Improvement of the grid dependency of the momentum coupling and the droplet collision modeling in the Arbitrary Lagrangian-Eulerian method for spray simulations

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Abstract

In the simulation of liquid spray penetrating into gaseous phase, the conventional computational fluid dynamic (CFD) code adopts the Arbitrary Lagran-gian-Eulerian (ALE) method. In this ap-proach, the continuous gaseous phase is calculated in the Eulerian view point by solving the conservation equation of mass, momentum and energy, and the dispersed liquid particles are tracked in the Lagrangian view point. This algorithm has been proved to be very useful for IC engine spray simulations. However the ALE method has inherent grid dependency problem causing serious numerical errors. The grid dependency is generally induced when calculating the momentum coupling between gaseous and liquid phases, and applying the droplet collision algo-rithm. Thus, this study investigates the strategies for reducing the grid sensitivity involved in the momentum coupling and the droplet collision modeling. In order to achieve the goals, the gas-jet model was implemented in the KIVA code, and the calculated results were compared to the ap-propriate experimental results. Then the feasibility of the models for the spray simulations was discussed. In addition, the advanced algorithm of the droplet collision modeling which can over-come the grid dependency problem was applied to the KIVA code. By simultaneously consider-ing the momentum coupling and the collision modeling, successful reduction of the grid sensitiv-ity could be accomplished in the prediction of spray pene-tration and Sauter Mean Diameter (SMD)

Introduction

Spray dynamics has a multiphase and the complicated physical phenomena such as ambient gas dynamics, liquid droplet breakup, heat and mass transfer, and momentum transfer between two different phases. With its phenomenological consideration, the spray must be described by distinguishing between gas phase and liquid phase. The gas phase can be described in a continuum because its quantities change continuously in space. On the other hand, the liquid phase exist as a disperse phase, accordingly the density of the fluid is zero in the volume between gas and liquid elements. Especially in the high-compressed injection spray, the liquids remain as a number of droplets. For this reason, two phases must be dealt with different way in the CFD method in order to get reasonable simulation results. With this consideration, the Arbitrary Lagrangian-Eulerian (ALE) method has been commonly used to simulate the spray penetrating into gaseous atmosphere. In this method, the quantities of continuous gas phase are solved using the Navier-Stokes equations in an Eulerian view point. On the other side, since the Eulerian formulation is not appropriate for the description of the liquid phase because of no continuum, the Lagrangian description is used. In this point of view, the droplets are treated individually by tracking their exact position. Their quantities such as size, velocity, and temperature are resolved by sub-models that considers breakup and collision, aerodynamic droplet drag and evaporation. Then, some quantities of both phases are coupled by source terms in the conservation equations of the gas phase because they always transfer their mass, momentum, and energy each other.

In the use of CFD for spray simulations, it is well known that the predicted results are relatively sensitive to the mesh size [1], because the Eulerian field can not be properly computed in the vicinity of liquid droplets due to the inadequate space resolution. In such a diesel engine simulation, the nozzle diameters are a few hundred micrometers, while the bore size of engine cylinder generally has tends of thousands times of nozzle diameter. For this reason, the maximum grid resolution that is practically feasible in the vicinity of nozzle is limited by the expensive computational cost. The inaccurate grid resolution causes an over-estimation of diffusion, resulting in inaccuracies in calculation of the source terms in the Eulerian phase. Then the inaccurate gas quantities bring in erroneous calculations of droplet sub-models, i.e. droplet drag model and breakup model.

In the droplet collision modeling, O'Rourke's collision model [2] is currently the standard model for Lagrangian spray simulations and widely used because the model does not have a high computational cost. But many researchers have reported that the model has some serious problem on the impractical collision regimes and the grid

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dependency. In order to solve the problems, numerous researchers [3,4,5] have developed alternative collision models which reduce the grid sensitivity and enhance the prediction of practical collision regimes.

This study shows the issues of improving the numerical accuracies with consideration of the grid sensitivity and the droplet collision modeling. First, in order to reduce the grid dependencies, momentum transfer between droplets and gas phase was modeled using the gas-jet model [6] and the Nordin's concept [3] for droplet collision. In addition, to consider the practical droplet collision phenomena, the Munnannur's collision model [5] was used. The computation was conducted for high-pressure diesel injection by implementing the models in the KIVA-3V code [7].

Numerical concepts for standard KIVA simulation

Standard KIVA code [7] solves mass and momentum conservation equations for continuous gas phase. Eqs. (1) and (2) have source terms that describe the effect of liquid particle presence and the chemical reaction. Eq. (1) assumes that all evaporated and chemically reacted mass from fuel droplets is distributed within a cell containing the droplets. In the same way, the momentum gain from the spray is assumed to be uniformly distributed over the cell. Thus, this possibly causes the spray evolution to be dependent on grid size.

