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# A New Model for Diesel Spray Impaction on Walls and Comparison with Experiment

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## ABSTRACT

This paper considers the problem of calculating the impaction of a diesel spray onto a wall. The spray is calculated using a discrete droplet model, in which representative drops move through and interact with the gas phase. Eulerian partial differential equations in two or three dimensions are solved by finite volume means for the gas phase, whilst Lagrangian ordinary differential equations are solved by finite difference means for the drops. The coupled sets of algebraic equations are solved by a fast non-iterative implicit solution scheme.

A new sub-model is developed for the impaction process, based on the approach Weber number of the drops. The basic model was found not to match the observed dispersion of the drops after impact. A new drop-drop collision model is therefore developed for thick spray regions which allows the dispersion to be modelled.

Comparison with experiment shows that the model is encouraging, giving good results for wall spray shape and development, particularly for normal impaction.

## INTRODUCTION

The study of diesel spray impaction on engine walls is assuming greater importance than hitherto. Direct injection diesel engines are becoming more compact as more applications are made to small automobiles. Although the gas flow in such engines is often highly swirled in order to aid the mixing of fuel vapour and air, much of the fuel spray still reaches the engine walls. It is believed that this obstructs the mixing process of fuel with air and leads to incomplete combustion and therefore, higher hydrocarbon emissions (1).

Over the last decade studies of diesel spray have shifted from highly empirical methods, based on gas flow analogies, to fundamentally-based computational fluid dynamics methods. In the latter case the full multi-dimensional partial differential equations governing the gas and spray flows are solved using finite-difference or finite-volume methods. Two-phase applications solve either Eulerian equations for both phases or Lagrangian ones for the non-gas phase. In diesel engines, where, for the most part, the spray is atomised into discrete droplets, the second approach seems more appropriate.

The first application of a stochastically-based discrete droplet model (DDM) to diesel sprays was by Ducowitz (2). His model was subsequently extended to thick sprays by O'Rourke and Bracco (3), who introduced sub-models to account for droplet collisions. Droplet break-up models were later developed by Reitz and Diwakar (4).

Recently Naber and Reitz (5) introduced sub-models to account for spray impaction on walls. Three different models were employed. The drops striking a wall were made either to (i) rest near the wall (STICK), (ii) rebound specularly (REFLECT), or (iii) travel tangentially along the wall at their approach speed (JET). In all cases the drops continued to reside in the gas, no wall wetting was accounted for. Shattering of the drops on impact was also neglected. Comparisons were made with photographic data on sprays impacting either normally or at an angle on a flat plate in a constant-volume room-temperature bomb, or on the walls of a single cylinder research engine. The best predictions were obtained using the JET model.

Subsequently Naber et al (6) applied this model to impaction very close to the injector. It was found not to match experimental evidence. In particular the spray failed to disperse after impaction. The subsequent motion through the gas (the 'wall' was a small flat land on the pip of a piston bowl) was greatly overpredicted. Better results were obtained by departing from the wall jet model and giving impacting droplets a randomly sampled velocity component normal to the wall after impact. Shattering of the drops was also introduced, although this had a smaller effect than ascribing the normal velocity component.

The present authors and colleagues have been developing computer methods for diesel sprays, using the DDM, for a number of years (7). The major difference between these models and those cited previously lies in the solution methodology. Here a non-iterative implicit solution scheme, based on the PISO method (8) is employed, instead of iterative implicit methods or the semi-implicit method used in the KIVA code (9), for example. Substantial savings in computer times are claimed (8). Full details of the solution methodology applied to two-phase flows are presented in (7).

In this paper, a different sub-model to either (5) or (6) for spray impaction on walls is presented. This is based on an extension of the drop-drop collision sub-model of O'Rourke and Bracco (3). Results are presented of simulations of room temperature experiments of sprays injected, either normally or at an angle, onto flat plates.

## MATHEMATICAL MODEL

For the gas phase, Eulerian partial differential equations are solved for the conservation of mass, momentum, energy, and for vapour mass fraction and for the $k$-$\epsilon$ turbulence model.

Lagrangian ordinary differential equations defining the droplet position, velocity, mass and energy are solved for each droplet in the flow. Two-way transfer of mass, momentum and energy between the phases is accounted for, including dispersive effects on the droplets due to the gas phase turbulence. Following Ducowitz (2) each of the 'drops' actually represents a parcel of many thousands of drops, each having the same position, velocity, temperature, etc.

