Lagrangian-Eulerian Fuel Spray Modeling and Near-Nozzle X-Ray Data

SUBTASK 1.2H: Fuel Spray Modeling for Diesel Combustion and Simulation

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Abstract

The Lagrangian discrete particle method (DPM) provides the most straightforward means for spray simulation in the dilute parts of sprays if the grid spacing is much larger than the droplet radius. Yet, the method is typically applied even in the dense spray region which is optically inaccessible for many experimental methods. Although very reasonable results for the fuel spray can be achieved with the DPM especially in a $k-\epsilon-$type of framework, the problems of applying the method near the spray nozzle become apparent when moving on to time and space accurate calculations such as Large Eddy Simulation (LES). Another problem in time and space accurate spray modeling is that, despite the vast number of experimental and computational studies on sprays, the atomization processes including primary and secondary breakup are generally not known well enough for creating breakup models that would be generally applicable. The existing droplet breakup models are also difficult to validate in practice so that the attempt of making a 'realistic' simulation of a certain type of a spray system using the DPM becomes actually a very peculiar task. Yet, in order to carry out a larger scale simulation of e.g. combustion of diesel fuel, some type of droplet breakup models are needed which give a reasonable description of the physical spray and include the physical properties of the droplets. In this paper some of the properties of two droplet breakup models, the KHRT-model and the CAB-model are discussed and usefullness of the x-ray method for simulations considered.

1 Introduction

Despite the vast literature of experimental work on sprays, modeling the spray formation including primary and secondary breakup is still unclear. In principle, the atomization process can be viewed as a complex combination of inner nozzle disturbances and cavitation, exit velocity, fuel properties as well as the properties of the gas into which the spray is injected. From the viewpoint of the flow field, the fuel spray works as a fluctuating source of momentum. These factors couple to form the global spray that is often characterized in terms of parameters including the penetration depth, moments of the droplet size distribution and the spray opening angle [1]. These issues form a complex field of modeling that, to date, does not seem to possess general means of simulation.

In diesel engines the fuel spray is very dense near the nozzle orifice. In this region the spray has been reported to form a 'fragmented liquid core' implying a complex core structure including the presence of voids inside the core [2, 3]. These observations have been obtained by means of an x-ray technique. The x-rays are highly penetrative in the optically inaccessible regions of dense fluid and the technique can be used to give a line-of-sight spatial mass distribution of the spray, i.e. information about the spray structure may be obtained [4, 5, 7]. Since the x-rays pass the optically accessible regions in the spray periphery, the visual definition of the spray opening angle differs when measured with optical and x-ray methods the latter giving a much smaller value for the angle [1]-[5].

From the viewpoint of spray modeling using the DPM all experimental information is important for describing the boundary condition at the nozzle exit since, to date, there does not seem to be any other

common way of initializing the spray than injecting droplets according to an initial size distribution and solving the equations of motion 'normally' even in the dense spray region.. It has been suggested that in high pressure diesel sprays the spray would be completely atomized very close to the nozzle orifice so that the aerodynamic secondary breakup would actually have a minor role in contrast to what has been assumed earlier [1]. Recent evidence of some type of core fragmentation has been provided by these authors [5] where the x-ray method was used to study the near nozzle region of a mini-sac type heavy-duty injector with a single axial orifice. In the NTP conditions, a simple analysis of the line-of-sight mass distributions implied that, within the distance of the orifice diameter $\sim 0.2mm$ from the nozzle, the void fraction might be of the order of 30% or even higher.

A straighforward method of simulating spray dynamics is the Lagrangian particle tracking scheme i.e. the discrete particle method where the equation of motion is solved for each computational particle separately. This approach is believed to give a good description of the spray in the dilute spray regime if the grid spacing is large enough in comparison to droplet size whereas the approach becomes unavoidably non-physical near the nozzle exit where the spray is very dense. The most evident problems appear in the near nozzle region which needs to be modeled in someway even with the DPM. Typically, the confronted problems are omitted by discarding the fine details of the core itself for calculation of which the Eulerian-Eulerian framework would be needed and simply injecting droplets according to some representative initial size distribution and then letting the droplets traverse in the gas even in the dense spray region.