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_V \rho_g \mathrm{d}V = \int_V \dot{\rho}_g^{\mathrm{spray}} \mathrm{d}V + \int_V \dot{\rho}_g^{\mathrm{chem}} \mathrm{d}V \qquad (1)$$

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_V \rho_g \mathbf{u} \mathrm{d}V = \int_S p\mathbf{n}\cdot\mathrm{d}\mathbf{A} + \int_S \boldsymbol{\sigma}\cdot\mathrm{d}\mathbf{A} + \int_V \mathbf{F}^{\mathrm{spray}} \mathrm{d}V + \int_V \rho_g \mathbf{g} \mathrm{d}V \qquad (2)$$

The momentum source term due to spray is solved by integrating the drag force of all the droplets contained in a cell. The droplet drag effect is represented by the droplet momentum equation given as:

$$\frac{du_l}{dt} = \frac{3}{8} C_D \frac{\rho_g}{\rho_l} \frac{1}{D}\left(u_l - u_g\right) \qquad (3)$$

where u_l and D is the droplet velocity and diameter, respectively. The droplet drag coefficient C_D is a function of drag coefficient of a sphere and droplet deformation quantity.

In the standard KIVA code, the binary droplet collision is described using the O'Rourke's model. The model follows the statistical approach in determining the collision probability and assumes that the collision occurs only if two droplets lie in the same computational cell. Once two droplets are in a cell, the probability of no collision, Eq. (4), is checked creating random number between 0 and 1. If the collision probability is satisfied, the collision regime is determined statistically according to the condition of Brazier-Smith et al. [8]. In this model, only two main outcomes, i.e. coalescence and stretching separation, are regarded.

$$P_0 = \exp\left(-\frac{N_2}{V_{cell}} \frac{\pi}{4} (d_1 + d_2)^2 U_{12} \Delta t\right) \qquad (4)$$

Modification of KIVA code

Gas-jet model

In order to reduce the inaccuracy of the momentum coupling, the gas-jet model [6] was implemented in the KIVA code. In contrast to the original concept, the axial component of the ambient gas velocity in the droplet momentum equation, Eq. (3), is modeled by gas-jet theory [9] as:

$$U_{axis} = \min\left[U_{inj}, 3U_{inj}^2 d_{eq}^2 \Big/ \left[32\nu_t x\left(1 + \frac{3U_{inj}^2 d_{eq}^2 r^2}{256\nu_t^2 x^2}\right)^2\right]\right] \qquad (5)$$

where U_{inj} is the injection velocity of the liquid jet and d_{eq} is the equivalent diameter of the gas jet defined as $d_{eq} = d_{noz}\sqrt{\rho_l / \rho_g}$, and ν_t is the turbulent viscosity. Using this relation, the droplet-gas relative velocity in the

KIVA code is calculated except in the droplet breakup model. On the other hand, the momentum lost by the droplets due to drag is gained by the surrounding gas phase through the conservation equations in the same way with the standard ALE method.

Nordin's mesh independent collision model

Nordin suggested a model that collision between two parcels occurs if their trajectories intersect and the intersection point is reached within an integration time step at the same time. In this model, the collision is assumed to occur if following two requirements are satisfied:

$$| \vec{u}_{12} | = (\vec{u}_2 - \vec{u}_1) \cdot \frac{(\vec{p}_2 - \vec{p}_1)}{| \vec{p}_2 - \vec{p}_1 |} < 0 \text{ , and } | \vec{u}_{12} | \Delta t > | \vec{p}_2 - \vec{p}_1 | - (r_1 + r_2) \quad (7)$$

Munnannur's fragmenting droplet collision model

Munnannur and Reitz [5] developed a collision model that focuses particularly on the fragmentation in stretching separation and reflexive separation. They modeled the fragmentation and the formation of satellite droplets under the assumption that the interacting droplets form an elongating ligament that breaks up into smaller droplets. The model regards all the possible outcomes, i.e. coalescence, bounce, stretching separation, and reflexive separation.

Rate of Influence (ROI) model

The ROI model suggested by Munnannur [10] is a concept for searching collision partners. While the O'Rourke's model causes the grid dependency due to the statistical determination of collision probability based on the grid cell size, this model introduces a collision cut-off distance for individual parcels to determine whether two droplets could collide. In this study, the cut-off distance for all the parcels was chosen as 2 mm.