Finite volume discretisation is employed to cast the gas-phase partial differential equations into algebraic forms. Within this process, Euler implicit discretisation is used for the time advancement, and the hybrid upwind/central difference scheme is used for the convective and diffusive fluxes in space. The droplet equations are also discretised using the Euler implicit scheme in time. The same time step is employed as for the gas phase equations.

## WALL IMPACTION SUB-MODEL

The main feature of this model is the application of experimental observations of drop-wall interactions. As (10) and (11) have shown, the outcome of a drop striking a surface depends on the value of the Weber number We. For We < 80, the drop rebounds from the surface, otherwise it attaches to the surface while shattering into a number of smaller drops (10). This criterion is used in this model under the assumption that, although the results of (10) are based on water droplets, they should still be applicable to fuel oil drops because the relation is in the form of the similarity parameter. This is provided that other parameters, like the surface conditions, are similar.

The momentum and energy losses due to drop-wall collision must also be considered. The results of energy loss of water drops falling onto a water surface were arranged in (11) into the equation

$$\frac{E_b - E_a}{E_b} = 0.05 \sin^2 \beta \qquad (1)$$

Where $E_b$, $E_a$ are the kinetic energy of the drops before and after impaction respectively. Here $\beta$ is the angle between the approaching drop and the normal to the surface. Both of these features are included in the sub-model. In the sub-model, when attachment takes place, the drop is left to float near the wall. Its tangential velocity is the same as that before impaction, its normal velocity is set to zero and the drop size is reduced by a factor of four to simulate the shattering process. These contrast with the JET model in (5) in which the tangential velocity after impact was set equal to the approach speed of the droplet and the drop size remained unchanged.

As will be illustrated below, this model itself is not adequate enough to obtain the dispersed wall spray shape as shown by experimental evidence. The droplets tend to accumulate close to the wall. This aspect was confirmed when reference (6) became available. However the remedy applied here is different from that adopted in (6). Rather than giving all impacting droplets a rebound velocity it is argued that the subsequent collision activity of the droplets near the wall generates normal velocity components away from the wall. This leads to an extended collision model.

## EXTENDED COLLISION MODEL

In the collision model of O'Rourke and Bracco (3) colliding droplets may either coalesce, thus reducing the number of drops, or swing around each other and continue with the same masses as previously. This is termed a grazing collision. In the latter case, linear momentum is conserved, but energy may be dissipated and the angular momentum of the drops may change. It is assumed in the model that the angle between the line of centres of the drops and the relative velocity vector remains unchanged by the grazing collision.

This model seems to work well in free sprays. However, it seems likely that for the very thick spray moving in a very thin layer close to the wall after impact there will be a preferential movement of drops away from the wall after undergoing a grazing collision, as a consequence of droplets swirling around each other. Movement in the other direction is of course restricted by the presence of the wall.

The new model assumes that droplets after grazing collision will move preferentially in the direction of the local gradient of the void fraction. In other words, drops move away from areas of local droplet concentration. Fig. 1 illustrates the model: there $\alpha$ is the angle between the direction of the void fraction gradient vector $\nabla\theta$, and that of the velocity vector $\bar{V}$ after collision, as predicted by the original grazing model of O'Rourke and Bracco (3). A new velocity vector $\bar{V}_n$ is computed which has the same magnitude as $\bar{V}$, i.e., $|\bar{V}_n| = |\bar{V}|$, but whose direction lies at an angle $\alpha_n$ to that of $\bar{V}$. A large number of droplets are involved during drop (parcel) collisions, and this should lead to a certain stochastic behaviour in the outcome of collisions. Therefore a random number P, uniformly distributed in the range [0,1], is generated. Thus, the actual formula used to calculate $\alpha_n$ is

$$\alpha_n = (1 - \bar{\theta}_i)P\alpha \qquad (2)$$

The drops, on collision, reside in a gas phase control-volume or cell, denoted here by the subscript i. Then $\bar{\theta}_i$ is the average value of the void fraction of cells surrounding cell i. $\bar{\theta}_i$ lies in the range [0,1] and approaches 1 for droplet-free cells.

In a region of thin spray, where $\bar{\theta}_i$ is very close to 1, equation (2) gives $\alpha_n$ approximately zero. The introduction of (2) thus does not appreciably influence the spray shape in such a region. However it will be seen below that for thick sprays, where $\bar{\theta}_i$ drops substantially below 1 in value, the effect on the spray shape is considerable.

