Reduction of Numerical Parameter Dependencies in Diesel Spray Models

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Abstract
Numerical grid and time-step-dependencies of Discrete Droplet Lagrangian spray models are identified. The two main sources of grid-dependency are due to errors in predicting the droplet-gas relative velocity, and errors in describing droplet-droplet collision and coalescence processes. For reducing grid-dependency due to the relative velocity effects, gas jet theory is proposed and applied to model diesel sprays. For the time-step dependency, it is identified that the collision sub-model results in drop size variation in the standard spray model. A proposed spray model based on the gas-jet theory is found to improve the time-step independency also along with the mesh independency. The use of both Eulerian (collision mesh) and Lagrangian (radius of influence) collision models along with gas-jet theory is found to provide mesh-independent results.

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Introduction

Sprays have been widely modeled by Lagrangian-Drop and Eulerian-Fluid (LDEF) and Eulerian-Liquid-Eulerian-Gas (two-fluid) models. Both the models predict spray structure, penetration and drop sizes for coarse CFD meshes. In both models, near nozzle resolution of the flow is required down to the order of the injector-hole size for better spray predictions. As the near nozzle resolution is reduced, the prediction becomes poorer. For large bore engines, for example Smarine engines, the nozzle diameter are few hundred microns and the bore size is few hundred millimeters. Hence, a coarser mesh size for a small engine might be the finest practical mesh size for a large bore engine. Hence, it becomes important to achieve fairly mesh-independent spray models if they are to be universally applicable. The present study we have adopts the LDEF method, which is already implemented in KIVA-3V [1] and a range of uniform mesh sizes from 1D to 16D is considered, where D is the nozzle diameter. The standard LDEF method over-predicts spray tip penetration for a fine mesh resolution of the order of nozzle diameter (~1D). This was found to be due to the ineffectiveness of the collision model at this scale. The smaller drop sizes impart higher rates of momentum transfer in the near nozzle resulting in high entrainment rates and hence the over-penetration. As the mesh is coarsened to the order of 4-6D, the penetration prediction improves due to an increase in the effectiveness of the collision model with its better prediction of drop sizes. Further coarsening of mesh to the order of 8-16D again predicts poor spray penetration due to the fact that momentum coupling between the droplets and gas phase becomes poor. Thus, there is an optimum mesh size that gives a minimum error in spray penetration when the error in both the collision and momentum coupling is exhibited through droplet drag.

Another inherent modeling issue is time-step independency which has rarely been reported in the literature. It is found that the O’Rourke collision model [2] is time-step dependent if it follows the assumed Poisson process. This is because the collision model is called at every new time-step of the simulation. Hence, for a fine time-step, the total number of collisions can exceed that obtained for a coarser time-step for the same elapsed time. So in the case of a fine-step, drop sizes can be larger due to the increase in the number of coalescences.

The atomization model employed in LDEF models popularly is based on considerations of Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT breakup) instabilities [4, 5]. Grid-dependency of spray models has been studied by Abraham [6] and Post et al. [7] who suggest that the nozzle region must be adequately resolved for obtaining an accurate prediction of the spray structure. Schmidt [8, 9] improved the O’Rourke and Bracco collision model by using a separate collision mesh, and further sampled collision partners so as to speed-up collision computations using the “no-time counter” (NTC) approach. Nordin [10] proposed a semi-deterministic collision model, wherein the droplets do not collide at all if they are traveling in opposite directions. For the momentum coupling between the two phases Beard et al. [11] identified that the relative velocity between the two phases can be mesh dependent and results in incorrect penetration predictions. They proposed a method to correct the relative velocity which is based on an expanding radius of influence concept between droplets and gas. Lippert et al. [12] proposed resolving the flow-field by using an adaptive mesh which resolves the near nozzle region finely enough to predict accurate spray structures. They also used a separate collision mesh based on the NTC model. However use of extra cells near the nozzle means significantly increasing computation times.

