Recent Advances in DI-Diesel Combustion Modeling in AVL FIRE – A Validation Study

R. Tatschl, P. Priesching, J. Ruetz
AVL List GmbH
Advanced Simulation Technologies
Graz, Austria

ABSTRACT

The ECFM-3Z combustion model is coupled with refined auto-ignition tables based on detailed chemical kinetics calculations and linked to models for NO and soot formation. The resulting model suite is implemented in the CFD code FIRE and validated with respect to its applicability to conventional and alternative Diesel combustion regimes. For this purpose the set of models is applied to the calculation of combustion and pollutant formation in a high-speed DI diesel engine for selected operating points performing a number of DoE based combustion system parameter variations. Assessment of the model performance is achieved via comparison of the calculation results with the corresponding experimental data. Good agreement of calculated and measured in-cylinder pressure traces as well as pollutant formation trends can be observed for both the conventional and alternative Diesel combustion modes for the investigated parameter variations.

MODELING

The commercial CFD code FIRE is used in the present study. The liquid fuel spray is modeled according to the Lagrangian discrete droplet method. Sub-models are used that account for the effects of turbulent dispersion, coalescence, evaporation, wall interaction as well as droplet primary and secondary break up. In the present study the blob-injection method in combination with the WAVE break-up model is used to model liquid fuel break-up downstream of the injector. The value of the break-up model parameters is chosen to fit the experimental spray propagation characteristics measured in a constant volume bomb.

For modeling the diesel combustion process the ECFM-3Z model is adopted which distinguishes between the three major regimes relevant during diesel combustion, namely auto-ignition, premixed flame and non-premixed, diffusion combustion [1]. The distinct modeling of the different ignition/combustion regimes makes the ECFM-3Z model applicable to conventional as well as alternative Diesel combustion modes.
For prediction of the auto-ignition process the present study adopts refined auto-ignition tables generated based upon detailed chemical kinetics calculations adopting the validated n-heptane mechanism of [2]. The values are stored as function of the parameters pressure, temperature, fuel/air equivalence ratio and residual gas content. The range of these parameters is chosen to cover the relevant conditions prior to combustion, i.e. pressure from 10 to 80 bar, temperature from 600 to 1500 K, equivalence ratio from 0.3 to 3.0 and residual gas mass fraction from 0 to 90%. During the CFD calculation the tables are accessed via a fast interpolation procedure ensuring minimized calculation time.

![Figure 1: Parameter surface of the ignition delay time as function of temperature and pressure](image)

The formation of thermal NO is modeled in the present study by the widely accepted extended Zeldovich mechanism, for calculating prompt NO a global kinetics mechanism is adopted. In order to avoid effects of liquid fuel break-up and evaporation, the model implementation and parameterization has been validated for gaseous jet diffusion flames [3].

The soot model applied in the present work is based on a flamelet library approach for the soot source terms [4]. Implementation of the soot model into CFD is achieved via calculation of additional transport equations for the mixture fraction and its variance and integration of the instantaneous soot formation rates in mixture fraction space via a presumed $\beta$-PDF in order to obtain their mean values. Since the source terms for the soot formation and oxidation are evaluated before the CFD simulation and are stored in a library, the model appears to be very time efficient despite its complexity.

**VALIDATION**

The engine used for the validation study is a single-cylinder research engine with electro hydraulic valve actuation and three intake ports with swirl flaps. An $\omega$-shaped piston bowl is used in this study. The main engine and injection system data are summarized in Table 1.

<table>
<thead>
<tr>
<th>Bore</th>
<th>85 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stroke</td>
<td>94 mm</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>16:1</td>
</tr>
<tr>
<td>Injection system</td>
<td>BOSCH Piezo CR</td>
</tr>
<tr>
<td>Number of injection holes</td>
<td>8</td>
</tr>
</tbody>
</table>

Table 1: Engine and injection system data
Validation of the adopted model suite is presented for two operating points. Operating point A pertains to conventional diesel combustion, whereas operating point B is an alternative diesel combustion mode. For these two operating conditions DoE plans are used for the design of the calculation campaign. This means that for each speed/load point a considerable number of combustion system variations are applied by simultaneously changing the parameters start of injection (SOI), residual gas amount (EGR), swirl level and injection pressure. The following table shows the main specifications and the range of parameter variations for both cases.

<table>
<thead>
<tr>
<th></th>
<th>Operating Point A</th>
<th>Operating Point B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine speed</td>
<td>3000 rpm</td>
<td>2000 rpm</td>
</tr>
<tr>
<td>IMEP</td>
<td>8.3 bar</td>
<td>2.55 bar</td>
</tr>
<tr>
<td>SOI</td>
<td>1 – 10 deg BTDC</td>
<td>1 – 30 deg BTDC</td>
</tr>
<tr>
<td>EGR</td>
<td>12 – 20 %</td>
<td>25 – 60 %</td>
</tr>
<tr>
<td>Swirl</td>
<td>0 – 74 %</td>
<td>0 – 74 %</td>
</tr>
<tr>
<td>Inj. presssure</td>
<td>1200 – 1600 bar</td>
<td>550 – 1000 bar</td>
</tr>
</tbody>
</table>