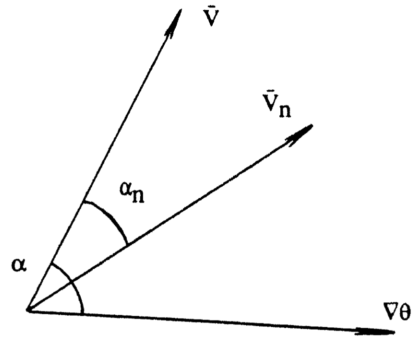

Fig. 1 Extended Grazing Collision Model

## SIMULATION CASES

A number of test cases, with different wall distances and injection conditions, were simulated in order to test the wall impaction sub-model. These test cases are summarised in Table 1.

Table 1 Details of Simulated Test Cases

| Case No. | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| Wall Distance(mm) | 24 | 63 | 50 | 63 | 63 |
| Trap Pressure(Mpa) | 1.5 | 6.28 | 2.64 | 6.28 | 6.28 |
| Injector Diameter(mm) | 0.3 | 0.29 | 0.25 | 0.29 | 0.29 |
| Injection Pressure(Mpa) | 14.3 | 37.3 | B* | 37.3 | 37.3 |
| Injection Duration(ms) | 1.2 | -** | 7.8 | -- | -- |
| Injection Angle(°) | 0 | 0 | 0 | 26.6 | 45 |

* Diagram Pattern B (14)
** Continuous Spray

The cases can be divided into two categories; (i) normal impaction, with the injector placed normal to the end wall, and (ii) inclined injection, with the injector placed at an angle to the end wall.

For the former category, a two dimensional code employing a cylindrical polar grid can be used because of the axi-symmetric nature of the flow. For the results presented below a 40 x 40 line grid in the axial and radial directions respectively has been employed.

For the second category, which lacks any symmetry, a fully three-dimensional code is used in which the grid is Cartesian. For the results shown here a 40 x 35 x 40 line grid, in the x,y,z directions respectively, has been employed, where the injector lies in the x-z plane, and z is normal to the wall.

The time step employed is 7μs for Cases 1 and 3, and 14μs for all other cases. Throughout the injection process 15 new droplet parcels are introduced at each time-step, resulting in more than 5000 parcels in all. At introduction the drop sizes are sampled from a Rosin-Rammler distribution with a Sauter mean diameter of 25μm. Droplet collision and break-up models (3)-(4) are fully activated.

## RESULTS AND DISCUSSION

Fig. 2 shows the free and wall spray developments for Case 1, in terms of spray plots, and Fig. 3 shows the wall spray radius and height developments. Comparison is made between calculations, (a) without and (b) with, the extended collision model, and (c) image processed sprays based on photographs (12). With each spray plot are shown the calculated Sauter mean diameter, the minimum and maximum droplet diameter, and the number of droplet parcels after collisions and break up.

