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An Ad-Hoc Procedure to Alleviate False Diffusion Effects in Computer Codes Using Discrete Droplet Models

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ABSTRACT

A three-dimensional computer model for the solution of gas flow and sprays represented by a discrete droplet model is employed to study the importance of false diffusion effects on the gas flow and spray penetration under various operating conditions. An ad-hoc correlation is presented to alleviate false diffusion effects on the predicted spray trajectory in cases of injection inclined to the computational grid. Application of this correlation over a wide range of gas pressures and injection angles shows satisfactory results for both the spray structure and penetration but its effect is less beneficial on the gas velocity field.

INTRODUCTION

Computer codes which solve multi-dimensional partial differential equations for two-phase flows are inevitably extremely complex. They are also very intensive users of computing resources. Many compromises must therefore be made in constructing such codes, between the requirements of obtaining high accuracy but at reasonable cost.

One such compromise lies in the selection of the method for approximating fluid fluxes across cell boundaries. Most large-scale codes use either the upwind scheme or upwind combined with central difference (the hybrid scheme), because of the enhanced stability provided. However, it is well known that such first-order accurate schemes contribute numerical or false diffusion when the flow is not aligned with the computational grid. This false diffusion may be many times larger than the physical (turbulent) diffusion.

A second compromise must be made when the grid itself is selected. In three dimensions it is currently not possible to provide a grid which is sufficiently fine that truncation errors are eliminated. Further, the distribution of the grid lines may not be ideal for calculating all the phenomena in i.c. engine cylinders. Body fitted grids must be used in order not to introduce unacceptably high truncation errors at the boundaries. In the remainder of the volume the constraints on the grid, even for codes with adaptive grids, such as the KIVA code (1), may be such that the grid lines cannot be aligned with fluid motion. This is likely to be so for sprays in diesel engines, because they are generally injected at angles of 25° - 40° with the cylinder head, down into a complex-shaped piston bowl. The inevitable result is false diffusion if upwind based schemes are used.

In this study the effects are examined of false diffusion associated with the upwind differencing scheme on the predicted results of sprays injected into quiescent gases at various pressures and angles of injection. An attempt is made to eliminate the false diffusion effects by introducing a correction factor which correlates the drag force to the local gas velocity inclination angle. The calculated results are obtained from the simulations of sprays in a test rig. The experimental research is conducted by Yule's group at UMIST, and (2) gives examples of early results obtained by them. The rig can be pressurised and the temperature raised. The injector, mounted in the roof of the rig, can be aligned such that the spray is injected into the rectangular cross-sectioned rig at a number of different angles. Further, fans allow the injected sprays to be subjected to a cross flow of gas. The simulations are made using a well documented three-dimensional code for calculating diesel sprays using discrete droplet models, see e.g. (3) and (4).

DESCRIPTION OF THE MODEL

In this model, the motion and heat transfer of the gas flow and the fuel vapour mass fraction are predicted by solving the unsteady, three dimensional conservation equations of mass, momentum, energy and the fuel vapour fraction in which allowance has been made for the presence of the liquid phase by introducing the void fraction into the relevant equations. The turbulence of the flow is calculated through the solution of the transport equations for turbulence kinetic energy (k) and its dissipation rate (ϵ). Liquid spray is modelled in a stochastic manner by representing it with discrete droplet parcels which can penetrate and interact with the gas phase. Each parcel contains thousands of spherical non-interacting droplets with the same size, velocity and temperature. The position, velocity, size and temperature of the individual droplets are respectively evaluated from the Lagrangian equations describing the trajectory, momentum, mass and energy of the droplets. The effect of turbulent motion on the droplets is stochastically modelled by including the fluctuating components of the gas velocity in the droplet momentum equations. The collision/coalescence and break up modelling of the droplets are also included in the code but are not employed in the present calculations.

The Lagrangian liquid phase equations are written in Euler implicit finite difference form. The gas phase partial differential equations are transformed into algebraic equations using the finite volume methodology in which the equations are integrated over a given control volume. During the process of integration, Euler implicit temporal discretization is used which results in a fully implicit solution method in which large time steps can be chosen without resulting in instability of the solution algorithm. The spatial discretization scheme used here is a hybrid of central and upwind differencing schemes proposed by Spalding (5). A second order accurate central differencing is used for low cell face Peclet numbers (Pe<2),

$$\varphi_{i+\frac{1}{2}} = \frac{\varphi_{i+1} + \varphi_i}{2} \tag{1}$$

where φ is any conserved scalar or velocity component.

