Eulerian Spray Modeling of Diesel Injection in a High-Pressure/High Temperature Chamber

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Abstract

Spray modeling using statistical particles is known to have several numerical problems associated with grid dependency and statistical convergence. To overcome these difficulties a new Eulerian spray model is presented and it is used to investigate the injection and ignition process of a diesel spray in a high pressure/temperature cell. To model the chemistry and the chemistry-turbulence interaction a flamelet model is employed. Ignition delay and spatial soot distributions are compared between experiment and simulation.

Numerical Model

For Diesel simulation spray modeling plays a very important role as it strongly influences all subsequent processes such as mixture formation, ignition, heat release and pollutant formation. The most common approach in CFD codes for engine modeling is the use of stochastic Lagrangian spray models. The spray is represented by parcels which then constitute the statistical distribution of location, velocity, size and temperature of the spray droplets. A detailed description can be found in [1]. Despite its popularity there are a range of mainly numerical difficulties associated with Lagrangian spray models and the associated submodels to describe the physical processes such as breakup, collision, turbulent dispersion and evaporation. The models for turbulent dispersion and collision e.g. show a strong sensitivity with respect to the CFD grid. Several attempts have been made to fix these problems, see e.g. [2]. Another problem is to reach statistical convergence which may require a huge number of particles. Krüger [3] pointed out that maybe the largest problem is the coarse mesh resolution of the CFD code especially close to the nozzle. Velocity gradients cannot be properly resolved which leads to an underestimated turbulence intensity which then leads to an underestimation of the turbulent diffusivity. This however is balanced by the increased numerical diffusivity due to the coarse mesh resolution.

An example for the mesh resolution dependency is shown in Fig. 1. The penetration of the gas phase over time is plotted for an injection of n-heptane into a high-pressure/high-temperature chamber. The mesh size has been varied and the cell size is given as a multiple of the nozzle diameter. The simulation data shows a strong dependence of the penetration depth on the resolution. In practice this leads to tuning of spray parameters on a given grid to achieve the correct penetration depth. It should be noted that the number of statistical parcels for these calculations was kept constant.

A different way to model diesel sprays was proposed by Wan and Peters [4] which they called Interactive-Cross-Sectionally-Averaged (ICAS) spray model. Eulerian boundary layer equations for the gas and the liquid phase are formulated and integrated over the cross-section of the spray. This leads to the instationary, one-dimensional
Figure 1: Penetration depth for different mesh resolutions compared to experimental data, Lagrangian spray model.

CAS-equations. As an example the continuity equation for the gas and liquid phase read

\[
\frac{\partial (\hat{\rho}(1 - \hat{Y}_f)b^2)}{\partial t} + \frac{\partial (\hat{u}_g\hat{b}(1 - \hat{Y}_f)b^2)}{\partial x} = \rho_g\beta \hat{b}\hat{u}_g + \hat{\omega}_{vap}b^2, \text{ (gas)},
\]

(1)

\[
\frac{\partial (\hat{\rho}\hat{Y}_f b^2)}{\partial t} + \frac{\partial (\hat{u}_l\hat{Y}_f b^2)}{\partial x} = -\hat{\omega}_{vap} b^2, \text{ (liquid)},
\]

(2)

where the \(< \cdot >\) denotes the cross-sectional average, \(\hat{\rho}\) the density of the mixture, \(\hat{Y}_f\) the liquid fuel mass fraction, \(b\) the half-width of the spray, \(\hat{u}_g\) the gas velocity, \(\rho_g\) the density of the entrained air, \(\beta\) the spreading coefficient, \(\hat{\omega}_{vap}\) the evaporation rate and \(\hat{u}_l\) the liquid velocity, respectively. Similar equations are formulated for the momentum, the energy/enthalpy of the gas and the liquid phase. Also an equation for the diameter of the droplets is solved. This model has also been extended to multiple so-called droplet classes. The spatial coordinate \(x\) corresponds to the spray axis. The entrainment is prescribed by the spray radius \(b\) for which an empirical correlation obtained from measurements is used. These equations are solved in a separate spray code.