It is evident that in when it comes to droplet size distributions the x-ray method does not provide any information for modeling. However, it could be possible to extract other type of information such as near nozzle dynamics from the transient x-ray data to be used in conjunction with the DPM. Recently, the experimental studies carried out with the x-ray technique were compared with computations [5, 8]. These studies indicated that matching the x-ray results with the simulated values is not straightforward in the spray periphery and methods for improved adjustment have been suggested resulting in better matching of the experiments and computations [8]. Recent computational studies have made the picture of these findings more clear indicating that, indeed, the capability of the x-rays to capture the actual line-of-sight mass density would become soon weaker when moving away from the spray axis. Yet, these newest findings also clearly demonstrate that, the simulated and the experimentally measured centerline mass fluxes are in reasonable agreement [5]. The findings made in [5] make matching of the x-ray data i.e. mass distributions with the fuel mass distributions to be simulated somewhat questionable.

Motivated by the previous x-ray-related experimental and computational studies, in this work the usefullness of the x-ray data for spray modelling is critically discussed. In addition to this the modeling of the near nozzle region is discussed. The main objective is to demonstrate how two different secondary breakup models, the KHRT-model (Kelvin-Helmholz and Rayleigh-Taylor) and the CAB-model (Cascade Atomization and Breakup) behave in the near nozzle region and use the models for gaining deeper understanding on the issues related to atomization. As will be later discussed, the simulated situation has many non-physical features including the breakup models themselves. Thus, we basically aim at demonstrating how the models behave near the spray nozzle, what kind of qualitative behaviour can be seen from them and finally, we will draw some conclusions about the models and breakup modeling in general.

2 Experiments

Over the past few years, Argonne National Laboratory researchers have developed the x-ray radiographic technique to overcome the limitations of optical measurements in the near-nozzle region [4, 7]. Basically, the technique offers the means of creating the spatial line-of-sight mass distribution image of the spray by focusing a very thin monochromatic x-ray beam on the other side of the spray and then estimating the fuel mass within the beam volume by recording the intensity on the opposite side of the spray. The exponential relation $I/I_o = \exp(-\mu m)$ is assumed in this analysis where I is the recorded intensity, I_o the incoming intensity, μ the attenuation constant and m the evaluated mass/area. An example of such a distribution can be seen in the Figure 1. These images consist of hundreds of pixels each of which corresponds to an average over 50-60 successive measurements.

Initially, the spray chamber was filled with nitrogen and the pressurized to the NTP conditions.

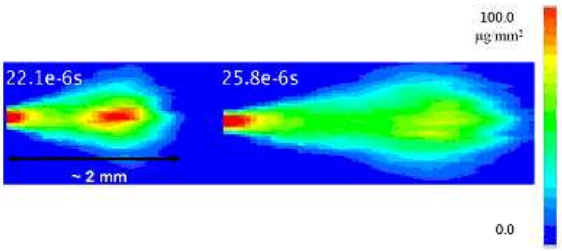

Figure 1: *Spatial eye-of-sight mass distribution. The red blobs correspond to mass density of approximately* $100\mu g/mm^2$ *whereas the large surrounding green regions corresponds to mass density of approximately* $50\mu g/mm^2$.

The orifice diameter of this heavy-duty injector was $d_o = 182\mu m$ and it was operated at 1000 bar injection pressure. The measured injection duration is $\sim 2.95ms$. The mass of the fluid injected during each experiment was $23mg$. As noted, the spray opening angle is difficult to deduce from x-ray data but a direct calculation from Figure 2 gives an estimate of $\sim 15deg$ and serves as a best guess. The viscosity of the calibration fluid is $2.45-2.75mm^2/s$ at $T = 313K$ whereas the surface tension is $29.9dynes/cm$. The density of the fluid is $0.820-0.830g/cm^3$. These values are fairly close to typical diesel values. We note that using these parameter values, including the amount of injected fuel, one would get about 6000 large droplets with diameter of the orifice if only large droplets were present.

It has been shown that the data at $z = 0.2mm$ fits well the ellipse $m \sim \sqrt{r_o^2 - r^2}$ which corresponds to the theoretical distribution of a smooth round liquid tube very close to the nozzle orifice with radius $r_o = 91\mu m$ [5]. Later on, around $z = 2mm$ the profile fits well with a Gaussian [7]. In this region the jet disintegrates and starts spreading apart. Using the system dimensions and the recorded mass value, an easy calculation shows that the density of the fluid would be $0.530g/cm^3$ at the nozzle exit implying the presence of voids [5]. Since the x-rays are highly penetrative we believe that what is actually seen in Figure 1 is a liquid core which is optically totally inaccessible. Basically, our current understanding on the x-ray method is that if a non-zero value of mass is obtained, then this part of the spray is indeed optically inaccessible and belongs to the liquid core.