For higher values of cell Peclet numbers, where central differencing results in unstable solution, the first order accurate but highly stable upwind differencing scheme is employed, that is,

$$\varphi_{i+\frac{1}{2}} = \begin{cases} \varphi_i \quad , \text{ if } u_{i+\frac{1}{2}} > 0 \\ \varphi_{i+1} \quad , \text{ if } u_{i+\frac{1}{2}} < 0 \end{cases} \tag{2}$$

where $u_{i+\frac{1}{2}}$ is the fluid velocity at the cell face. This practice ensures the stability of the numerical scheme but the upwind difference part of it, as shown by de Vahl Davis and Mallinson (6), leads to false or numerical diffusion if the flow direction is not aligned with the grid lines. For a two dimensional situation it has been shown (6) that false diffusion is given by:

$$\mu_f = \frac{|V|\rho \ \delta x \delta y \ \sin 2\theta}{4(\delta y \ \sin^3\theta + \delta x \ \cos^3\theta)} \tag{3}$$

where δx and δy are grid spacings, V is the resultant gas velocity and θ is the angle between the flow direction and the x-direction grid lines.

The Engine-PISO solution algorithm, which involves a series of predictor and corrector steps, is employed to handle the pressure-velocity coupling and solve the differenced equations in a non-iterative manner. Details of the equations and the solution procedure employed in this study are fully reported in (4) and (7).

RESULTS AND DISCUSSION

In order to investigate the role of the injection angle on the predicted results a number of calculations were made for sprays injected into a 32.5 bar gas pressure and room temperature quiescent environment with injection angles of α_z=0°, 15°, 30° and 45° to the vertical axis using the non-uniform grid shown in Fig. 1. The number of grid lines employed is fairly typical of the numbers used for three-dimensional calculations. In all cases the injector was located at plane K=2, and between planes 9 and 10 in both the I and J directions. In all the calculations a 25 μm Sauter mean diameter and a Rossin-Rammler distribution was assumed for the droplets at nozzle exit and no further break up and collision was allowed for.

Fig. 2 shows the predicted penetration curves obtained for various injection angles. It is seen that by increasing the inclination angle the penetration rates are markedly reduced at first and then more gradually until the minimum penetration is reached for the maximum angle (α_z=45°). Moreover, it is seen from Fig. 3 that the predicted gas velocity fields become wider in breadth and shorter in length as the injection angle is increased. The prime reason for this phenomenon probably lies in false diffusion which occurs in the directions perpendicular to the injection direction and causes the gas velocity dispersion in these directions. So the momentum transfer from the droplets to the surrounding gas is distributed over a wider area as the injection angle is increased and this creates smaller local gas velocities. These subsequently lead to greater drag on the droplets and hence smaller penetration. The second contributing factor is the cell sizes which become coarser as α_z is increased. This has the effect of reducing the penetration and it also increases the numerical diffusion, see eqn. (3). To show the importance of the false diffusion, Fig. 4 shows the ratio RDIF of false diffusion to the maximum physical (turbulent) diffusion for the 30° angle case. The latter is characterised by the turbulent viscosity and the former is calculated from the approximate two dimensional equation (3). Clearly the false diffusion dominates physical diffusion over much of the spray region.