Test conditions for high pressure diesel injection

The computational test condition was referred to the experimental condition [11]. In order to validate the grid independent models, predictions of spray tip penetration and Sauter mean diameter (SMD) were compared to the experimental results. The test was conducted at two-dimensional mesh and three different grid resolutions were selected as 2x2 mm^2, 3x3 mm^2, and 4x4 mm^2. The 2-D mesh is a cylindrical mesh with a 0.5 degree sector. For comparison of results of the different CFD mesh size, a time-step of 2 μs was used.

Results and discussions

Results of standard KIVA code

Fig. 1 shows the calculated spray shapes at t =3 ms after start of injection and tip penetration as a function of time according to the different grid resolutions in the case of standard KIVA code. As the grid resolution becomes lower, the spray tip penetration is longer. Thus it can be found that the uniform distribution of the momentum gain over the cell volume leads to an unphysical diffusion momentum. If the cell volume is large, the change of gas velocity due to the momentum transfer becomes small, then the relative velocity between gas and next coming droplets is high. The high relative velocity causes the high drag force and decelerates the droplet velocity. This phenomenon can be found in Fig. 3. Therefore the spray tip penetration becomes shorter with lower grid resolutions. Fig. 4 is the local distribution of SMD according to the axial distance. The result of turned off collision model case shows the grid dependency of standard momentum coupling method with no effect of collision model concept. As can be seen here, in the case of the smaller the mesh size, the fewer droplets are atomized. The reason is the same with that of spray tip penetration results. The higher gas velocity gives rise to reduce the lower relative velocity, resulting in less aerodynamic force. On the other hand, in the case of turned on collision model, the result of SMD distribution is highly dependent on the grid resolutions.

Results of modified KIVA code

Figure 5 shows the spray shapes at t =3 ms calculated by using the modified KIVA code which includes the gas-jet model and the grid-independent collision models. Figure 6 illustrates the predicted spray tip penetration as a function of time with various grid resolutions. From the inspections, it can be found that the modified KIVA code gives an improvement of grid sensitivity and well predicts the spray tip penetration. This is because with the improvement of momentum transferred from the gas phase with no regard of grid resolutions. In the modified KIVA code, the ambient gas velocity is not calculated from the conservation equation but modeled from the gas-jet model so that the relative velocity is identical with regardless of mesh size. As can be seen in Figure 7, the droplet mean

velocity distributions of all the cases are almost similar with variation of mesh size. In order to illustrate the improvement of grid-independent collision models compared to standard model, the SMD distribution according to the axial distance from the nozzle is shown in Figure 8. In the case of turned on Munnannur's collision model with Nordin's model, the grid sensitivity is considerably reduced, but there is a little difference between three grid resolutions. This is because the relative velocity in the breakup model is assumed not to be calculated using the gas-jet model, but it is calculated by the standard method, thus the relative velocity in the breakup model is still dependent on the grid size, brings in influence of the breakup characteristics. On the other hand, the composition of the gas-jet model and the O'Rourke's model shows remarkable dependency on the grid size, because in the O'Rourke's model the collision probability is determined in basis of the grid cell size.

Conclusions

This paper shows the improvement of grid dependency of the spray simulations with use of several advanced spray model. From the results, the present study has concluded as follows:

1. The standard CFD code for spray simulation tends to give dependencies on the grid resolution because inherent assumption on the momentum coupling such that it leads to an unphysically fast diffusion of momentum.
2. The statistical approach on the calculation of collision probability in the O'Rourke's model is dependent on the grid cell size. And it shows impractical increase of SMD result because of limitation of its assumption on the collision regime.
3. The gas-jet model well improves the grid dependency problem on the calculation of the droplet momentum because the axial component of ambient gas velocity is modeled, not calculated by the original CFD method. This improvement on calculation of gas velocity can reduce the grid sensitivity of the droplet drag effect.
4. The improved collision model comprised of the Nordin's collision model and the Munnannur's collision model give a better SMD distribution with no dependency of the grid resolutions. This is because the Nordin's model determines the practical collision probability not dependent on the mesh size, and the Munnannur's model can predict the all the possible collision outcome and formation of satellite droplets.