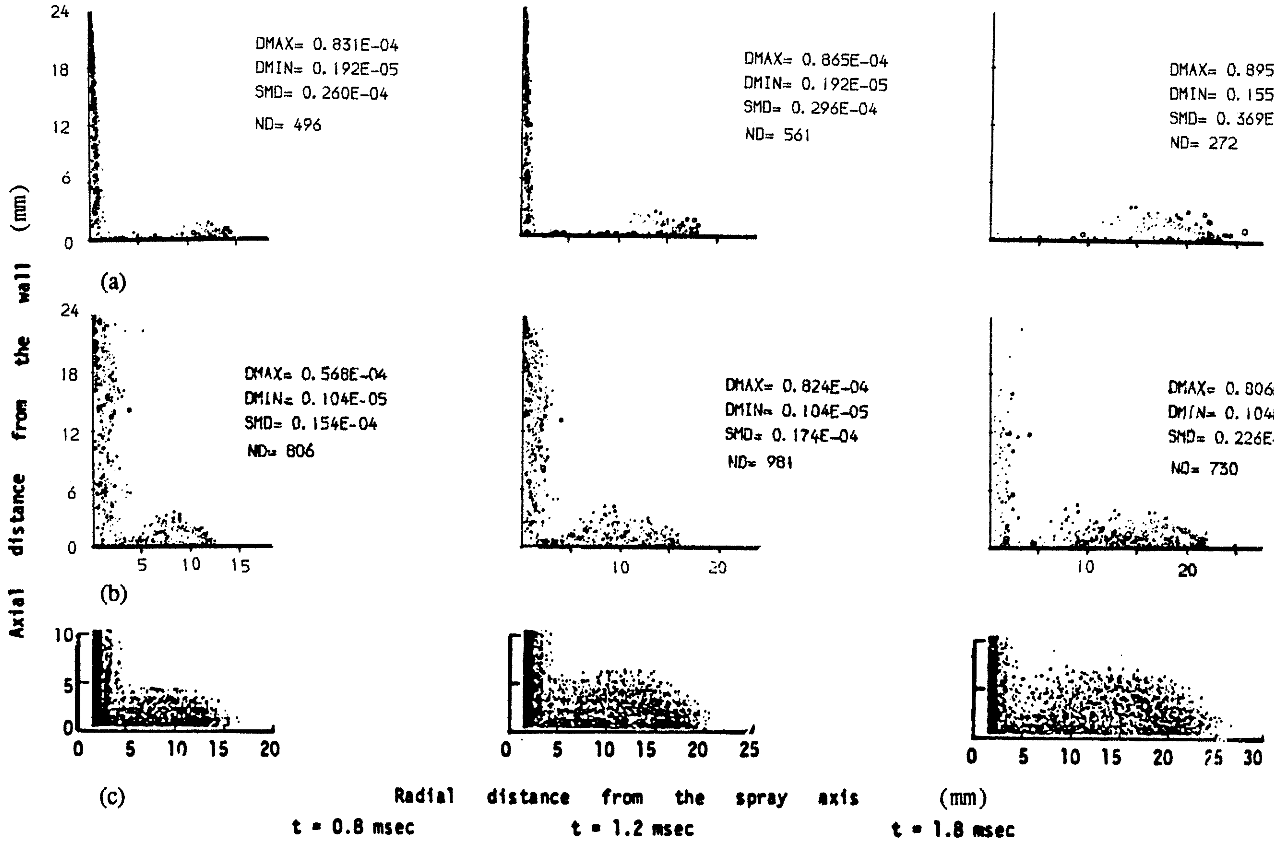

Fig. 2 Spray Shape Developments for Case 1
(a) without extended collision model
(b) with extended collision model
(c) image processed sprays (12)

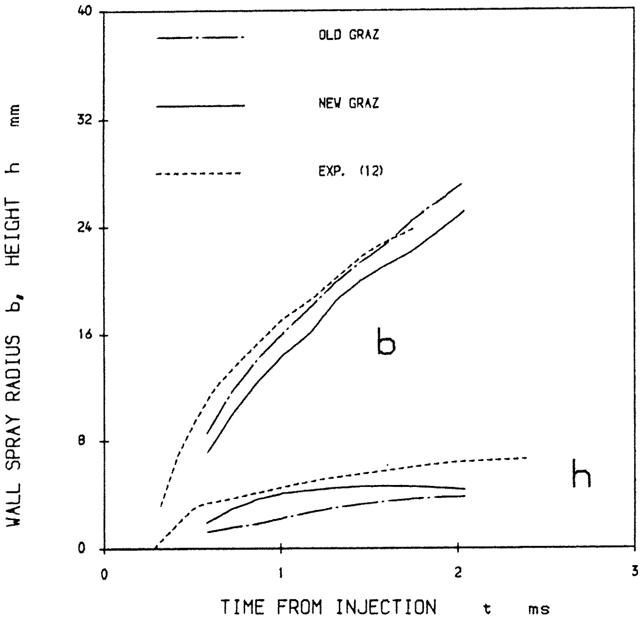

Fig. 3 Wall Spray Development for Case 1

A common feature among Fig. 2(a)-(c) is that the contour of the wall spray is wider, and the spray is denser, near the tip and that there is a concave region closer to the impacting stream.

Using the original collision model the development of the wall spray radius b is well predicted, but that of the wall spray height h is far from satisfactory. This is largely because b is determined by convection, while h, or more generally, the wall spray shape, is more dependent on the mass diffusion process. Indeed the spray height, using this model, is determined by convection in the spray tip vortex, which sweeps droplets away from the wall.

In contrast the extended collision model allows the wall spray to become much more dispersed, and the spray shape, as well as the wall spray height, are in much better agreement with the experimental results.