In the present model no extra cells are added as per the adaptive mesh technique. Instead it is proposed that the air entrainment can be modeled according to gas jet theory [13, 14]. With this information the axial component of the droplet relative velocity is corrected using the assumption that the relative velocity is that of the liquid droplet in a gas jet. This corrects the momentum exchange between the droplets and the gas phase, and is independent of mesh resolution. To prove the concept, a fixed collision mesh and the standard O’Rourke and Bracco collision model is used first. That is, for all CFD mesh sizes, a separate collision mesh is considered as previously suggested [7, 8, and 11]. This separates consideration of collisional processes from mesh resolution issues. The results show that the mesh dependency is greatly reduced in terms of spray penetration, drop size, number of parcels and the spray structure. Next, an improved collision treatment is proposed that dynamically computes the collision process without the need for a separate collision mesh.

Diesel Spray Model

The basic idea of the present model is depicted in figure 1. The spray flow has two components; the group of droplets which forms the liquid phase and the air entrained which forms the gas phase. For grid-independency either of the phases could be corrected since they are coupled by their respective transport equations. Previous researchers have focused on minimizing errors in the liquid phase [10, 11], but with corrections mostly based on intuition and have not been tested and proved enough to work at different conditions. Others have increase the accuracy of the gas
phase prediction with increased mesh refinement at the cost of increased computational time [12].

The LDEF stochastic spray model considers a group of identical droplets known as a drop parcel which is tracked in a Lagrangian approach. The gas phase is modeled using an Eulerian approach. The conservation equation for a droplet parcel is represented by the conservation equation of a single droplet in that parcel. As mentioned above, the axial component of the gas phase velocity in the droplet equations is modeled using gas-jet theory. Hence the droplet momentum equation is given as:

\[
\frac{d\mathbf{U}}{dt} = \frac{3}{8} C_D \frac{\rho_s}{\rho_l} \frac{1}{D} \left( \hat{\mathbf{U}} - \mathbf{V}_{\text{gas}} \right) \left( \hat{\mathbf{U}} - \hat{\mathbf{V}}_{\text{gas}} \right)
\]  

(1)

where \( \mathbf{U} \) is the droplet velocity vector, \( D \) is the drop diameter and \( \mathbf{V}_{\text{gas}} \) is the surrounding gas phase velocity vector. The drag coefficient, \( C_D \), is assumed to be a function of droplet Reynolds number [1]. \( V \) is given as \( V = (V_x, V_y, V_z) \). \( V_x \) and \( V_y \) are the perpendicular components of the surrounding gas-phase velocity obtained from the CFD solution and the axial component (considered as the z-direction here) is given by gas-jet theory as [13, 14]:

\[
V_{\text{gas}} = \min \left( U_{\text{inj}}, \sqrt{\frac{3 U_x^2 d_{\text{eq}}^2}{32 \nu_t^2 \left( 1 + \frac{3 U_x^2 d_{\text{eq}}^2 r^2}{256 \nu_t^2 z^2} \right)^2}} \right)
\]

(2)

where \( U_{\text{inj}} \) is the injection velocity of the liquid-jet which is also assumed to be the injection velocity of the gas-jet. \( z \) is the axial distance of the droplet parcel from the injector tip and \( r \) is the radial distance of the parcel from the spray axis. Thus, the relative velocity between the droplets and the gas phase in the near-nozzle region is zero. \( d_{\text{eq}} \) is the equivalent diameter of the gas jet defined as [13]:

\[
d_{\text{eq}} = d_{\text{nec}} \sqrt{\frac{\rho_l}{\rho_g}}
\]

(3)

where \( d_{\text{nec}} \) is the effective nozzle diameter and \( \rho_l \) and \( \rho_g \) are the liquid and gas-phase densities, respectively. \( \nu_t \) is the turbulent viscosity for jets given as [13]:

\[
\nu_t = C_t \pi^{0.5} U_{\text{inj}} d_{\text{eq}} / 2
\]

(4)

\( C_t \) is the entrainment constant, as reported by Abraham [13] who used \( C_t = 0.0161 \). In the present case \( C_t = 0.0247 \) was selected by trial and error to optimize predictions of spray tip penetration.

