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Author(s)	Kikuta, Kazushige; Chikahisa, Takemi; Murayama, Tadashi et al.
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Necessary Grid Size Conditions for Accurate Diffusion and Convection Calculations with KIVA-II

Kazushige KIKUTA* Takemi CHIKAHISA* Tadashi MURAYAMA*
and J. K. MARTIN**

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Abstract

This paper investigates the effect of grid size on the accuracy of simulations of fuel spray penetration in KIVA-II, a three-dimensional simulation program for flow and combustion in engines. The analysis was made semi-theoretically for the momentum diffusion in a two dimensional gas jet. Predictions were compared with numerical simulations. The results of the comparison partially validated the semi-theoretical predictions, identifying the necessary grid size condition for diffusion and convection calculations. However, because of unexpected flow pattern changes with different grid geometries, the evaluation of the semi-theoretical prediction could not be fully completed. The reason for these flow pattern changes is not clear, but they may be partially due to insufficient simulation of the top of the spray.

1. Introduction

The KIVA or KIVA-II programs are widely used three-dimensional simulation programs for combustion and fluid flows in internal combustion engines. However they do not provide a sufficiently high level of accuracy. For example, the simulated heat release in the initial stage of combustion is much larger than is actually the case and the simulated spray penetration is weak, with the result that mixing of fuel and air appears extremely weak late in the combustion¹⁾. One reason for the poor simulated spray penetration is thought to be that inappropriate grid sizes are used in the calculations. When the grid size is too large, momentum diffuses significantly in the computational cell, resulting in extreme reductions in the penetration.

To research grid size effects, Allocca et al. have shown the effect of the grid spacing on numerical results by comparing measured and computed tip penetrations of the spray using KIVA-II with and without a breakup submodel²⁾. Gonzalez et al. conducted a study of the grid resolution effect for non-vaporizing and vaporizing sprays without combustion, and vaporizing sprays with combustion³⁾. Sugiyama et al. investigated the penetration and the shape of the spray using KIVA-II for different grid sizes⁴⁾.

* Department of Mechanical Engineering, Faculty of Engineering, Hokkaido University.

**University of Wisconsin-Madison, U. S. A

The purpose of this research is to investigate the effect of grid size on the calculated spray penetration distance and to identify maximum possible grid sizes. To establish that grid sizes are sufficient to approximate spatial gradients, one approach is to reduce grid spacings until further reductions produce negligible changes in the calculated quantities. However, this is not adequate for KIVA-II, as engine problems are complex, involving complicated geometries and numerous length and time scales. In this research, a theoretical analysis of the maximum grid size required to maintain simulation accuracy was performed based on an analysis of two dimensional free gas jets.

In this paper, an equation for a two-dimensional steady-state gas jet was non-dimensionalized, and similarity was applied to enable simplification to a one-dimensional problem. The set of equations was then solved numerically, and compared with the theoretical velocity distribution in the jet. The two-dimensional jet problem was examined because sprays injected into the combustion chamber appear to require the finest grid and as the phenomena are primarily similar to a gas jet problem.

The results of the semi-theoretical analysis showed that large grids resulted in reduced calculated jet penetrations. To obtain satisfactory calculation accuracy, KIVA programs do not require extremely small grid sizes : approximately 5 nodes are adequate for the width of a jet. To confirm this semi-theoretical evaluation, simulated results were compared with the semi-theoretical analysis. However, because of unexpected flow pattern changes with different grid geometries, the evaluation of the semi-theoretical prediction could not be fully completed. As it seems to be important to point out problems in the simulation at this moment, the paper presents the unrealistic phenomena observed in the simulations.

2. Computational method and conditions

The KIVA-II used in the present research was developed for a Fujitsu computer, and the Fujitsu VP2600 Super Computer at Kyoto University was used. The NISA-II post processor, a structural analysis program, was used for displaying the calculated results.

The analysis was for the non-combustion state. Fig.1 shows the mesh geometries for the calculations. The top is a planar mesh and the bottom a sector mesh of a cylinder similar to the mesh in the semi-theoretical analysis. Different mesh sizes of each geometry were compared, for a two-dimensional space of 10mm thickness with slip condition on both sides. The planar mesh had one cell in the thickness direction, while the sector mesh of the cylindrical coordinate had 4 cells to enhance calculation stability, as the calculations were unstable with only 1 cell. The reasons for this instability is still unclear.