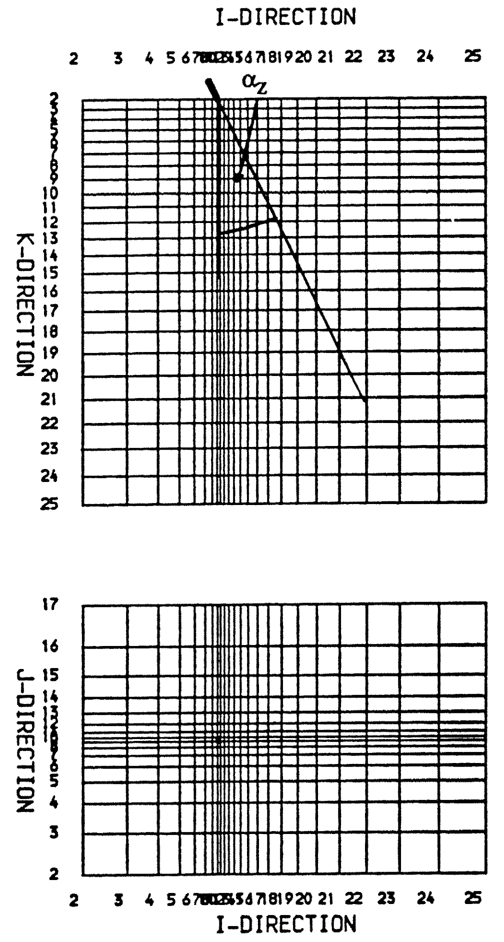

Fig. 1: Computational grid and injector position

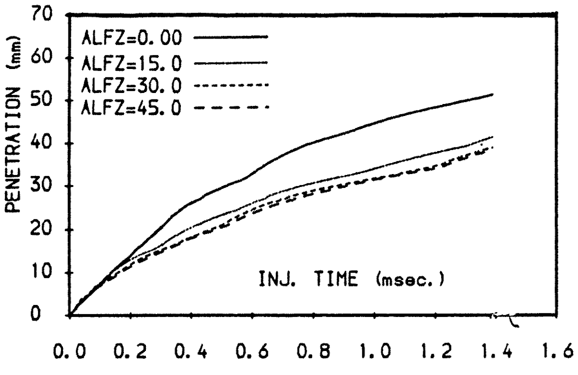

Fig. 2: Effects of inclination angle on penetration

As mentioned above some of the underprediction of the penetration for the inclined angle cases is due to the drops and gas passing through much larger cells at larger values of I and K (see Fig. 1), than for the vertical case. To eliminate this effect as far as possible, further calculations

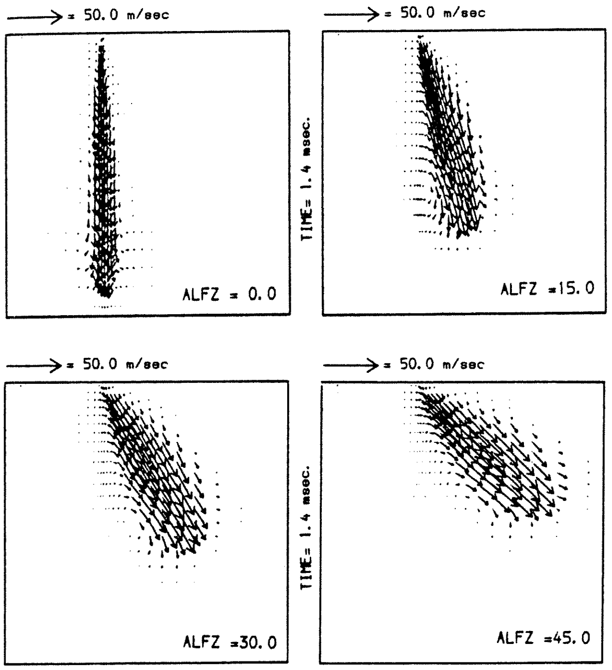

Fig. 3 Effects of inclination angle on the flow field

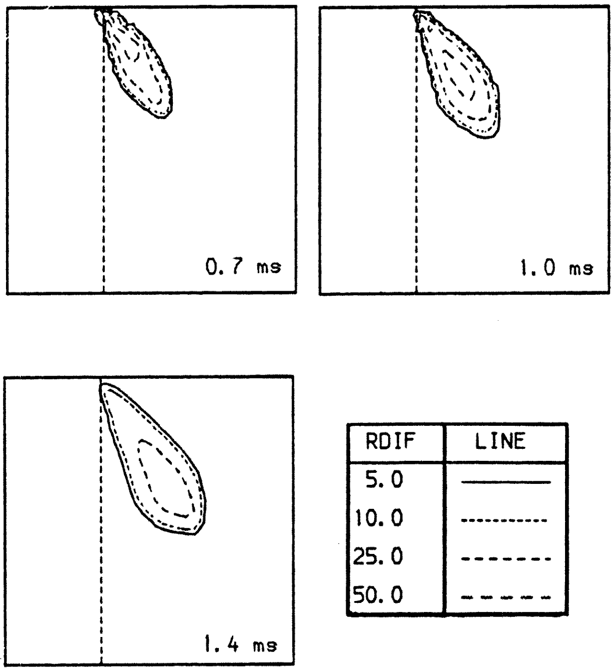

Fig. 4 Development with time of ratio of false to physical diffusion

were made with the uniform grid shown in Fig. 5. Penetration predictions are shown in Fig. 6. Because of the increased coarseness of the grid here the predicted penetration rates are reduced compared with those shown in Fig. 2.