On the gas side we use the Representative Interactive Flamelet (RIF) model. The flamelet equations are solved in a separate code flamelet code. The coupling of the various codes is shown in Fig. 2. The CFD code, which is KIVA for this investigation, interacts with the spray code as well as the flamelet code. The coupling of the CFD and the flamelet code has been described in detail in a number of papers [5-8] and only a brief description is given here. The flamelet parameters scalar dissipation rate and pressure are passed to the flamelet code which computes the instationary flamelet solutions for that time step. These solutions, being a function of the mixture fraction variable, along with the probability density function of the mixture fraction can be used to compute the mean temperature and species profiles in the 3D field. The chemistry which also includes pollutant formation processes is completely solved within the flamelet code. The soot model is also completely incorporated into the framework of the flamelet concept.

The spray code interacts in a similar way with the CFD code. Boundary conditions such as temperatures and species mass fractions at the edges of the spray are passed to the spray code which then solves the radially integrated equations for the gas and the liquid phase along the spray axis. The source terms for the fuel, the momentum, the turbulent kinetic energy and dissipation for that time step are then passed to the CFD code. The CFD code only indirectly sees the liquid phase through these source terms.
Figure 2: Coupling of the CFD code with the Eulerian Spray code and the flamelet code.

These placement of these source terms depends on the axial coordinate $x$ and the half-width $b(x)$. A second grid for the spray which is usually much finer is generated and each computational cell is associated with a KIVA cell which then controls the placement of the source terms in the KIVA code.

Figure 3: KIVA mesh and the ICAS exchange mesh.

Figure 3 shows a typical KIVA mesh with an embedded ICAS mesh which shows the fine resolution of the spray grid compared to the CFD grid. This is very beneficial especially close to the nozzle. It has been shown by Krause and Peters [9] that refining the KIVA grid now leads to convergent behavior in terms of gas and liquid penetration in the KIVA code. No unphysical behavior such as in Fig. 1 is found any more.
<table>
<thead>
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<td>Diesel</td>
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<tr>
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<td>300 K</td>
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<tr>
<td>nozzle</td>
<td>single hole nozzle</td>
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<tr>
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<tr>
<td>injected mass</td>
<td>6 mg</td>
</tr>
<tr>
<td>ignition delay</td>
<td>1.2 mg</td>
</tr>
</tbody>
</table>

Table 1: Experimental conditions.

Results

In the following we will present results for injection and ignition in a high pressure chamber. The experimental conditions are summarized in Tab. 1. Further details on the experimental setup and technique can be found in [10].

The fuel in the experiments is diesel which is modeled using a two-component model fuel being a mixture of 70% n-decane and 30% α-methylnaphthalene. It has been shown previously [6, 7] that this so-called IDEA fuel yields good results for ignition delay and pollutant formation when compared to real diesel fuel.

The simulation is carried out on a 2D sector mesh with 40 x 150 cells for a domain of 2 cm x 8 cm. The experimental ignition delay of 1.2 ms is well predicted by the combined ICAS/RIF model.

The emphasis of the experimental work was on measuring soot by means of light extinction techniques. Therefore in the following we compare measured and the computed soot profiles. On the one hand soot computations are a very challenging task but on the other hand it can be used to assess the performance of the combined model as both the mixture formation which directly depends on the spray and the flamelet modeling strongly influence the soot results.

In Fig. 4 the soot distributions are shown for three instants, 2 ms, 2.5 ms and 3 ms. In the upper half the experimental result is plotted and the simulation data is shown in the lower half of each picture. The color coding is slightly different for experiments and simulations. As the maximum values are different for experiment and numerics and due to the nonlinear subdivision of the contour-levels we found that the present color-coding is the best compromise. The maximum values should not be adjusted as there may be several reasons for deviations of these maximum values such as real vs. model fuel as well as experimental uncertainties. It seems more important to compare the spatial soot distribution.

In general the agreement between experiment and simulation is reasonably good considering the complexity of soot modeling. There are some deviations especially at the spray tip which are due to some modeling issues in the tip region. Krüger[3] proposed a solution for that problem but this has not been used here.

Summary

In order to overcome some of the numerical problems associated with Lagrangian spray models an Eulerian spray model was developed and coupled to a CFD code. This combined model was applied to the simulation of the injection and ignition of a diesel spray in a high pressure, high temperature chamber. The simulated ignition delay is in good agreement with the experimental value. Two-dimensional soot profiles are compared for three instants. The maximum values are of the same order of magnitude when compared to the experimental data and in general the spatial distributions show reasonably good agreement.
Figure 4: Soot distributions, comparison between experimental (upper half) and the numerical (lower half) results for 2.0 ms (top), 2.5 ms (middle) and 3.0 ms (bottom)
References