The fuel was octane injected by a 0.0031mm wide slit nozzle for 100m/s to maintain the two-dimensional phenomena. It was verified that the results correspond to the penetration of a 0.2mm diameter hole nozzle. The spray angle was 5 degrees and represented by a DDM model in KIVA-II. The particles were distributed by Sauter mean diameters. For all the simulations, the time step for every cycle during the calculation was kept constant at 2×10^{-6} sec. to eliminate errors due to time step irregularities.

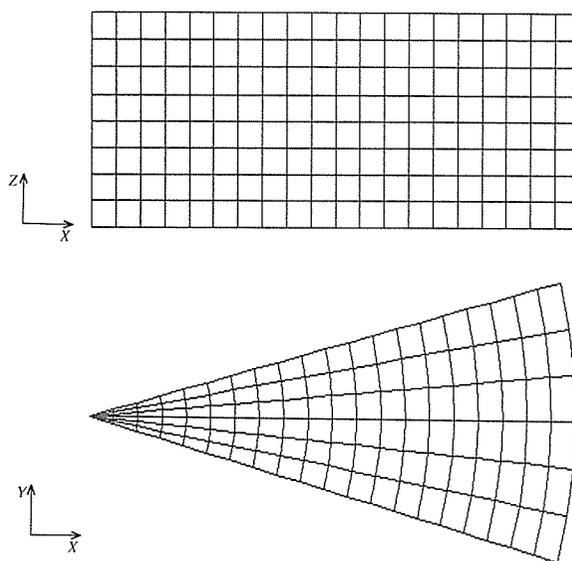


Fig. 1 Mesh geometries for computations (Top : PLANAR, Bottom : CYL. SECTOR)

In KIVA and KIVA-II, there are three optional models for differentiation of the convection term. A comparison was made of the differences in the influence of the grid size with these models. In KIVA, there are two models : 1) The Full Donor Cell model (abbreviated as FDC) which considers the transport of enthalpy and mass in the cell uniform. It is the most stable calculation method, however the diffusion of momentum, internal energy, and species are excessively strong. 2) The Interpolated Donor Cell model (IDC) which considers the gradient of the enthalpy and mass concentration in the cell, and solves the transport amount using a weighting factor corresponding to the flow speed. Compared to the FDC model, the diffusion speed is moderate but the calculation is not very stable. In KIVA-II there is a further Quasi-Second Order Upwind Differentiation method (QSOU) option, which partially overcomes the shortcomings of the two other models by estimating gradients in the cell to be relatively continuous⁵⁾.

3. Theoretical analysis of grid size

3. 1 Methods of analysis

As mentioned in the introduction, a direct numerical calculation is not appropriate to determine maximum grid sizes, and theoretical simplifications were made for the analysis.

The spray behavior is generally similar to a gas jet, and large parts of the spray (except for the tip) are assumed to be in a nearly steady state, wherefore the analysis was made for a steady state gas jet. When adopting the explanation below, the problem can be further converted to a one-dimensional velocity distribution problem, and it becomes possible to evaluate the degree of momentum diffusion by the spread of the velocity profile.

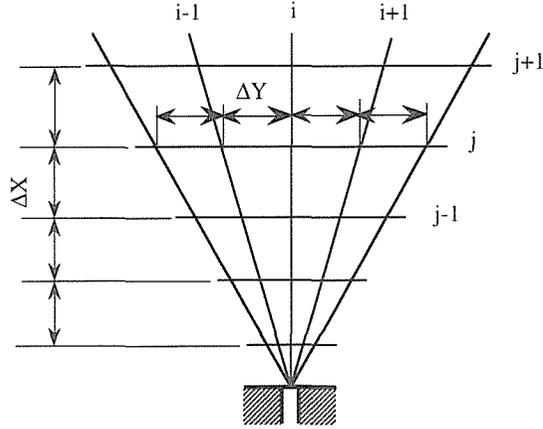


Fig. 2 Mesh geometry for theoretical analysis of mesh size effects

Fig.2 is the grid geometry used in the theoretical analysis of a two-dimensional jet. It consists of straight lines radiating from the nozzle tip, with parallel lines perpendicular to the spray center. The horizontal grid spacing Δy and the axial grid spacing Δx are constant, regardless of the i and j coordinates. The grid spacings were non-dimensionalized by the one half velocity boundary width, $\Delta y_{1/2}$, for the Y direction and the nozzle slit width, bn , for the X direction, and defined as Δy^* and Δx^* .

The assumption made in the theoretical analysis was that there is similarity in the velocity distribution in the radial direction at any X section, and the spreading of the boundary is in a straight line even in the numerical analysis.