Perhaps the best solution to the problem of false diffusion is application of a non-diffusive scheme, such as QUICK (8) in place of first order upwind schemes. However the QUICK scheme is much less stable and requires longer computing times for complex flows. An alternative ad-hoc procedure is to apply a correction factor to the drag coefficient which eliminates as far as possible the effects of false diffusion.

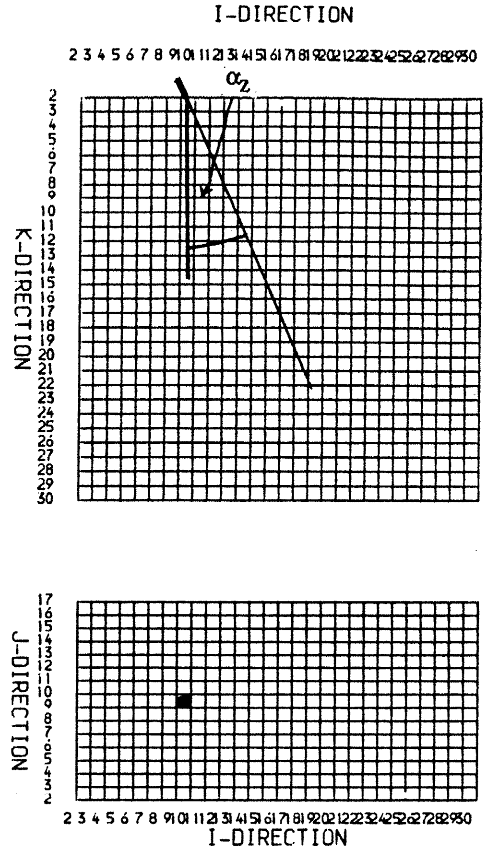

Fig. 5 Uniform computational grid

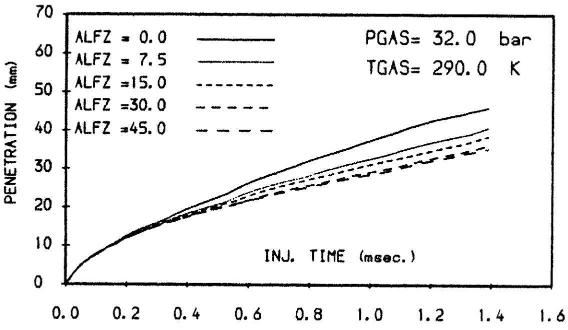

Fig. 6 Effects of inclination angle on penetration using the uniform grid

For each of the inclined injections, a number of additional runs were made in which the drag coefficient was reduced by a constant factor. The factor which provided closely the same penetration curve as the vertical injection case was obtained for each of the injection angles. Using the least squares method a third order polynomial was obtained to best fit these values. This polynomial is:

$$f(\alpha) = 1.068 - 4.796\alpha + 9.12\alpha^2 - 5.52\alpha^3,$$

where α is the inclination angle in radians.

There are other circumstances in which false diffusion arises, as for example, with a spray in a cross-flowing gas stream, in which the 'inclination' angle is not known. To account for these circumstances the function is employed with α being given by the arctangent of the ratio of the local velocity components.

This correlation was then applied to simulate sprays into chambers at room temperature and four different pressures, namely 11.5, 21.5, 32.5, and 53.0 bar using the grid shown in Fig. 1. For each case different values of α_Z between 0.0° and 45.0° were examined and the penetration curves obtained for all the angles were compared with the corresponding vertical penetration curves. As shown in Fig. 7 the calculated penetration curves obtained for angled injection are reasonably close to the vertical ones for all chamber pressures and angles of injection. Fig. 8 shows that the predicted spray structure for $\alpha_Z = 30°$, using the correlation, is now similar to that of vertical injection.

However the effect on the gas field is not as beneficial. Less momentum is now transferred from the droplets to the gas. As a result the gas velocities are smaller than hitherto. This is illustrated in Fig. 9, where the 30° case is shown with and without using the correlation. It is seen that the gas velocity field is less spread than before indicating a diminished effect of false diffusion. But overall, as comparison with Fig. 3 shows, the flow field is still very different from the vertical injection case.

CONCLUSIONS

An ad-hoc method has been presented preventing false diffusion effects on gas flow from affecting the prediction of the spray trajectories when using a discrete droplet model. A single correlation for reducing the drag force on droplets has resulted in almost perfect agreement of predicted penetration rates over a very wide range of back-pressures and injection angles. The corresponding effects on the gas velocity field are however less beneficial.

