}\right) \tag{8}$$

The soot formation model currently implemented in FIRE is based upon a combination of suitably extended and adapted joint chemical/physical rate expressions for the representation of the processes of particle nucleation, surface growth and oxidation.

$$\frac{dm_{soot}}{dt} = \frac{dm_{form}}{dt} - \frac{dm_{oxid}}{dt} \tag{9}$$

$$\frac{dm_{form}}{dt} = A_f m_{fv} p^{0.5} \exp\left(-\frac{E_a}{RT}\right) \tag{10}$$

$$\frac{dm_{oxid}}{dt} = \frac{6M_c}{\rho_s d_s} m_s R_{tot} \tag{11}$$

D. Numerical Model

The numerical method used in this study is a segregated solution algorithm with a finite volume-based technique. The segregated solution is chosen, due to the advantage over the alternative method of strong coupling between the velocities and pressure. This can help to avoid convergence problems and oscillations in pressure and velocity fields. This technique consists of an integration of the governing equations of mass, momentum, species, energy and turbulence on the individual cells within the computational domain to construct algebraic equations for each unknown dependent variable. The pressure and velocity are coupled using the SIMPLE (semi-implicit method for pressure linked equations) algorithm which uses a guess-and-correct procedure for the calculation of pressure on the staggered grid arrangement. It is more economical and stable compared to the other algorithms. The upwind scheme is employed for the discretization of the model equations as it is always bounded and provides stability for the pressure-correction equation. The CFD simulation convergence is judged upon the residuals of all governing equations. This "scaled" residual is defined as:

$$R^\phi = \frac{\sum_{cells} p \left| \sum_{nb} a_{nb} \phi_{nb} + b - a_p \phi_p \right|}{\sum_{cells} p \left| a_p \phi_p \right|} \tag{12}$$

Where ϕ_p is a general variable at a cell p, a_p is the center coefficient, a_{nb} are the influence coefficients for the neighboring cells, and b is the contribution of the constant part of the source term. The results reported in this paper are achieved when the residuals are smaller than 1.0×10^{-4}.

IV. RESULTS AND DISCUSSION

Fig. 3 shows the comparison of simulated and experimental cylinder pressures at -9 degrees ATDC injection timing for the Caterpillar diesel engine. Overall the computed cylinder pressures are in good agreement with the measured data. In

particular, the simulation correctly models the time of auto-ignition and the peak pressures in this case.

Fig. 4 and Fig. 5 show the total in-cylinder soot and NOx variation with crank angle. It is seen that most of the NOx is predicted to be produced after the peak heat release (i.e., after peak cylinder pressure).During this time soot oxidation accounts for the decrease in the in-cylinder soot levels. Figs. 4 and 5 also allow a comparison between the predicted and measured engine-out soot and NOx values. The data are seen to agree well.

The evolution of the NOx distribution within the combustion chamber is shown in Fig. 6 at 20, 25, 30, 40, 50 and 60 degrees ATDC. NOx is seen to be highest in the region where the ignition occurred and the gas has been exposed to high temperatures for the longest time.
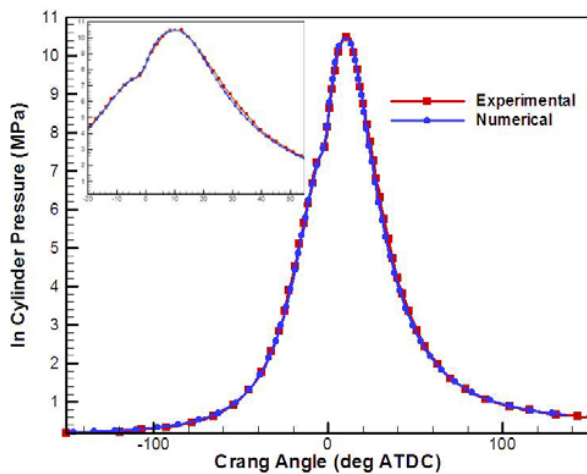