Then the velocities of the different planes in the X direction, $(j-1)$, j , and $(j+1)$ can be expressed with the velocity of the j -plane as :

$$\begin{aligned} u_{i,j+1} &= \Phi_1 \cdot u_{i,j} & v_{i,j+1} &= \Phi_1 \cdot v_{i,j} \\ u_{i,j-1} &= \Phi_2 \cdot u_{i,j} & v_{i,j-1} &= \Phi_2 \cdot v_{i,j} \end{aligned} \quad (1)$$

With momentum conservation in the x -plane, the similarity coefficients, ϕ_1 and ϕ_2 , become :

$$\begin{aligned} \Phi_1 &= \sqrt{x_j^*/(x_j^* + \Delta x^*)} \quad , \quad \Phi_2 = \sqrt{x_j^*/(x_j^* - \Delta x^*)} \\ \therefore x^* &\equiv \frac{x}{bn} \quad \Delta x^* \equiv \frac{\Delta x}{bn} \end{aligned} \quad (2)$$

With these equations, the two-dimensional velocity distribution can be converted to a one-dimensional problem in the j -plane. The non-dimensional differential equation for momentum includes the turbulent Reynolds number defined for an eddy viscosity, μ_t , as in :

$$Re_t \equiv \frac{\rho u_m y_{1/2}}{\mu_t} = \frac{u_m y_{1/2}}{\epsilon_t} \quad (3)$$

When substituting an empirical eddy viscosity of the Prandtl mixture length theory shown in reference(6) into Eq.(3), the turbulent Reynolds number becomes constant regardless of grid size.

The analysis is performed in two steps. First, the sensitivity of the diffusion term for the grid size was investigated. The numerical differentiation of the diffusion term in KIVA-II is an implicit method as shown in Eq.(4), and the speed of diffusion during one calculation time step was compared for different grid sizes. In the second step, the steady state velocity profile was calculated according to the numerical method used in KIVA-II, and it was compared for different grid sizes. In this case, the diffusion term was calculated explicitly because of the steady state.

$$(M)_{ij} \frac{u_{ij}^{(t+\Delta t)} - u_{ij}^{(t)}}{\Delta t} = \sum_{\beta} [\phi_D \sigma(u_{ij}^{(t+\Delta t)}) + (1 - \phi_D) \sigma(u_{ij}^{(t)})]_{\beta} \cdot A_{\beta} \quad (4)$$

$$\because \sigma_{i,j} = \mu_{t,i,j} \frac{\partial u_{i,j}}{\partial y} \quad M \equiv \rho V_{i,j}$$

3. 2 Results of the theoretical study

Fig.3 shows the calculated effect of grid size on the diffusion term based on the semi-theoretical analysis detailed above. It shows the velocity change after one calculation time step, Δt , with the Eq.4. This is for diffusion term alone, and corresponds to the velocity change in a Lagrangian phase. A steady state velocity profile was used as the initial velocity and the semi-empirical eddy viscosity was used to determine the diffusion coefficient. In the figure, the curve of the subgrid explicit method was calculated by subcycling the time step with very small grids and it is considered to be the exact solution. As Fig.3 shows, there is almost no effect of grid size on the diffusion term in calculations with KIVA-II.

The effect of grid size on the calculated convection term was also investigated. Fig.4 shows the velocity distribution of a two-dimensional steady free jet for various grid sizes determined like with the KIVA-II numerical calculations. In this case, the QSOU differentiation model was used. When the grid size is very small, $\Delta y^* = 0.1$, the calculated results agree well with the theoretical velocity profile, indicating that the numerical differentiation

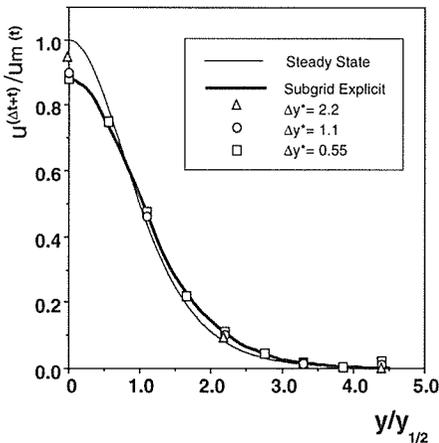


Fig. 3 Mesh size effect on momentum diffusion calculation in implicit method

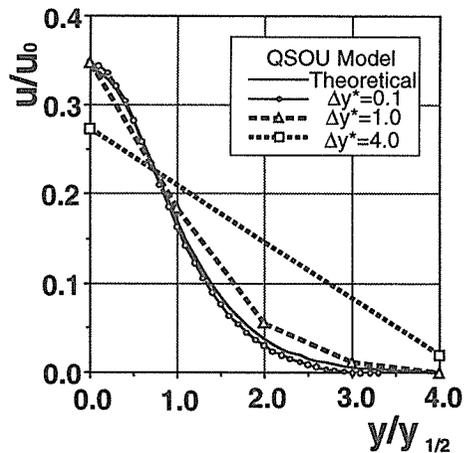


Fig. 4 Mesh size effect on velocity profiles of steady state 2-D gas jet (QSOU model, node centered on spray axis)