Another question concerns secondary breakup: would it be possible that the spray would be almost completely atomized already in the near-nozzle region? Does an intact liquid core starting from the nozzle exit even exist? Since the transverse length scale varies only within a few nozzle diameters in Figure 1 and since the recorded mass is typically of the same order of magnitude within this region this information does not really seem to allow any straigthforward conclusions about complete atomization although in this respect it seems quite unlikely. One scenario would be the presence of an intact core and a surrounding dense cloud of droplets and fuel ligaments. On other hand, from the viewpoint of the DPM and spray modeling the x-ray method could be usefull; especially in finding out the lengthscales of the dense spray region where the DPM is definately not valid. Other issues, that could be found out with the x-ray method is for instance transient jet oscillation that, however, was not obtained here.

Our observations from this particular example indicated that the dense spray region observed with the x-ray method exceeded up to $10mm$ from the nozzle exit. This is a drastic observation since, in light of these considerations, it totally invalidates the use of the DPM near the nozzle exit for this particular case! The near nozzle region nor the related fluctuations reflected to the flow field can not be modeled by just injecting round droplets to the chamber and then using the spray as a momentum source originating from the drag force. This is basically more or less evident but they are typically not taken into account when using the DPM. We note that probably the mentioned problems are minor if there are dominating effects taking place in the simulations such as combustion. However, the near nozzle problems can not be omitted when moving on to LES where the flow field structure is essential and formed by the boundary conditions among many other things.

3 Fuel Spray Modeling

In this work a qualitative comparison between two breakup models, the KHRT model and the CAB model is made taking the guidelines from previous studies regarding the models and the parameters [5]. The KHRT and the CAB models have the capability to adapt the droplet sizes to fuel viscosity. The models were implemented to the simulation code KIVA3Vrel2 CFD-code designed especially for in-cylinder simulations of internal combustion en-

gines. The simulations of this work were carried out using the RNG k-ϵ-turbulence model as implemented to the KIVA3vRel2 code by Han and Reitz. The CAB model implementation follows the guidance given by Tanner whereas the KHRT implementation follows the guidance of Nordin [11]. No new parcels are created in the present implementation of the KHRT model used in this study.

The KHRT (Kelvin-Helmholz and Rayleigh-Taylor) breakup model has been developed by Reitz et al. and it is a well known and widely used breakup model in spray combustion simulations. The KHRT model is based on the idea of surface waves that can be formed on the droplet surface by two different mechanisms, the KH-mechanism which originates from shear velocity between gas and droplet or the RT-mechanism.originating from two interpenetrating fluids. The RT-mechanism is a large scale mechanism whereas the KH-mechanism accounts for the surface waves. The model is then based on defining the growth time scales Ω_{RT} and Ω_{KH} as well as the wavelengths Λ_{RT} and Λ_{KH} of the fastest growing waves. An issue to note is that the RT-mechanisms are assumed to be explicite functions of droplet acceleration so that $\Lambda_{RT} \propto a^{-1/2}$ and $\Omega_{RT} \propto a^{3/4}$ whereas the KH-mechanisms are explicite functions of Weber and Ohnesorge numbers and given in terms of correlation formulae. Thus both modeling mechanisms have their weaknesses: modeling of the KH-mechanism might fail if We and Oh are computed incorrectly whereas modeling of the RT-mechanism might fail if modeling of the drop acceleration fails. Thus, whatever the case, calculation of the momentum source term will have a major role in model functioning.

The magnitudes of the resulting droplets can be controlled with the model parameters. The KH-instability includes two model constants B_o and B_1 for controlling wavelength and the time constant respectively. Also the RT-instability contains two model constants C_2 and C_3 for controlling the time constant and the wavelength. In this work we give the constants the values $B_o = 0.61, B_1 = 1.0, C_2 = 1.0$ and $C_3 = 5.33$. Essentially, the point in the KHRT model is to consider that during each timestep a droplet may undergo a transition to the RT breakup mode. This 'deformation transition' may begin if the computed RT-wavelength is smaller than the droplet radius. As the deformation for a particular particle has started it's duration is being tracked and a RT-breakup may occur if the deformation time exceeds the RT-timescale. A KH-instability may occur at any time and since it's timescale is typically much smaller than the RT-timescale the mass stripped from the surface of the droplets may be calculated and taken into account. In this implementation of the KHRT-model no new parcels are produced.

