MODELING OF COMBUSTION AND POLLUTANT FORMATION IN A SINGLE-CYLINDER DIRECT-INJECTION DIESEL ENGINE

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Introduction

Chemical and physical processes accompanying combustion in Diesel engines are very complex and interrelated [1]. Chemical processes include numerous oxidation reactions of fuel, reactions of NOx and soot formation, etc. Physical processes include transient molecular, turbulent, and convective heat and mass transfer in a gas phase, liquid spray disintegration, drop gasification, etc. Particular issues are the flame ignition and extinction phenomena. Multidimensional Computational Fluid Dynamics (CFD) modeling of these processes helps understanding the importance of relevant parameters for the overall engine performance. As a result of the research summarized in this paper, the critical points in the underlying mathematical models have been identified.

Computational Approach

The engine under consideration is a high-swirl, 5-spray, direct-injection, 4-stroke, deep bowl-in-piston, turbocharged Diesel engine with 85-millimeter bore, 96-millimeter stroke, and 17:1 compression ratio to approximately model the conditions of [2]. Figure 1 shows the assumed geometry (one-fifth part of the cylinder) and the computational grids of the combustion chamber at the top dead center (TDC), (a), and bottom
dead center (BDC), \((b)\). With the motion of the piston, the computational grid is properly interpolated between those shown in Figs. 1a and 1b.

The governing equations are the Favre-averaged Navier–Stokes equations for the equivalent gas-phase mixture supplemented by the averaged equations of energy and species conservation, \(k-\varepsilon\) model of turbulence, and the model of combustion based on the presumed bi-modal probability density function of temperature in the turbulent flame brush [3]. The chemical kinetic mechanism applied takes into account fuel \(\text{C}_{14}\text{H}_{30}\) decomposition to \(\text{C}_{1}-\text{C}_{2}\) hydrocarbons and their further oxidation accompanied with NO and soot formation. The equivalent flame concept has been applied [4]. The main implication of this concept is based on the finding that the rate of chemical transformation of the dispersed fuel is smaller than the corresponding rate in the premixed fuel–air mixture. Therefore, it appears possible to represent the two-phase flame by the equivalent gas-phase flame with properly corrected rates of reactions and heat release. The reason for diminished values of reaction rates in two-phase flames lies in the fact that drops exhibit smaller volumetric rates of combustion than the premixed gas due to finite-rate diffusion processes.

Initially (in the BDC), the cylinder is filled with pure air at pressure \(p_0\) and temperature \(T_0\) corresponding to the conditions of turbocharging. A swirl is initially introduced into the cylinder by

\[\text{Figure 1}\] The computational grids with the piston positioned in the bottom \((a)\) and top \((b)\) dead center. With the motion of the piston, the computational grid is properly interpolated between those two grids.
means of initial angular motion of the fluid. In terms of the velocity, the fluid circulation speed in the cylinder attained 40–50 m/s.

Fuel injection is triggered by means of changing the boundary conditions at the nozzle openings from rigid-wall-type to inlet-type boundary conditions and vice versa. Injection timing is the input parameter of computations. The total amount of fuel injected is controlled by the injection velocity and duration, nozzle diameter and density of the fuel jet. Injection velocity is as high as 200 to 300 m/s to ensure deep jet penetration into the bowl. Injection duration was fixed at 25° of crank angle. Ignition is triggered by applying a semi-empirical relationship [1]:

$$\int_{0}^{t_i} \frac{dt}{\tau} = 1$$

(1)

where $\tau$ is the ignition delay time at local instantaneous values of pressure, temperature, and species concentrations, $t_i$ is the actual ignition delay in the cylinder. At time $t > t_i$, during the preset (relatively short) time interval $\Delta t_i$, mixture portions that satisfy Eq. (1) were allowed to burn according to the prescribed fuel depletion law. Further development of combustion was governed by the equations and models mentioned above. In the course of calculations, cylinder-mean concentrations of pollutants (CO, NO, and soot) were continuously monitored.

The problem was solved by the finite volume method with two-stage pressure correction. As a platform for calculations, FIRE code developed by AVL LIST GmbH (Austria) was used with the authors' modules of ignition, turbulent flame propagation, and pollutant formation chemistry integrated into the code.

Results of Calculations

The initial pressure and temperature, $p_0$ and $T_0$, were taken 1.82 atm and 347 K to approximately represent the operating conditions described in [2] for the Diesel engine operating at speed of $n = 4000$ r/min. Wall temperature was taken equal to $T_w = 400$ K.

Figures 2 and 3 show the predicted spatial distributions of fuel mass fraction and temperature in the cylinder cross-section (just above the bowl) at different crank angles. It follows from the figures that igni-
Figure 2 Typical spatial distributions of fuel mass fraction in the cylinder cross-section (just above the bowl) at different crank angles. Ignition occurs at $\varphi = 167.5^\circ$. 

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Figure 3 Typical spatial distributions of temperature in the cylinder cross-section (just above the bowl) at different crank angles. Ignition occurs at $\varphi = 167.5^\circ$.

Combustion occurs in multiple spots with premixed fuel-air mixture at about $\varphi = 168^\circ$ or $12^\circ$ before TDC, that is in a good agreement with the experimental data of [2]. This rapid combustion phase is responsible for high values of energy release and maximum local temperatures. After ignition, there exists a short period of decrease in the maximum temperature that is explained by the transition from the premixed-combustion phase to the mixing-controlled combustion. During mixing-controlled combustion phase, a highly turbulent flame traverses the combustion chamber resulting in the increase of the mean local temperature to 1500–1600 K at the late combustion stage. At this late stage, the distribution of residual fuel and temperature is almost homogeneous.
throughout the whole cylinder. Note that before completion of the mixing-controlled combustion stage, there exists large amounts of CO (up to 5%-6%) in the cylinder. This CO oxidizes to CO₂ during the late combustion phase (at $\varphi > 200^\circ$–$210^\circ$).