Similar pictures are presented for Case 2 in Figs. 4 and 5. Here the wall is at a much greater distance from the injector. The calculated results of Naber and Reitz (5) are also included, as are experimental data (13). The new grazing collision model improves the prediction for the spray height, although the improved prediction of h is still not as good as for (5). Examination of the computer output shows that far fewer grazing collisions take place in the wall spray of Case 2 than for Case 1. Hence the new model is less effective. Methods are being investigated of changing the balance between collisions which result in coalescence and those which result in grazing.

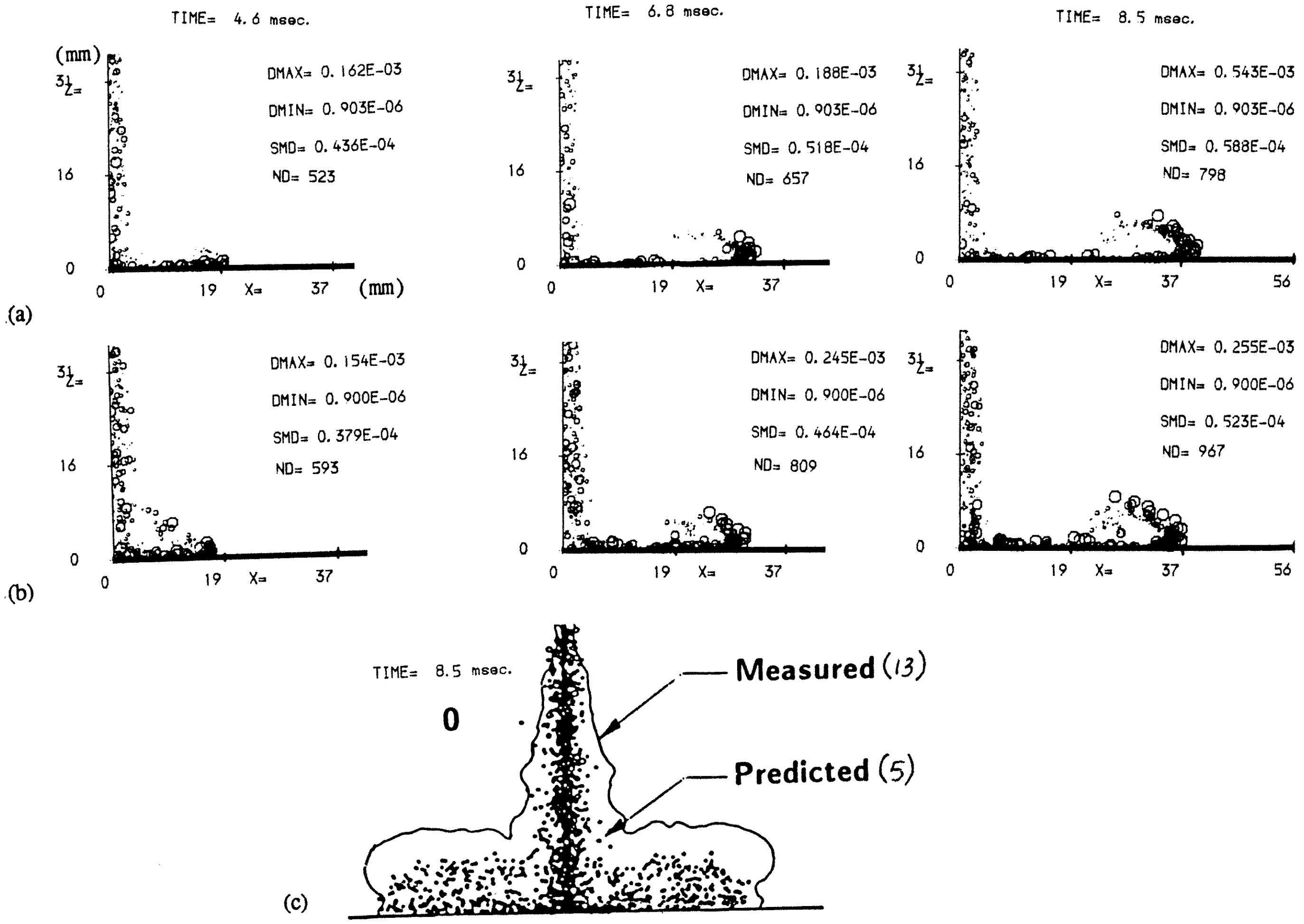

Fig. 4 Spray Shape Developments for Case 2
(a) without extended collision model
(b) with extended collision model
(c) photographic outline (13) and calculations (5)