The momentum lost by the droplets due to drag is gained by the surrounding gas-phase through the source terms in the conservation equations. The axial component of the source terms is modeled using the modified relative velocity with Eq. 2. The droplet-gas relative velocity is modeled in this way everywhere except in the spray (KH-RT) break-up model. This is because if the relative velocity is very low near the nozzle, then the predicted breakup would be slow and the droplet size large. Thus, for the break-up model only, the gas phase velocity from the CFD prediction is considered. This is also justified by the fact that the gas-jet theory is based on a quasi-steady assumption. Hence, the velocity given by Eq. 2 only applies after some time. Since there is no simple way to evaluate what fraction of the quasi-steady state velocity causes break-up, the surrounding gas velocity from the CFD mesh is used to represent the external force in the jet breakup.

The collision model is based on O’Rourke’s Model [2, 3] that allows collision of droplets located in a collision cell that is traditionally considered to be the CFD cell itself. However this gives rise to further mesh-dependency. Hence, we first adopt the proposal of Schmidt [8] of using a separate collision mesh (but without the NTC algorithm). To study mesh-dependency related to drop drag, we use a single collision mesh for all CFD meshes considered.

If the size of the collision mesh is small, there will be fewer potential collision partners for a parcel and there may even be no collisions at all if the mesh-size is of the order of the drop diameter. A large collision mesh size will give numerous coalescences but breakup of the resulting large drops is expected due to RT-breakup mechanism. Hence, collision mesh size was selected based on a sensitivity study, as will be discussed later in the results section. As a second approach, we also consider use of a collision cut-off distance for the parcel as a criterion to decide whether two parcels should collide, as is the practice in molecular dynamic simulations [15]. This is a Lagrangian Collision Model based on each droplet’s position, as opposed to the traditional collision model that was a fixed collision mesh (Eulerian). This is an important consideration in non-uniform injection cases. This cut-off distance (henceforth termed ‘radius of influence’ (ROI)) of a parcel is the distance to the most distant parcel that can collide with it in the present time step. There are many ways to estimate ROI. In one approach, the computation of radius of influence involves checking whether the distance \( x_{rel} \) between a parcel and its collision partner is such that,
\[ x_{rel} \leq u_{rel}dt , \]  

where \( u_{rel} \) is the relative velocity between the drops and \( dt \) is the computational time step. Another approach would be to use a completely deterministic model with contact time estimation [16]. In the present study, the radius of influence was estimated as follows. For each gas-phase computational cell, the mean and standard deviations of velocities of the drops within the cell are estimated. Then, the velocity of a fictitious representative parcel \( (u_{fic}) \) is calculated assuming a Gaussian distribution of drop velocities within the cell. The distance that this parcel will have to travel in order to collide with a parcel that has equal, but opposite velocity is \( 2u_{fic} dt \), is used as the characteristic collision distance for all the parcels contained in that cell.

**Experimental Conditions**

A constant volume chamber experiment by Naber and Siebers [17] was considered in the present study. Only non-evaporative conditions were used to compare with the computational results. Experimental data corresponding to a range of ambient densities was considered. The injection profile is uniform and more details are given in Table 1.

**Computational Mesh and time-step details**

Six two-dimensional and uniform computational meshes were considered with cell sizes of 4 x 4, 3 x 3, 2 x 2, 1 x 1, 0.5 x 0.5, 0.25 x 0.25, mm² respectively. The separate collision mesh had, a uniform cell size of 4 x 4 mm², which was chosen based on sensitivity study of collision mesh size. If the standard CFD (standard KIVA) cell size is considered, then for the fine mesh of 0.25 x 0.25 mm² there would be very few collision partners and hence, the predicted drop sizes could be very small. KIVA-3V [1] is used for the computations with the modifications of the new model implemented. The 2-D mesh is a cylindrical mesh with a 0.5 degree sector. The dimensions of the domain are 10 cm in the axial direction and 4 cm in the radial direction.