of KIVA is appropriate. When the grid size is equal to the half velocity boundary width, $\Delta y^* = 1.0$, the velocity distribution still agrees fairly well with the theoretical curve. This shows that KIVA does not require an extremely small grid, and that reasonably accurate calculations are possible with cells of the whole half velocity boundary width. However, when the grid size becomes four times the half velocity boundary width, $\Delta y^* = 4.0$, the calculated velocity distribution becomes linear and the numerical diffusion of momentum is excessive.

The grid size in the jet axial direction, Δx^* , was also investigated. The results showed that the effect of Δx^* is smaller than that of Δy^* , and confirmed that the grid may be large in the injection direction for a steady jet calculation.

Fig.5 shows the effect of nodal points relative to the spray center, where the nodes are symmetrical with respect to the jet axis and without nodes on the axis. In Fig.5, the calculation shows a significant loss of velocity on the center axis and the penetration of the spray is notably reduced. Thus, nodes should be centered on the jet axis, and the injection should not be directed toward the center of the cell. When there is swirl flow, nodes should be on the axis of injection because numerical diffusion can be significant in the region close to the nozzle.

Fig.6 shows the FDC, IDC, and QSOU differentiation models of convection. The IDC model did not give numerical convergence for $\Delta y^* = 4.0$ in this calculation scheme, and the data is not shown: this lack of convergence appears to be due to the velocity

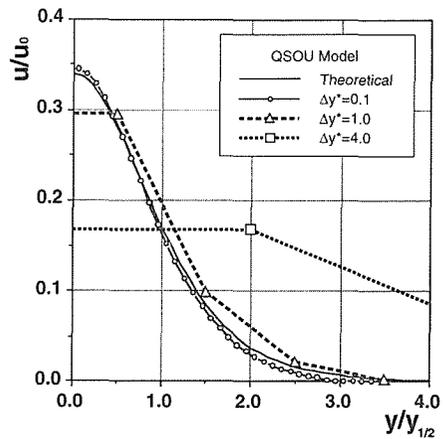


Fig. 5 Effect on node position relative to jet axis

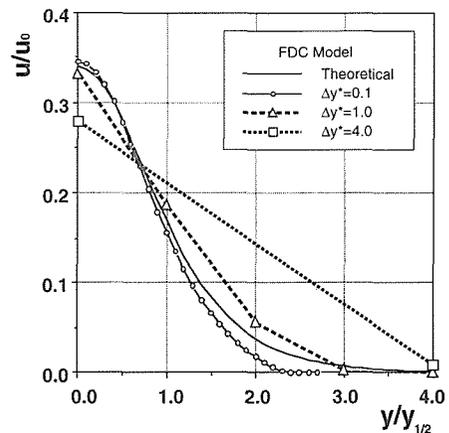
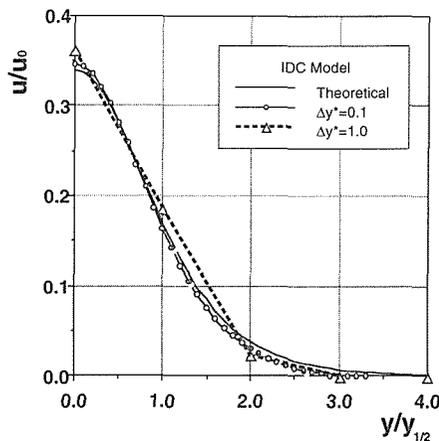


Fig. 6 Comparison of differencing model in convection calculation
Left : IDC model.
Right : FDC model

profile of the solution not being similar to the assumptions in the simplification. There are no large differences among these differentiation models of the jet simulation. This appears to be because the flow is directed outward in the center region and inward in the outer region of the jet, and that these two opposite flows compensate each other. All models are sufficiently accurate with $\Delta y^* = 1.0$, half the velocity boundary width.