Fig. 3 Comparison of predicted and measured engine cylinder pressure for the Caterpillar diesel engine
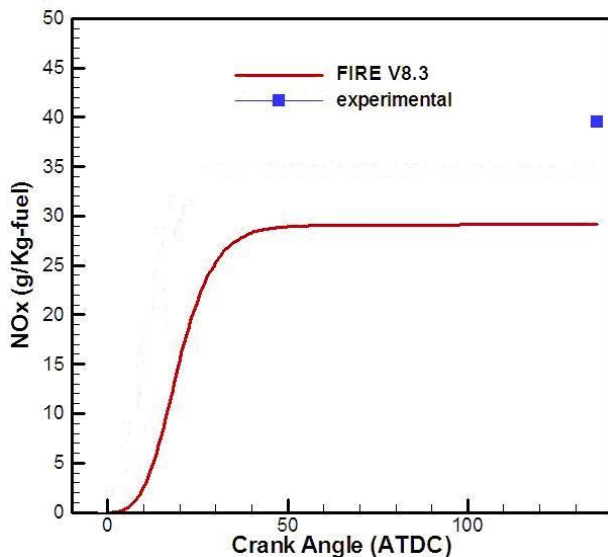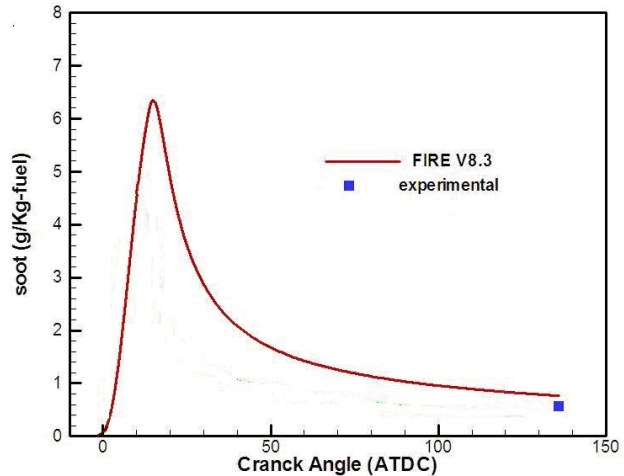

Fig. 5 Predicted total in-cylinder and measured engine-out soot data for the Caterpillar diesel engine

The evolution of the soot distribution within the combustion chamber is shown in Fig. 7 at 0, 4, 10, 20, 35, 50 degrees ATDC. Soot concentrations are the highest in the rich regions of the spray near the cool piston surface.

According to Figs. 6 and 7 the majority of the soot is located near the bottom of the bowl, while the NOx is located closer to the injector. Note that the NOx mass fraction high contour values increase significantly (an order of magnitude) while the soot decreases only slightly (by a factor of about two) due to oxidation.
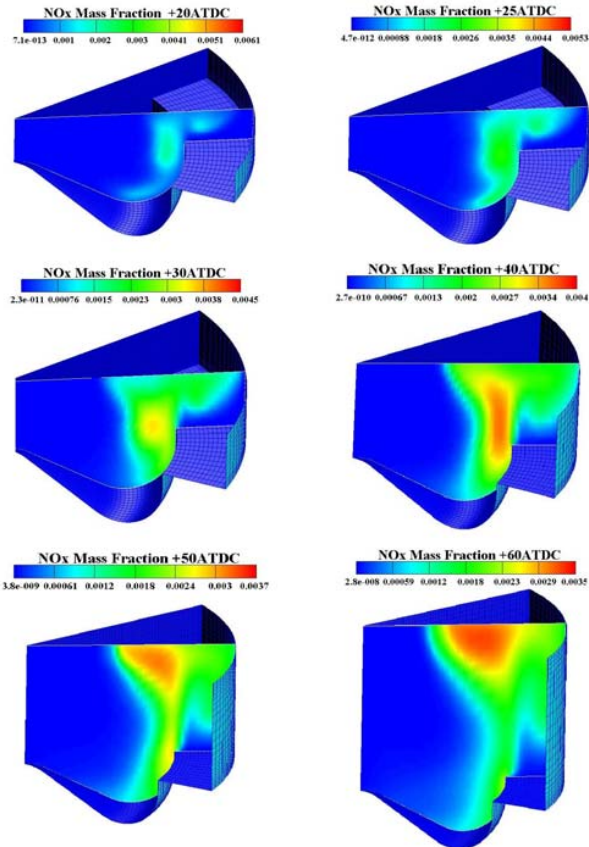