Acknowledgement

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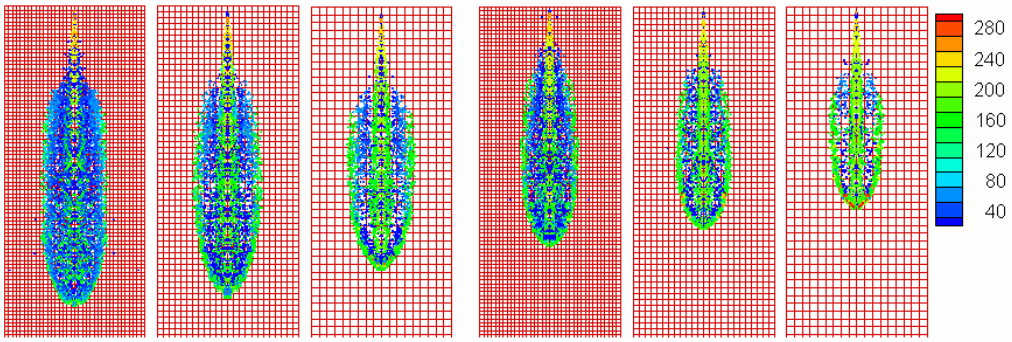
References

1. Kim, S., Chon, M. S., and Lee, C. S., *11th Annual Conference on Liquid Atomization and Spray Systems – Asia*, Taipei, Taiwan, November 2007, pp. 181-188.
2. O'Rourke, P. J., "Collective Drop Effects on Vaporizing Liquid Sprays", Ph. D. Thesis, Princeton University, 1981.
3. Nordin, N., "Complex Chemistry Modeling of Diesel Spray Combustion", Ph. D. Thesis, Chalmers University of Technology, 2001.
4. Ko, G. H., Lee, S. H., Ryou, H. S., and Choi, Y. K, *Atomization and Sprays*, 13:251-272 (2003)
5. Munnannur, A., and Reitz, R. D., *International Journal of Multiphase Flow*, 33:873-896 (2007)
6. Abani, N., Kokjohn, S., Park, S. W., Bergin, M., Muuannur, A., Ning, W., Sun, Y., and Reitz, R. D., *SAE 2008 World Congress, Detroit, USA, April 2008,* SAE2008-01-0970.
7. Amsden, A. A., "KIVA-3V: a block structured KIVA program for engines with vertical or canted valves", Los Alamos National Laboratory Technical Report No. LA-13313-MS.
8. Brazier-Smith, P. R., Jennings, S. G., and Latham, J., "The interaction of falling rain drops: coalescence", Proc. R. Soc. London, Ser. A 326:393-408 (1972)
9. Abraham, J., *Numerical Heat Transfer*, Part-A 30:347-364 (1996)
10. Munnannur, A., "Droplet Collision Modeling in Multi-Dimensional Engine Spray Computations", Ph. D. Thesis, Department of Mechanical Engineering, University of Wisconsin-Madison, 2007.
11. Naber, J. D., and Siebers, D. L., *International Congress and Exposition, Detroit, Michigan, USA, Februaru 26-29 1996,* SAE960034.

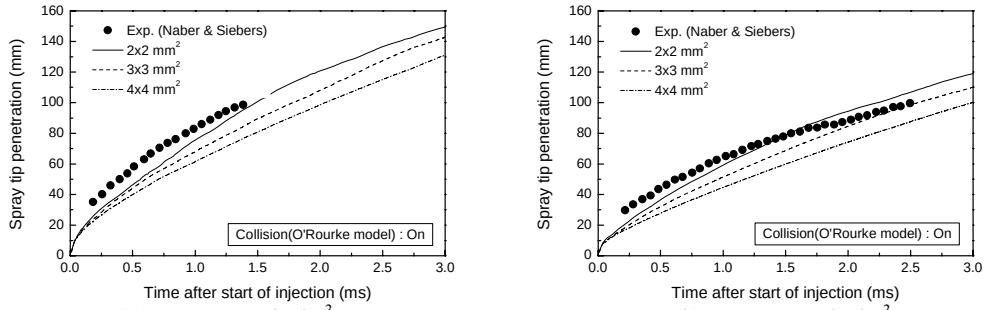
Table 1. Test condition for high-pressure diesel injection

Fuel	Diesel fuel
Ambient gas	Nitrogen
Density[kg/m^3]	844-0.9(T_l -289K)
Fuel temperature, T_l [K]	313
Injection duration [ms]	3
Nozzle diameter [μm]	257
Ambient gas density [kg/m^3]	14.8, and 30.2
Ambient gas temperature [K]	451
Injection pressure difference [MPa]	137
Discharge coefficient of nozzle	0.62



(a) ρ_g = 14.8 [kg/m^3] (b) ρ_g = 30.2 [kg/m^3]

Figure 1. Calculated spray shapes of the standard KIVA code



(a) ρ_g = 14.8 [kg/m^3] (b) ρ_g = 30.2 [kg/m^3]