For the different CFD mesh sizes, a time-step of 1 \( \mu \)s was used. For time-step sensitivity studies, five different time steps were used, namely 10, 5, 1, 0.5 and 0.1 \( \mu \)s. The time-step study was done on the 4 x 4 mm² mesh after establishing mesh independency.

**Results and Discussion**

Results for mesh and time-step dependency are presented separately. First results from the standard KIVA/LDEF code are presented and the sub-models are identified that cause mesh dependency. The discussion and comparison of mesh dependency is based on comparison of spray tip penetration (defined as the location from the nozzle of the leading droplet comprising 95% liquid mass in the domain), overall Sauter-mean diameter, (i.e., the average drop size of all drops in the spray, regardless of their location), the number of drop parcels in the domain and the spray structure. In the same section we discuss the sensitivity of the collision mesh and chose a collision mesh size based on this sensitivity study. Results of the improved model with a collision mesh and the radius of influence are presented next. Then the improved results from the new model are presented and compared with the standard KIVA results.

A. Mesh Independency:

1. **Standard KIVA/LDEF results:**

   Results from the standard KIVA models for the six different mesh sizes showed significant mesh dependency. Figure 2 shows the spray structure at \( t=3 \) ms after the beginning of injection and Fig. 3 shows the spray tip penetration as a function of time compared with the experimental penetration. The 4 x 4 mm² mesh shows an under-predicted tip-penetration and the fine mesh (0.25 x 0.25 mm²) shows over-predicted penetration. Figure 3 shows the predicted overall drop size and Fig. 4 shows the total number of parcels in the chamber. It can be observed that the drop sizes are reduced as the mesh size is reduced. This is because with the reduction in mesh size, the number of collisions gets reduced. In the limit of 0.25 x 0.25 mm², the collision model becomes in-effective and the predicted drop size become of the order of 1 micron. The total number of parcels increases for the smaller sized mesh due to fewer coalescences, and effects due to collision with the bottom wall beyond \( t=1.5 \) ms.

   The over-penetration at small mesh size can be explained as follows. The small drops produced after break-up do not collide and coalesce if collision cell is confined to the small CFD cell. Thus, in the vicinity of nozzle, large numbers of smaller drops exist having large momentum (equal to the jet momentum). These smaller drops are also subjected to higher drag forces and lose their momentum in a small distance from the nozzle. This results in higher gas-phase momentum near the nozzle which causes the liquid droplets being injected at later times to over-penetrate. This is a cumulative process from the injector location to positions downstream of the injector. Hence, the gas-phase momentum or the air entrainment rate is over-predicted for the fine mesh case as a consequence of the ineffectiveness of the collision model.

   In case of the coarse mesh (4 x 4 mm²), the spray tip penetration is under-predicted, even though the drop sizes are not unreasonably low. This is due to the fact that the gas-phase momentum is under-predicted and results in incorrect penetration. However, in a large cell the group of droplets exhibits little transfer of mo-
mentum to the gas, leading to over-prediction of droplet-drag.

Thus, a correct prediction of the gas-phase momentum is crucial in order to get accurate spray tip penetration. The collision model also affects the drop size, and to overcome this problem the improved model is presented using a separate collision mesh of a uniform cell size of 4 x 4 mm$^2$.

2. Sensitivity study of collision Mesh:

The improved spray model was studied at different collision mesh size keeping the same CFD mesh. This would lead to the sensitivity of the collision mesh size on the drop sizes. 9 different collision mesh sizes were chosen, with smallest collision mesh size of 2 x 2 mm$^2$ and largest being 10 x 10 mm$^2$. The results show that after about the size of 4 x 4 mm$^2$ there is less variation in drop sizes, as shown in Fig. 6. Figure 7 shows a bar-chart of total number of coalescences with increase in collision mesh size. As can be observed, after about 4 x 4 mm$^2$ collision mesh size, the slope of increase in the total number of coalescences is constant. At the same time Fig. 7 shows that there is no significant increase in the drop size with increase in collision mesh size. This is due to a balance between the RT-breakup and coalescence that produces nearly the same drop size. Thus, a collision mesh of 4 x 4 mm$^2$ was chosen.