Fig. 4 Predicted total in-cylinder and measured engine-out NOx data for the Caterpillar diesel engine

Fig. 6 Predicted NOx mass fraction contours at20, 25, 30, 40, 50 and 60 degrees ATDC
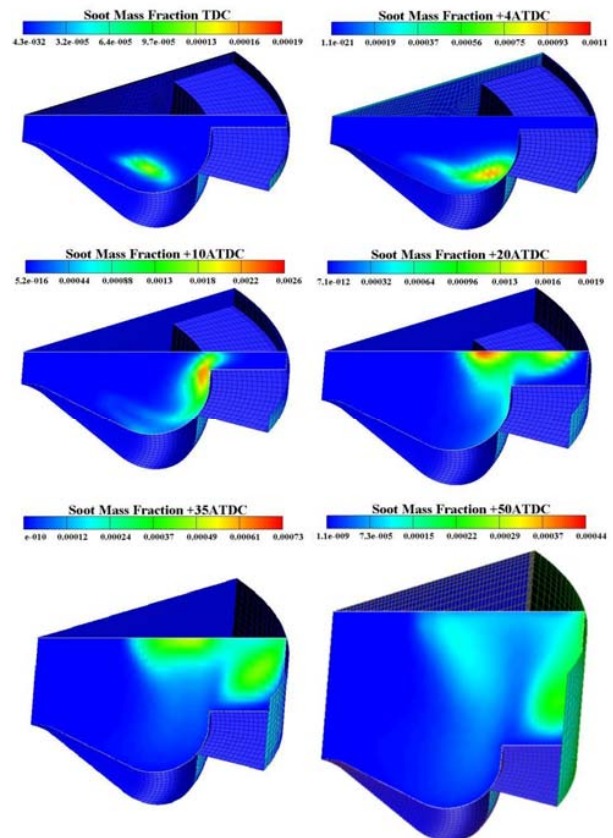

Fig. 7 Predicted soot mass fraction contours at 0, 4, 10, 20, 35, 50 degrees ATD
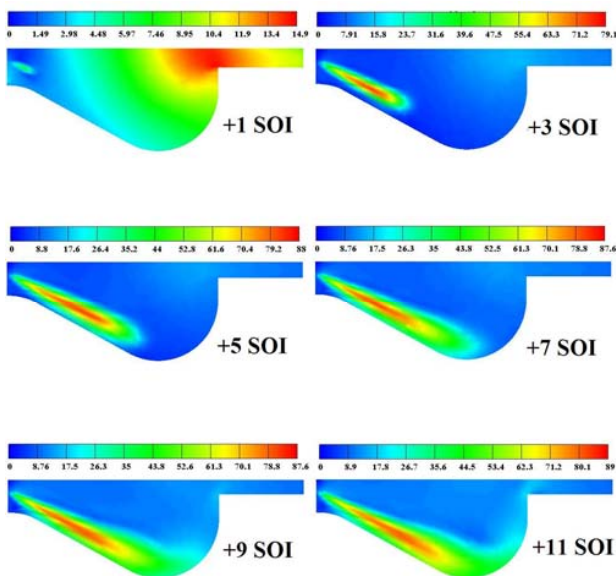

Fig. 8 Predicted spray velocity contours at 1,3,5,7,9 and 11 crank angle degree after start of injection

Fig. 8 shows the predicted spray velocity profiles for the Caterpillar diesel engine using the wave breakup spray model. This figure shows fuel spray tip penetration at various crank angle degrees after start of injection. Researchers [11] have found hat even though the liquid fuel has limited penetration into the combustion chamber, the vapor continues to penetrate ahead of the liquid fuel into the combustion chamber. Hence, the present predictions by the wave model seem to capture this accurately.

V. CONCLUSION

To simulate Diesel injection and combustion the CFD code FIRE has been used by submodels for atomization and spay-wall-interaction. The simulation was performed from intake valve closing (IVC) to exhaust valve opening (EVO).The models implemented in FIRE code for secondary break-up, droplet collision, turbulent dispersion and evaporation were validated by comparison to published experimental data. A good agreement between the predicted and experimental values ensures the accuracy of the numerical predictions collected with the present work.

The results reported in this paper illustrate that the numerical simulation can be one of the most powerful and beneficial tools for the internal combustion engine design, optimization and performance analysis.

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