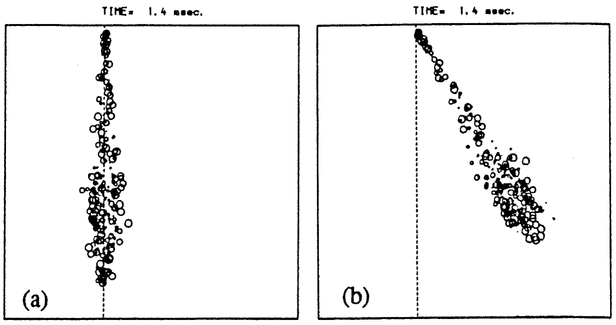

Fig. 8 Comparison of spray structures
(a) vertical injection
(b) inclined (30°) injection with correlation factor

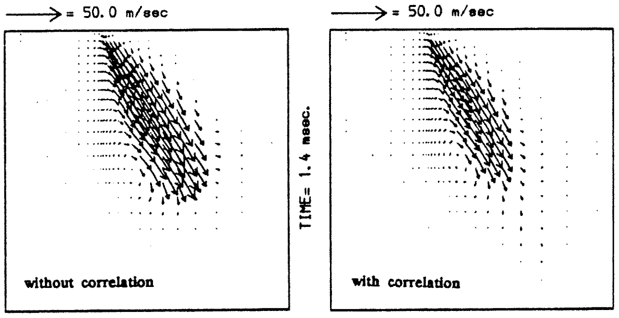

Fig. 9 Comparison of gas velocity fields for 30° inclination with and without the correlation factor

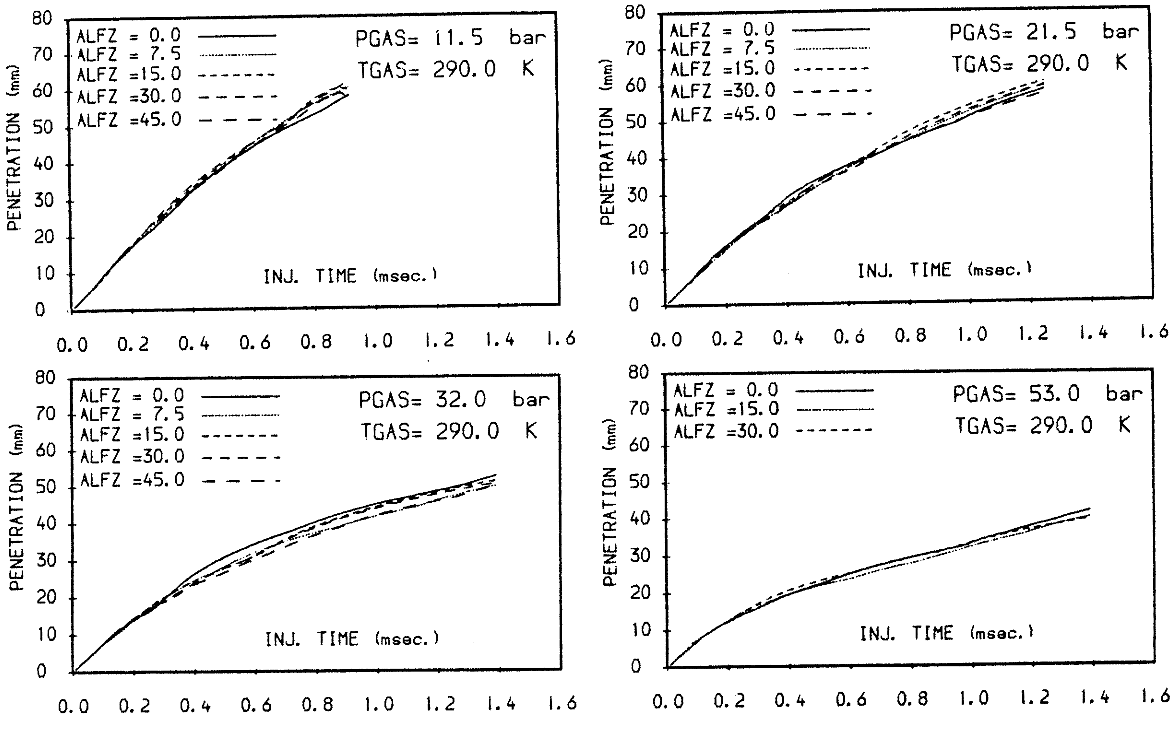

Fig. 7 Penetration calculations at various gas pressures and inclination angles, using the drag factor correlation

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