3.a Improved Diesel Spray Model results with collision mesh:

The improved spray model assumes that air entrainment can be modeled as a gas-jet. This at least ensures that the correct gas-phase momentum is used and hence a better prediction of the droplet relative velocity results. As discussed earlier, only the axial component of the droplet relative velocity is corrected based on the gas-jet theory.

Figure 8 shows details of the spray structure at t=3.0 ms for $\rho_{amb}=60.6$ kg/m$^3$. Figure 9 shows the predicted spray tip penetrations as a function of time. Both figures show vastly improved mesh-independency in the spray structure and penetration as compared to the standard KIVA/LDEF model. Since the collision mesh is same for all six CFD meshes, the effect of the collision model is eliminated. The drop size and total number of parcels are shown in Fig. 10 and Fig. 11 and also show improved grid-independency. In particular, the fine mesh case does not predict unreasonably small drop sizes, as observed for standard KIVA/LDEF models. Thus, it can be concluded that using the gas-jet theory in conjunction with a consistent/separate collision mesh, mesh-independent results can be obtained.

3.b Improved Diesel Spray Model results with collision Radius of Influence (ROI):

The radius of influence was selected based on the collision mesh sensitivity results. In the previous section it was found that the collision mesh of 4x4 mm$^2$ and above is insensitive to the spray drop size primarily due to a balance achieved in the RT-breakup and coalescences. The similar idea of a separate collisional volume was extended for the Lagrangian approach of considering a radius of influence of 2mm which is half the size of chosen collisional mesh size, i.e. 4x4 mm$^2$.

Figure 12 shows the spray tip penetration with the improved spray model and the collisional radius of influence. The spray tip penetration shows mesh-independent results. Figure 13 shows the corresponding drop size variation with difference CFD mesh sizes with the ROI collision model. The drop size variation is less as compared to the standard LDEF/KIVA case.

B. Time-step Independency:

After establishing mesh-independent results using gas-jet theory and the fixed and ROI collision meshes, an assessment of time-step dependency was made. First results from standard KIVA are presented for the five different time-steps (10 to 0.1 $\mu$s). Only the coarse mesh was used since the new model was proved in the previous sections to be fairly mesh-independent.

1. Standard KIVA/LDEF results:

The results from standard KIVA help to identify the sub-models responsible for the observed time-step dependency seen in Fig. 14. A non-linear trend is seen where, for $\Delta t = 1 \mu$s the spray tip penetration is maximum and for finer and coarser time-steps, the tip-penetration reduces, respectively. Figure 15 shows the drop sizes and the time-step has a major effect. For smaller time-steps, the drop sizes are larger as compared to those at the coarser-time steps. This is due to the fact that the collision model is based on the assumed Poisson distribution. For finer time-steps, the collision model repeatedly calculates collisions each time-step increment. For the same number of droplets, more collisions and coalescences result. This results in an increase in droplet size for finer time-steps. For the range of coarser-time steps between 1 and 10 $\mu$s, this trend is not very severe. Figure 16 shows the number of parcels in the domain. Using a fine time-step results in fewer parcels as more coalescence takes place. Thus, it can be concluded that for the standard KIVA/LDEF spray model using a very fine time-step will result in fewer parcels and large drop sizes. This can be critical for evaporating sprays (not considered in the present study).
2. Improved Diesel Spray Model results:
The improved model predicts a more accurate relative velocity between the droplets and gas and also utilizes a separate collision mesh. Thus, at any given instant of time, irrespective of mesh size, the relative location of droplets will be same. This results in mesh-independency. For the time-step independency, the model is also expected to give an accurate prediction of spray-tip penetration. Figure 17 shows the spray tip-penetration and provides a relatively good prediction at all time-steps. Figure 18 shows the drop size. The variation of overall SMD is reduced considerably as compared to the standard KIVA case (Fig. 11). This is due to the fact that the air entrainment is modeled consistently and thus, for two droplets as potential collision partners, the droplet-droplet relative velocity is the same irrespective of the time-step. This ensures a more consistent outcome of the collision model at different time-steps as compared to the standard KIVA/LDEF model. Figure 19 shows the total number of parcels in the chamber. The variation in number of parcels is not as pronounced at different time-steps as compared to the standard KIVA results.