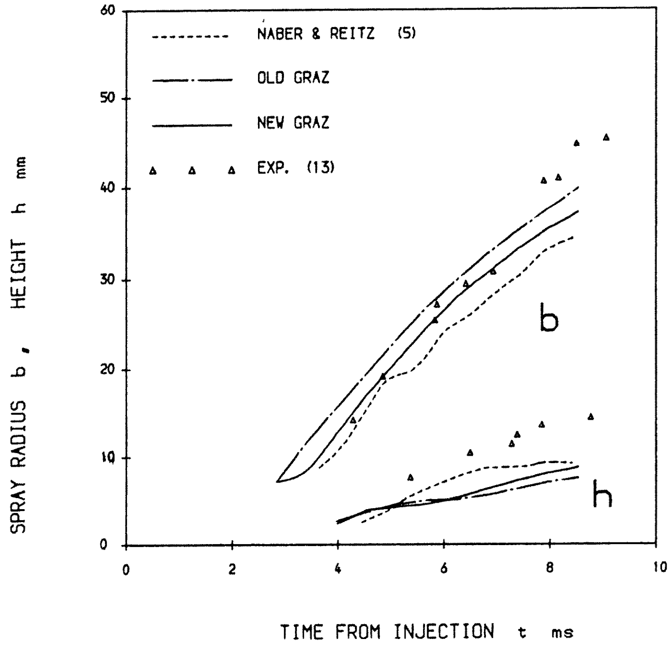

Fig. 5 Wall Spray Development for Case 2

All other calculated results presented here use the extended collision model. Some results for Case 3 are shown in Fig. 6. Here the actual injection pressure diagram was available (14) for use in the simulation. In all the other cases a uniform injection pressure has been assumed. Fig. 6 compares the predicted spray outline, at 3.9ms after the start of injection, with that from the experiment (14). It is apparent that, not only is the spray outline well predicted, but also the spray concentration is too. For the experimental results, the thick hatching shows fuel rich zones, thin hatching shows moderately fuel weak zones, and no hatching shows very weak zones.

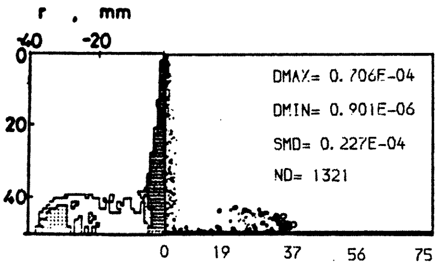

Fig. 6 Comparison of Experimental and Calculated Spray for Case 3

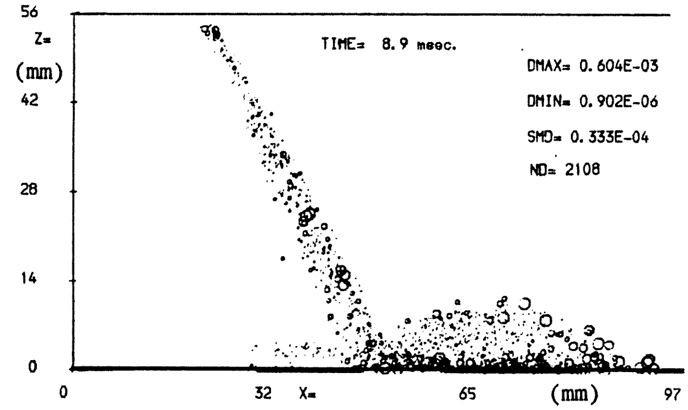

Fig. 7 Calculated Spray for Case 4

Figs. 7-10 show the results of simulations of sprays injected at different angles onto a flat plate. Good agreement is obtained with the experimental variations of wall spray radius b and height h with time (13), but both are under-predicted. One possible reason for this may be that the grid used is relatively coarse, compared with that which is used for the axi-symmetric calculations. The KIVA code, with which the results of (5) were obtained, has a greater geometric capability than the code used here. In KIVA the grid lines can be placed along the spray, whereas here the spray is at an angle to the grid lines. A separate paper (15) in this symposium discusses in detail problems of grid spacing and false diffusion effects resulting from the spray crossing grid lines at large angles. One major effect is that the penetration of the spray is under-predicted more and more as the angle increases. Here the time to impaction is calculated as being considerably more than the experiment shows. This results in the calculated lines in Figs. 9 and 10 being shifted to the right.