The CAB model has been developed by Tanner [8] and it is based on viewing the droplet as a harmonic oscillator driven by the aerodynamics and damped by the surface tension and viscosity. The model is a modified version of the ETAB (Enhanced Taylor Analogy Breakup) model developed earlier by Tanner. The main differences between CAB and ETAB are the introduction of a new catastrophic breakup regime and omitting the model constant for spray angle. In a way, the CAB-model also tries to capture the presence of the fragmented liquid core by delaying the first breakup event using the model constant C_λ. We note that the CAB model has very many details that have been explained elsewhere [8]. The model can be viewed as an improved version of historical secondary breakup modeling development used for instance in the KIVA codes. Evidently, due to it's many details the CAB-model is quite artificial and deterministic model due to for instance the fact that the droplets are viewed as harmonic oscillators. Yet, it's advantage is to take into account the fact that a droplet may also regain it's stability and the breakup occurs only after a critical threshold transition deformation has occured. The CAB model has also been successfully used in earlier spray simulations with the KIVA3vRel2 CFD code and it has prooved out to be capable to describe different types of sprays and to adapt to fuel properties.

In this work the spray simulations were carried out in a polar mesh with cylinder geometry injecting the computational particles i.e. parcels from the other end of the chamber. Each parcel represents an ensemble of identical physical droplets with equal temperature, velocity and diameter. The parcels are tracked in the gas phase by solving the Newtonian equations of motion for each of the parcels separately. In this study the Weber number is based on the droplet radius and defined as $We = \frac{\rho_g |U - U_g|^2 r}{\sigma}$, where ρ_g is the gas density, r the droplet radius, $|U - U_g|$ the magnitude of the relative velocity between the phases and σ is the surface tension.

4 Results

In this Section we shall show some examples of typical near-nozzle simulations. The simulations

were carried out on a cylindrical mesh by injecting droplets from the other end of a closed cylinder [10]. The Figure 2 shows snapshots of the instantaneous spatial variation of droplet radii, Weber number between the KHRT- and the CAB-models and in the Figure 3 the same comparison is made between the radii and relative velocities from a given cut plane along the spray axis. A comparison between the panels (a) and (c) in Figure 2 demonstrates the clear difference between the CAB and the KHRT models: in the CAB model a power law initial size distribution is used for droplet sizes wheras in the KHRT model implementation all the injected droplets are of the same size. The initial size distribution of the CAB model manifests itself as a colorful mixture of droplet sizes in the Figure 2 (a).

As the spray penetrates deeper the droplets start breaking up at some characteristic distance $z \approx 0.8cm$ which can be controlled with the model parameter C_λ in the CAB model as seen in the Figure 2(a). Here this parameter was set to the value $C_\lambda = 1.5$. For this specific simulation case if C_λ is increased for instance to the value $C_\lambda = 5.5$ the breakup would begin much later around $z \approx 1.7cm$ [5]. As seen in the Figure 2(c) in the case of the KHRT-model the breakup process begins almost immediately from the nozzle and the droplets that are initially of the same size break very rapidly since the value of C_3 forces the RT-wavelength to be small. Around $z \approx 2cm$ both of the models contain rather much small droplets, yet there are also large droplets present in the case of the CAB model.

In Figures 2 and 3 the spatial variation for Weber numbers and relative velocities have been plotted. The most evident observation is that when comparing the KHRT and CAB models the magnitudes between Weber numbers and relative velocities differ in the spray region. In the KHRT-model the correlation pattern between the droplet radii and the mentioned quantities is clear. However, in the case of the CAB-model the correlation patterns are somewhat more complicated due to the initial size distribution that is changing the situation. Another observation is that the relative velocity and observed Weber number might be considerably different in the near nozzle region despite the same mass flux injected into the chamber. Since these issues are formed as a consequence of the spray momentum source term, this observation is closely related to the fact that the momentum transferred to the gas is calculated in an unphysical way. Namely, since the droplet drag coefficient depends strongly on it's radius, the computed acceleration terms will be affected and thereof the computed momentum source terms will depend on the initial size distribution. Then, if the secondary breakup model or a part of it is sensitive to e.g. We or acceleration, the result of the breakup cascade might be dependent on these issues.