Conclusions
A new spray model based on the assumption that the component of the gas velocity in the spray direction can be imposed using gas-jet theory has been implemented and tested with the standard KIVA/LDEF methodology. The model predicts more accurately the relative velocity of the droplets and gas and also gives improved entrainment rate predictions. For the spray, mesh-independency over meshes in the size range of 1 to 16 times the nozzle diameter has been demonstrated in terms of spray tip-penetration, drop size, number of parcels and spray structure. The improved spray model was also tested with a separate collision mesh and a radius of influence approach surrounding the droplets. Both the models reasonably predict mesh-independent spray predictions. It is believed that for a non-uniform spray injection (not studied here), the radius of influence approach will give better spray predictions and will be the focus of future work.

Time-step dependency of LDEF spray models is rarely investigated. It was observed that time-step dependency of standard LDEF models results in large variations in predicted drop sizes, primarily due to the collision model. For small time-steps, the collision model predicts increased collision and coalescences and hence the average drop sizes are larger as compared to those with coarser time-steps. However, the new spray model also reduces the time-step dependency. This is because the droplet-droplet relative velocity is also more accurately predicted and hence coalescences are not over predicted. The time-step dependency of LDEF models is critical for evaporative spray predictions and will be the focus of future research to further improve the time and mesh independency.

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References
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Table 1: Experimental data by Naber and Siebers [17]: Non-evaporative conditions.

![Schematic of New Diesel Spray Model](image1)

**Figure 1.** Schematic of New Diesel Spray Model.

![Standard KIVA: Spray Structure at t=3.0 ms. $\rho_{amb} = 60.6\text{ kg/m}^3$](image2)

**Figure 2.** Standard KIVA: Spray Structure at $t=3.0$ ms. $\rho_{amb} = 60.6\text{ kg/m}^3$
Figure 3. Standard KIVA: Spray Tip Penetration. Experimental data from [14], $\rho_{\text{amb}} = 60.6 \text{ kg/m}^3$

Figure 4. Standard KIVA: Overall Sauter Mean Diameter. $\rho_{\text{amb}} = 60.6 \text{ kg/m}^3$
Figure 5. Standard KIVA: Total number of Parcels. $\rho_{\text{amb}} = 60.6 \text{ kg/m}^3$
**Figure 7.** Total number of coalescences in the domain with increase in collision meshes size

**Figure 8.** Improved model: Spray Structure at t=3.0 ms.
Figure 9. Improved Model: Spray Tip Penetration. Experimental data from [14], $\rho_{\text{amb}} = 60.6$ kg/m$^3$.

Figure 10. Improved Model: Overall Sauter Mean Diameter. $\rho_{\text{amb}} = 60.6$ kg/m$^3$. 

Figure 11. Improved Model: Total number of parcels. $\rho_{\text{amb}} = 60.6 \text{ kg/m}^3$

Figure 12. Improved Model (ROI collision model): Spray Tip Penetration, $\rho_{\text{amb}} = 60.6 \text{ kg/m}^3$
Figure 13. Improved Model with ROI collision model: Overall Sauter Mean Diameter, $\rho_{\text{amb}} = 60.6 \, \text{kg/m}^3$

Figure 14. Standard KIVA: Spray Tip Penetration at different time-steps. (4x4 mm mesh).
**Figure 15.** Standard KIVA: Overall SMD at different time-steps. (4x4 mm mesh).

**Figure 16.** Standard KIVA: Total number of parcels at different time-steps. (4x4 mm mesh).
Figure 17. Improved Spray Model: Spray Tip Penetration at different time-steps. (4x4 mm mesh).

Figure 18. Improved Spray Model: Overall SMD at different time-steps. (4x4 mm mesh).
Figure 19. Improved Spray Model: Total number of parcels at different time-steps. (4x4 mm mesh).