The semi-theoretical study showed that the half velocity boundary width is an adequate grid size and that approximately 5 nodes across the width of the jet is sufficient. With a diesel engine, this corresponds to about 120 divisions in the azimuthal direction, because the spray angle is around 14 degrees. Nodes should be placed on the axis of the spray, as there is a large loss of center velocity when the nodes are placed across the center line.

4. Comparison between the theoretical prediction and the simulated results

4.1 Effect on spray penetration of the models of evaporation, breakup, collision, and droplet sizes

Fig.7 shows the calculated penetration distances of sprays with each model for evaporation, breakup, collision and coalescence in KIVA-II. These were calculated in a 72 degree sector mesh with 200 mm radius and 10 cells in the radial direction and 18 in the azimuthal direction. The Sauter mean diameter of the initial injected particles were 10mm in all the calculations. The curve for non-evaporating spray does not include the models of breakup, collision and coalescence, but they are included in the curves for the evaporating spray.

Differences between the non-evaporating and evaporating sprays appear just after the injection, and the penetration decreases due to diffusion of momentum and decreased droplet size by evaporation in the evaporating spray.

With the evaporating spray with the model of collision and coalescence, the penetration increases due to increased particle size. With the model of breakup, the penetration obviously decreases due to smaller broken up particles than in the case of evaporation alone. With all of the models, the penetration resembles that of the evaporating spray with the model of breakup, stressing that the effect of the breakup on the penetration is very large. Since the spray model has a large effect on the penetration, the following calculations were made for the non-evaporating mode without the models of breakup, collision and coalescence.

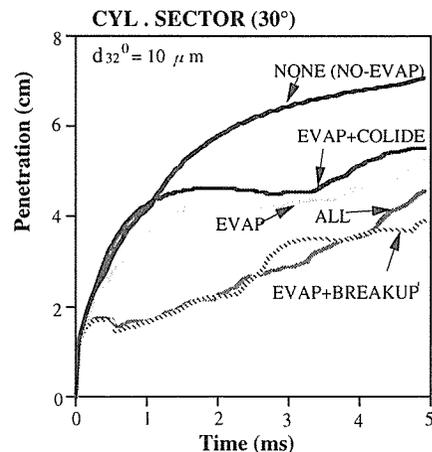


Fig. 7 Comparison of droplet penetration for different models ($P=0.12\text{MPa}$, $T=293\text{K}$ for non-evaporating spray and $P=0.32\text{MPa}$, $T=800\text{K}$ for evaporating spray)

Next, Fig.8 shows the calculated penetration distances of sprays for various droplet sizes. The calculations used the non-evaporating mode and in the same sector mesh and mesh sizes with Fig.7. The penetration decreased with decreasing droplet size. For the 60 μm dia. case, the penetration increases almost linearly, and decreases with decreasing droplet size, resulting in extremely weak penetration for 2 μm dia. droplets. This is an instance where the program provides insufficient simulation accuracy, because the penetration should converge to a gas jet penetration when droplet size decreases.

The reason for this result is not clear.

In the simulation, the 10 μm case appears to give the best fit, as smaller droplet sizes do not provide sufficient penetration while larger droplet sizes provide excessive penetration.

4. 2 Differences in Spray Penetration for Grid Size

Fig.9 shows calculated penetration distances using different grids with fuel injected into a two-dimensional space of 200x40mm and a cell width of 10mm. In these calculations, the mesh was square and the penetration was compared for 4 different grid sizes. At the beginning of injection there were no penetration differences, however, with the larger grid size the penetration distance decreases with time. The decrease in spray penetration for larger grid sizes appears to be due to instantaneous momentum diffusion of the gas in each cell, as the velocity gradient is considered uniform throughout a cell as shown in Fig.6. The

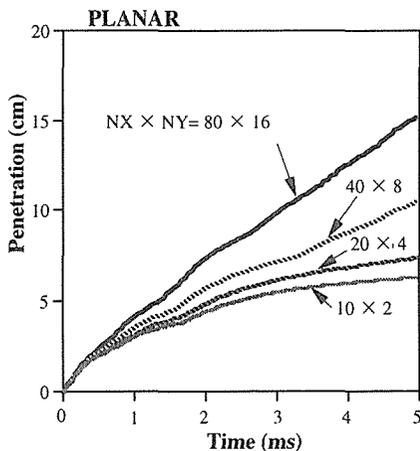


Fig. 9 Comparison of droplet penetration for different mesh sizes ($NX/NY = \text{const.}$ PLANAR)