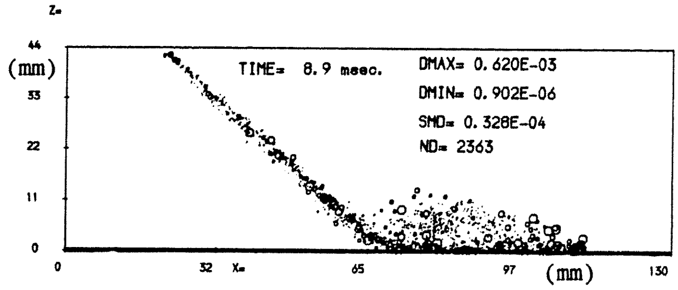

Fig. 8 Calculated Spray for Case 5

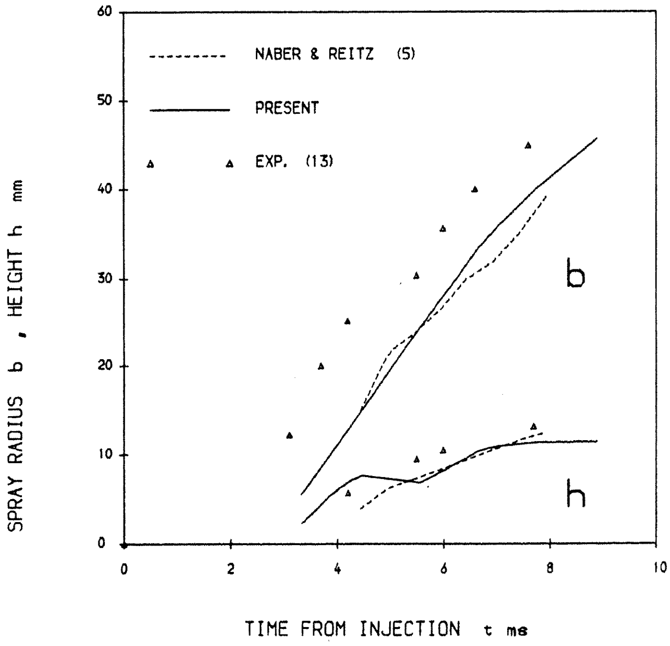

Fig. 9 Wall Spray Developments for Case 4

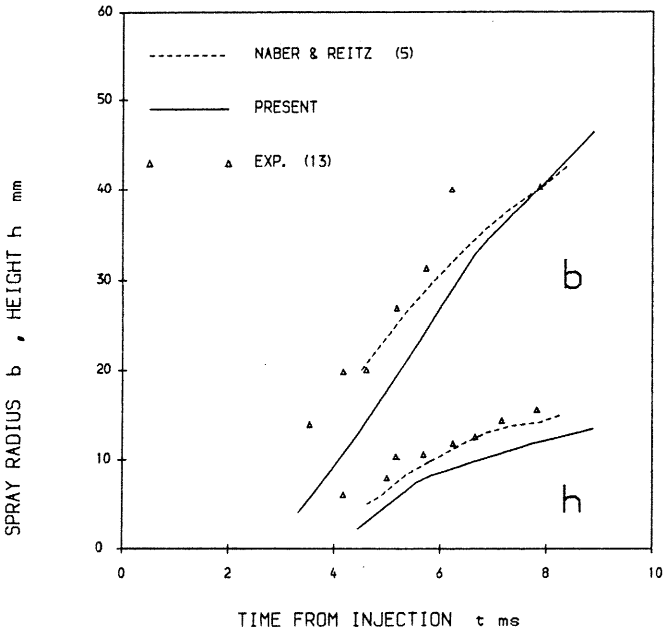

Fig. 10 Wall Spray Developments for Case 5

## CONCLUSIONS

A new sub-model has been developed to account for spray impaction on a wall. The basic sub-model was found not to give adequate mass diffusion effects in the wall spray. The collision model of O'Rourke and Bracco (3) has been extended in such a way that in very thick spray regions, the drops tend in a stochastic manner to move away from areas of high drop concentrations.

For normal spray impactions the new sub-model gives a good prediction of wall spray shape and development, particularly for walls near the injector.

For angled injections on relatively far walls, the comparison with experiment is not so good for the wall spray. This may be due in part to grid spacing and false diffusion effects.

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