Figure 2. Calculated spray tip penetration of the standard KIVA code

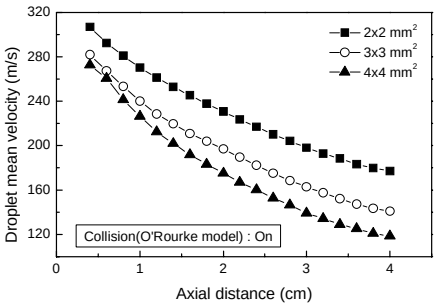


Figure 3. Droplet mean velocity according to the axial distance

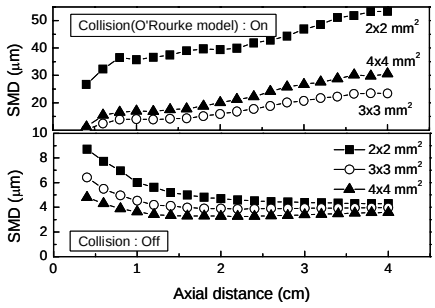
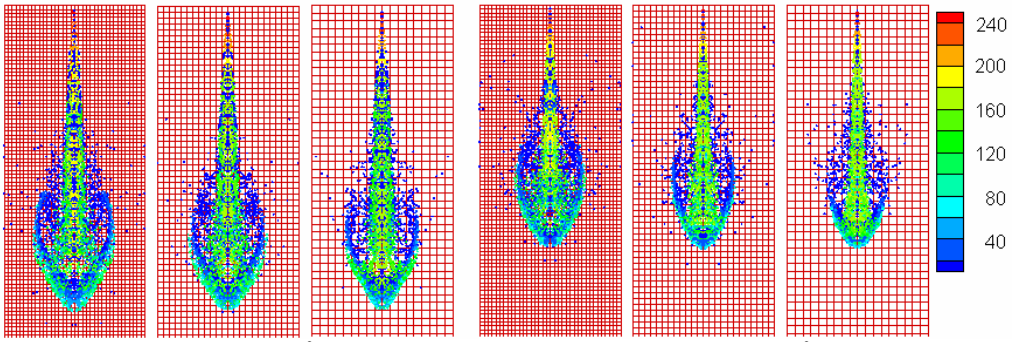
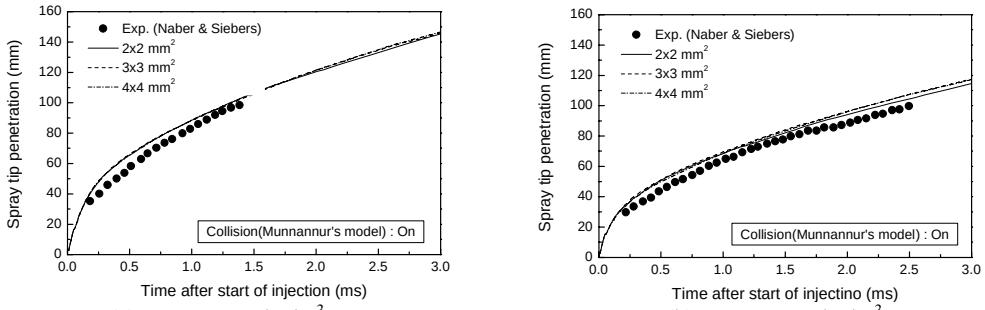


Figure 4. SMD distributions according to the axial distance



(a) ρ_g = 14.8 [kg/m^3] (b) ρ_g = 30.2 [kg/m^3]

Figure 5. Calculated spray shapes of the improved models



(a) ρ_g = 14.8 [kg/m^3] (b) ρ_g = 30.2 [kg/m^3]

Figure 6. Calculated spray tip penetration of the improved models

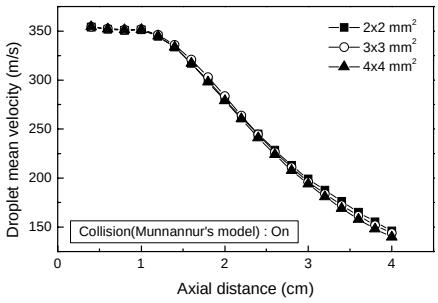


Figure 7. Droplet mean velocity according to the axial distance

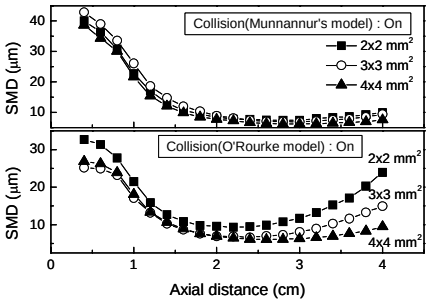


Figure 8. SMD distribution according to the axial distance