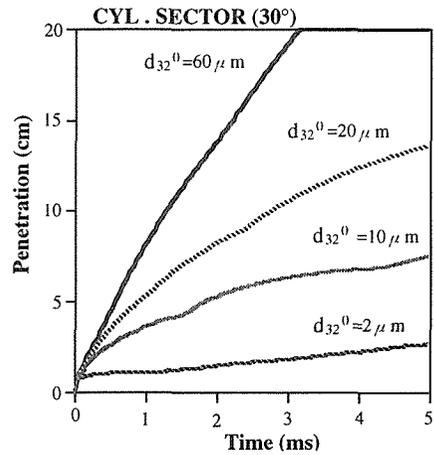


Fig. 8 Comparison of droplet penetration for different droplet sizes

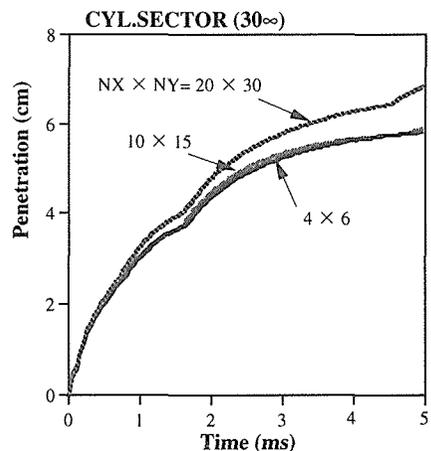


Fig. 10 Comparison of droplet penetration for different mesh sizes (CYL. SECTOR (30°))

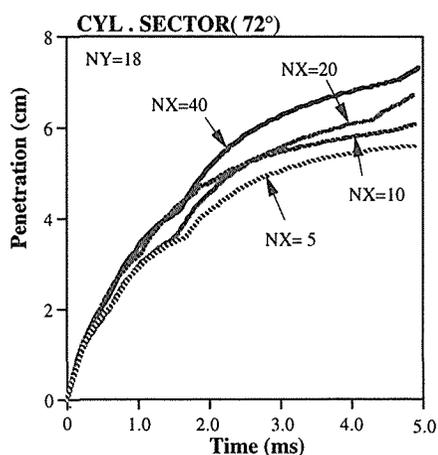


Fig. 11 Comparison of droplet penetration for different mesh sizes ($NY = \text{const. CYL. SECTOR } (72^\circ)$)

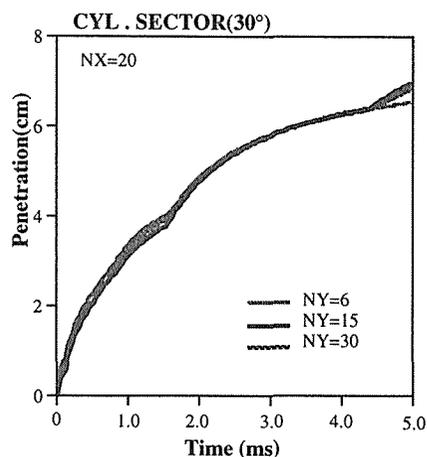


Fig. 12 Comparison of droplet penetration for different mesh sizes ($NX = \text{const. CYL. SECTOR } (30^\circ)$)

spray momentum transfers to the gas in the cell, and the velocity of the gas in the vicinity of the spray does not increase greatly due to the fact explained above, when the cell mass is large, resulting in a larger drag force on the droplet.

The penetration distances were compared with the cylindrical sector mesh like in the semi-theoretical analysis. Here the fuel is injected into a two-dimensional space of radius 200 mm and angle 30 degrees, giving the results in Fig.10. The penetration distance is shorter for the larger grid size, however, the effect of the mesh size in the Y direction (vertical to injection) is not significant as with the planar mesh. It is thought that the numerical diffusion of momentum near the nozzle, even for a comparatively coarse grids, is controlled by the sector mesh as these regions consists of fine grid spacing with the cylindrical sector mesh.

Fig.11 shows the effect on spray penetration of changing mesh sizes in the X direction (direction of injection) without changing the mesh size in the Y direction. Here the effect of the X direction mesh size is larger than with the planar mesh, giving a shorter penetration distance for the larger grid size.

Fig.12 shows the effect of the spray penetration when changing the mesh size in the Y direction without changing it in the X direction. All the penetration distances are very similar, showing that the difference in Fig.10 is due to the mesh size in the X direction.

This result does not agree with the semi-theoretical analysis. The reason for the disagreement between the theoretical predictions and the simulated results is not clear, however it appears to be partially due to inaccurate calculations at the top of the spray. Further investigation of the calculation method for the tip of the spray will be necessary.