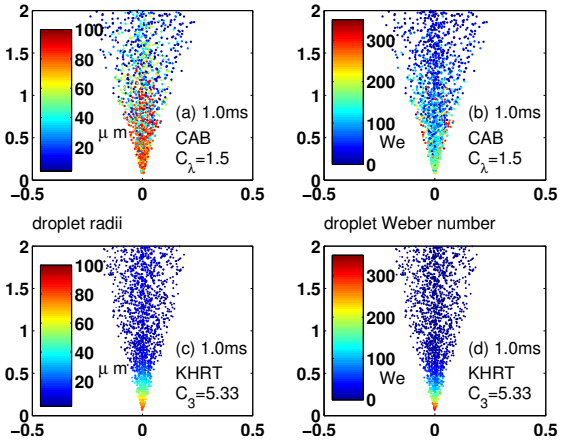

Figure 2: *The spatial distribution of droplet radii (left) and Weber numbers (right).*

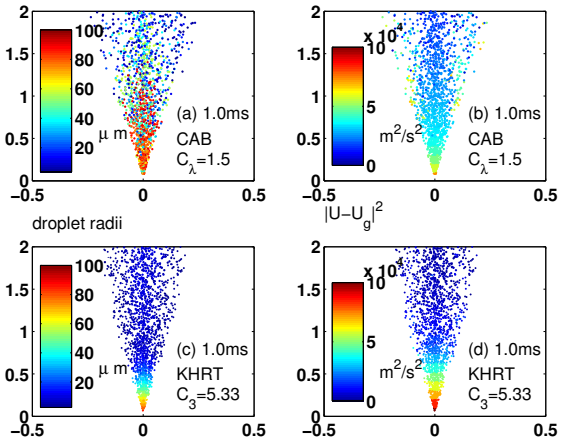

Figure 3: *The spatial distribution of droplet radii (left) and the square of relative velocity between the gas and droplets (right).*

5 Conclusions

When making a simulation of diesel combustion and choosing a suitable breakup model one should have an idea on the role of secondary breakup. Namely, if aerodynamics plays a major role in carrying out the secondary breakup, special emphasis should be

put on modeling the physics of the breakup cascade. It seems that in this case the breakup mechanisms of the KHRT model are closer to physics than those assumed in the implementation of the CAB model. In contrast, if secondary breakup due to aerodynamics is of a minor role which could be the case in high pressure atomizers [1] it could be enough to only make assumptions about the droplet size distribution in the whole spray. In that case it could be possible to even neglect the secondary breakup. Yet, the near-nozzle region would still need special attention.

This study has shown that there are many problems in the modeling of the near-nozzle region and using the DPM in this region. For instance, the momentum source term becomes calculated in a very vague manner if using the DPM near the nozzle where an intact liquid core could exist. In diesel sprays the core could be even $10mm$ long as noted in the x-ray experiments. This basically totally invalidates the modeling of the momentum source using the value of drag calculated with the spherical particle assumption. We also note that using a falsely calculated boundary condition might result in the whole flow field structure. It could be that these effects are not that important if there are dominating processes such as high temperature evaporation or combustion present or if a robust turbulence model such as the $k-\epsilon-$model is being used. However, the proper modeling of the nozzle boundary condition becomes more and more important when moving to LES that requires high spatial accuracy and that is philosophically quite different from the $k-\epsilon-$framework.

We note that these simulations have mainly served as an aid for developing further ideas for carrying out a successfull spray simulation. We believe that an important principle that should be kept in mind in further spray modeling would be to keep the breakup models simple. The KHRT-model is a very promising candidate since it basically offers the two main breakup mechanisms for breakup modeling. These mechanisms are related to initializing droplet distortion which is an important issue that should be looked at in the context of secondary breakup in contrast to e.g. the droplet shape. Making 'realistic' spray simulation would require time and space accurate calculations such as LES. In the future studies special emphasis in our laboratory will be put on developing and studying spray boundary conditions with the DPM and developing a LES environment for realistic simulations of fuel sprays.

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