Table 2: Engine operating conditions and DoE parameter variation range

In order to enable the large number of calculations of the DoE matrix to be performed within reasonable time, the CFD calculations are done on an engine segment mesh covering 1/8 of the cylinder/piston bowl arrangement around one single fuel spray assuming cyclic symmetry. The engine segment calculations for each DoE matrix point are started at the time of inlet valve closure and are finished at opening of the exhaust valves. The gas side initial conditions at the time of inlet valve closure, i.e. in-cylinder pressure, temperature and residual gas mass fraction, as well as the wall temperature boundary conditions are taken from 1D cycle simulations adopting the BOOST code. A solid body rotation of the in-cylinder flow field at the time of inlet-valve closure is prescribed, with the swirl levels and turbulence intensities extracted from preceding FIRE calculations of the entire intake stroke. The fuel side boundary conditions, i.e. hydraulic injection timing and injection rates for the different injection pressure levels are obtained on the basis of 1D hydraulic simulations with HYDSIM. Parameterization of the hydraulic model is conducted on the basis of selected three-dimensional nozzle flow simulations using FIRE.

RESULTS AND DISCUSSION

Conventional Diesel Combustion – Operating point A

The whole set of operating conditions form the DoE plan is calculated using the model parameters of the baseline case. In Figure 1 the calculated in-cylinder pressure trace and heat release rate from the CFD calculation are shown for the baseline reference case in comparison with the corresponding data from a 1D cycle simulation.

The good quantitative agreement of the premixed combustion spike and the heat release rate during the main diffusion controlled combustion process is remarkably well captured by the presently adopted spray/combustion modeling approach. The good overall agreement of the cylinder-pressure trace during the compression, combustion and expansion phases also confirms the validity of the overall calculation methodology, based upon a combination of the different 1D and 3D CFD tools for a proper description of the initial and boundary conditions.
Figure 1: Pressure trace and heat release rate for baseline reference case

Figure 2 shows four additional cylinder pressure traces selected from the set of DoE points calculated during the present study, representing simultaneous variations of injection pressure, injection timing, swirl intensity and residual gas rate.

Figure 2: Pressure trace for variations of injection pressure, injection timing, swirl intensity and residual gas rate

The good agreement between calculated and measured heat release and hence cylinder pressure without need for individual model parameter adjustment is a necessary prerequisite for accurate calculation of the pollutant formation trends. In Figure 3 and Figure 4 a comparison between calculated and measured NO and soot levels is presented for a sub-set of the performed simulations.
Alternative Diesel Combustion – Operating point B

The same procedure as described in the previous chapter is applied for the second operating point as well. Also here the model parameters are properly set for the baseline case and then all other different DoE conditions are calculated using the same set of parameters. Figure 5 presents the cylinder pressure traces for two selected DoE parameter sets in comparison with measured data.
Due to the high residual gas rates the engine is operated in the present alternative combustion mode, the local charge temperatures are below the NO formation threshold, i.e. no significant amounts of NO are produced. Because of the long ignition delay time characteristic for alternative combustion conditions, the fuel vapor mixes well prior to the onset of auto-ignition and combustion. Hence, areas of fuel rich zones are minimized and, consequently, soot formation is negligible. The high residual content and the high degree of mixing of fuel vapor with air, however, may lead to incomplete combustion resulting in increased CO and unburned hydrocarbon formation during alternative combustion. The formation of CO and unburned hydrocarbons is the result of complex chemical kinetic processes and turbulence/chemistry interaction details. In order to assess the adopted combustion model with respect to prediction of CO and unburned hydrocarbons, Figure 6 and Figure 7 show a comparison of calculated with measured values of CO and unburned hydrocarbons for selected points of the investigated DoE matrix, respectively.

Figure 6: Comparison of calculated normalized CO formation trends with corresponding measured data

Figure 7: Comparison of calculated normalized unburned hydrocarbon formation trends with corresponding measured data

It can be seen in Figure 6 that the measured CO formation trends are reasonably well predicted by the reaction and equilibrium chemistry models adopted in the ECFM-3Z. Although a model for calculation of the formation of the different unburned hydrocarbon components is not available for the present study, Figure 7 shows reasonable agreement of the calculated gross amount of fuel left unburned and the measured values for tail-pipe emissions for unburned hydrocarbons. A fairly good correlation between the calculated and the measured trends of unburned
hydrocarbon formation can be observed in Figure 7, however, no fully consistent prediction over the entire set of results is achieved. This lack of predictive capability related to the unburned hydrocarbon formation calculation clearly indicates the need for future development of more complex chemical kinetics models for unburned hydrocarbon formation.

SUMMARY

In the present work the ECFM-3Z combustion model and advanced soot and NO formation models are implemented in the CFD code FIRE and validated for conventional and alternative diesel combustion application. Comparisons of the numerically obtained results with measured in-cylinder pressure traces and rates of heat release show good agreement with respect to the timing of auto-ignition onset and pressure rise as well as peak pressure levels for both investigated operating modes. For conventional diesel combustion the NO and soot formation trends are well reproduced by the adopted models. For the alternative diesel combustion mode the CO formation is reasonably well reflected by the heat release chemistry of the ECFM-3Z model. The unburned hydrocarbon calculation results clearly indicate the need for future implementation of more detailed reaction chemistry into the CFD combustion modeling to better match experimentally obtained trends.

REFERENCES