This section has shown that when the grid size becomes large, the penetration of the spray decreases due to numerical diffusion of the momentum as predicted by the semi-theoretical analysis. However, the changes are affected by mesh geometry and require further investigation.

4. 3 Evaluation of the differences with the semi-theoretical analysis and of the unrealistic phenomena

Fig.13 shows the velocity profiles 10 and 40 mm from the nozzle with the planar mesh. With a coarse mesh, the numerical diffusion of momentum is very large, and it can be observed to be in quantitative agreement with the semi-theoretical analysis. However, the velocity distribution of the gas was not very large as in the case of gas jets even 40 mm from the nozzle. This implies further investigation of the value of the eddy viscosity coefficient is necessary. The result also shows that the velocity is negative outside the spray extremities. This is partially due to macro phenomena in the flow injected into the enclosed space as shown in the upper figure in Fig. 15. However, larger negative flow in the vicinity of spray than along the wall is unrealistic.

Fig.14 shows the case with the sector mesh. The numerical diffusion of the momentum near the exit of the nozzle is slightly greater for the larger grid size, thus producing similar results as the planar mesh. However, 40 mm from the nozzle it differs from the results obtained for the planar mesh case and also from the semi-theoretical analysis, maybe due to

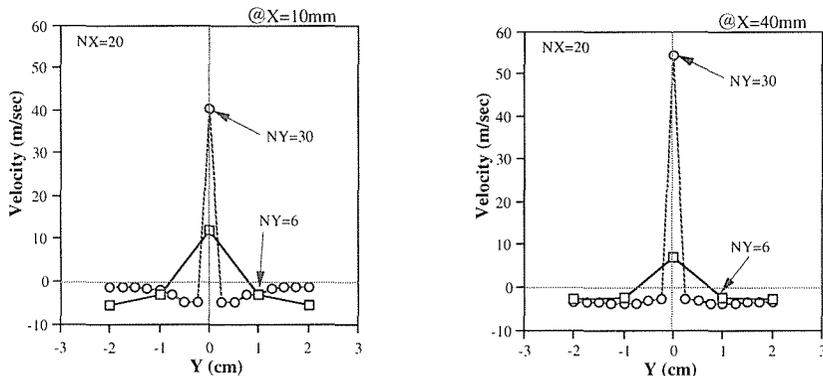


Fig. 13 Comparison of velocity profiles for different mesh sizes (NX=const. @ x= 10mm & 40mm, PLANAR)

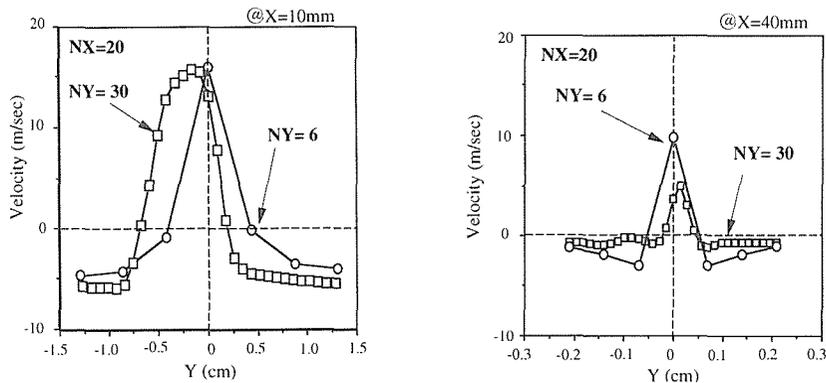


Fig. 14 Comparison of velocity profiles for different mesh sizes (@ x=10mm & 40mm, CYL. SECTOR (30°))

complicated flows.

Fig. 15 shows the velocity vector profiles of the different mesh types and sizes. Each figure is an enlargement of a 50x20 mm portion near the nozzle. For a 30 degree region with the sector mesh, there is back flow along the wall. With a 180 degree region for the same mesh type the flow near the nozzle should theoretically be similar to planar mesh, however, there is strong back flow near the nozzle. These results do not agree with the actual phenomena. Fig.16 shows the random flow pattern with the droplet diameter of 1mm at 5 ms after injection. When the droplet size is very small, the flow should be similar to that of a gas jet, however, this was not observed and only random flow pattern appeared. Further investigation of these points is necessary.