Figure 4 shows the predicted indicator diagrams for low ($p_i = 1.57$ MPa / $\Phi = 0.57$) and high ($p_i = 1.82$ MPa / $\Phi = 0.69$) engine loads. It follows from Fig. 4 that ignition always occurs $10^\circ$–$13^\circ$ before TDC that agrees with observations [2].

Figures 5a to 5c summarize the results of calculations of CO, NO, and soot emission, respectively, at $\varphi = 360^\circ$. When comparing these plots with the experimental data [2], one observes a satisfactory qualitative agreement between the predicted and measured results. Moreover, there exists a satisfactory quantitative agreement between predicted and measured CO and NO concentrations. If one takes into account that the exhaust valve opens at $\varphi \approx 300^\circ$, the predicted NO concentration will be of the order 1200–1300 ppm at low loads. The same level of NO has been registered in experiments [2].

Analysis

The results of calculations indicate that the most critical point in modeling engine performance is the combustion model. In many applications, sophisticated models of two-phase spray combustion are used which contain multiple empirical coefficients and approximations. In these models, the local mean reaction rate in the turbulent flow field is determined either on the basis of cell-averaged temperature and concentrations of fuel vapor and air or on the basis of the relationships for diffusion-controlled chemical processes.
Figure 5 Predicted dependence of NO (a), CO (b), and soot (c) emission on the mean indicated pressure.

As a matter of fact, the only computationally feasible way of modeling spray combustion is to treat the combustion chemistry in terms of mean reaction rates without detailed resolution of local flame structure around individual drops. Therefore, it is instructive to evaluate the relationship between the local instantaneous reaction rates in the gas surrounding a single burning drop with the instantaneous spatial mean reaction rates. The reaction rate of a gas-phase reaction is given by the formula:

$$w_{ij} = k_{ij} \prod_j n_j$$  \hspace{1cm} (2)

where index $j$ relates to the reactive species, index $i$ relates to the reaction number, $k_{ij} = A_{ij} T^{m_{ki}} \exp(-E_{ij}/(RT))$ is the reaction rate.
constant, $A_{ij} T^{m_{ij}}$ is the preexponential factor, $m_{ij}$ is the temperature exponent, $E_{ij}$ is the activation energy, and $R$ is the gas constant. At any time $t$, the average reaction rates $(\bar{\omega}_{ij})_t$ taken over the space around the burning drop, from the drop center ($r = 0$) to the "stoichiometric" radius ($r = r_{st}$), can be defined as

$$(\bar{\omega}_{ij})_t = \frac{3}{4\pi r_{st}^3} \int_0^{r_{st}} (\omega_{ij})_{r,t} 4\pi r^2 dr$$

The stoichiometric radius is the radius of the equivalent sphere, where the completely evaporated fuel is in a stoichiometric composition with air:

$$\frac{r_{st}}{r_{d0}} = \left[ \frac{\rho_l}{\rho_g} \right]^{1/3}$$

where $r_{d0}$ is the initial radius of the fuel drop, $\rho_l$ and $\rho_g$ are the densities of liquid and gas, respectively, and $v$ is the air-to-fuel mass ratio in the stoichiometric mixture (approximately 15 for heavy hydrocarbons).

In case of spray combustion, the mean reaction rate is usually taken as a function of mean species concentrations $(\bar{n}_{ij})_t$

$$(\bar{n}_{ij})_t = \frac{3}{4\pi r_{st}^3} \int_0^{r_{st}} (n_{ij})_t 4\pi r^2 dr$$

and mean temperature $(\bar{T})_t$

$$(\bar{T})_t = \frac{3}{4\pi r_{st}^3} \int_0^{r_{st}} (T)_{r,t} 4\pi r^2 dr$$

i.e.,

$$(\bar{\omega}_{ij})_t = k_{ij} \prod_j (\bar{n}_{ij})_t = A_{ij} (\bar{T})_t^{m_{ij}} \exp \left( -\frac{E_{ij}}{R(\bar{T})_t} \right) \prod_j (\bar{n}_{ij})_t$$

The ratio of mean reaction rates (3) and (4), $(\bar{\omega}_{ij})_t/(\bar{\omega}_{ij})_t$, is thus the measure of the error caused by using the mean temperature and species.
concentrations in available spray combustion models. The minimum error can be estimated by taking a maximum reaction rate of Eq. (4) during the entire drop lifetime. Thus, the factor \( (C_{ij})_t = (\overline{w_{ij}})_t/(\overline{w_{ij}})_{\text{max}} \) indicates the least discrepancy of the mean reaction rate of Eq. (4) from the true value of the mean reaction rate at time \( t \). Recent calculations [4] revealed that this factor can attain values exceeding \( 10^2 - 10^3 \), particularly, at the beginning of drop burning.

In view of this important finding, a simple equivalent flame concept adopted in this study seems to be more appropriate for multidimensional CFD modeling of Diesel engine performance than sophisticated spray combustion models. First, there seems to be no sense in modeling complex interactions in the spray if the error relevant to combustion chemistry is so large. Second, the equivalent gas concept takes into account a detailed chemistry of fuel oxidation and pollutant formation with due regard for the effect of turbulent fluctuations on the mean reaction rate. Third, this concept, when properly validated against experimental data for laminar and turbulent spray flames, can be used in multidimensional calculations without further modifications. The computational results presented herein illustrate the approach.

**Concluding Remarks**

Multidimensional CFD modeling of processes in a Diesel engine using the equivalent flame concept of [4] has shown a satisfactory agreement with experimental observations in terms of ignition timing and emission of CO, NO, and soot.

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**References**


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