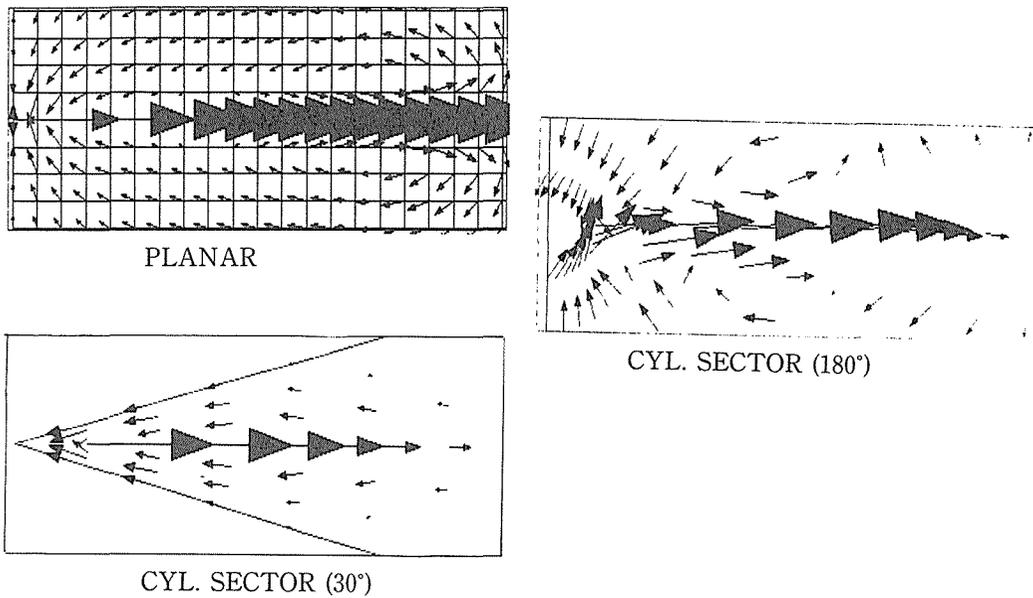


Fig. 15 Velocity vector profile

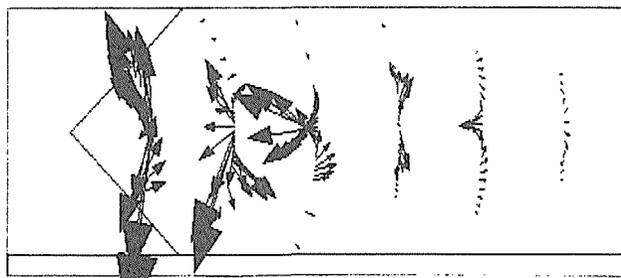


Fig. 16 Random velocity vector profile

5. Conclusions

Necessary grid size conditions were analyzed semi-theoretically and it was evaluated from simulation results. Although the evaluation of the theoretical prediction could not be fully completed, it should be useful to present some simulation problems as well as the results of the theoretical analysis at this moment. The research may be concluded as followings.

(1) The semi-theoretical analysis showed that when grids for jets and sprays are large, the calculated results show decreased spray penetration due to excessive diffusion of momentum by convection. Reasonably accurate calculations require about 5 nodes for the width of the jet. With a diesel engine, this results in a cell number of approximately 24,000 : 10 radially, 120 azimuthal, and 20 in the axial direction.

(2) The node of the calculation grid should be on the spray axis. When spray is injected into the center of cells the calculations result in a great loss of center velocity.

(3) The simulated results show agreement with the semi-theoretical predictions. However, unrealistic behavior in the calculated results prevented the full validity of the predictions questionable. The results appear to indicate that some components in the simulation program must be corrected before it is possible to make a quantitative comparison of the theoretical predictions and the calculations. The paper also points out results of unrealistic calculations, which will require further investigations.

This cooperative research between Hokkaido University and the University of Wisconsin was made possible with the assistance of the National Science Foundation of America.

Nomenclature

b_n : nozzle slit width

M : cell mass

u : velocity in axial direction

u_o : velocity at nozzle exit

u_m : velocity on center axis

V : cell volume

v : velocity in side direction

x : distance in axial direction

Δx^* : $\Delta x/b_n$

Δy^* : $\Delta y/y_{1/2}$

y : perpendicular distance from jet axis

$y_{1/2}$: 1/2 velocity boundary width

ϕ_D : implicit method coefficient

ϕ_1 : velocity ratio(u_{j-1}/u_j)

Re_t : Reynolds number

ε_t : eddy kinetic viscosity coefficient

μ_t : eddy viscosity coefficient

m_f : mass of fuel injection

t_{ini} : injection period

Subscripts

i : node in y direction

j : node in x direction

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