SPRAY PENETRATION AND VAPORIZATION IN DIESEL ENGINES: NUMERICAL SIMULATION AND EXPERIMENTS

S. M. Frolov[1], V. S. Ivanov[1], V. A. Smetanyuk[1], B. Basara[2], M. Suffa[2], and E. von Berg[2]

[1]N. N. Semenov Institute of Chemical Physics
Russian Academy of Sciences
Moscow, Russia

[2]AVL LIST GmBH
Graz, Austria

Introduction

One of problems inherent in commercial computational fluid dynamics (CFD) codes used for simulating liquid spray penetration and vaporization is grid dependence of computational results. To some extent, this dependence arises due to inadequate treatment of drop parcels representing some ensembles of drops with identical properties. In the standard parcel model, a parcel containing N drops is assumed to be located in the same computational cell where the representative drop is located. Therefore, when passing through the cells of different volume, the moving parcel exhibits artificial (nonphysical) compression/expansion, i. e., the ratio of the interphase surface area of all drops included in the fixed parcel to the cell volume changes depending on the cell volume. The latter is equivalent to physical variation of the local drop suspension density causing the variation of the local rates of mass, momentum, and energy exchange with the gas flow. As a matter of fact, suspension density should be independent of cell volume.

This paper offers a new model of drop parcel which allows minimization of grid dependence of spray penetration and vaporization.

Model

In the new model, each parcel is treated as a finite-size cloud of N identical drops. In general, the size of the cloud (and therefore, the drop number density in the cloud) should change in time only due to physical processes like turbulent dispersion, dilatation, compression, etc. It is natural to assume that initially, a parcel is nothing else as the dense agglomerate of N drops (as it is currently treated in commercial CFD codes) with the characteristic size on the order of $(mN)^{1/3}$ where m is a single drop mass. However, in the course of time, individual drops in the parcel disperse in space due to various physical processes, thus leading to the growth of parcel volume (and decreasing the drop number density in the parcel). Once a moving parcel possessing a finite volume crosses computational cells, its drop number density should not depend on cell volume. To ensure it, it is suggested to smear drop parcels over computational cells as shown in Fig. 1. Clearly, in this case, the drop number density in the parcel is independent of the computational grid. On the contrary, the standard treatment of parcel shown in Fig. 2 makes obviously the drop number density grid-dependent. Moreover, the standard parcel concept is intrinsically deficient: the smaller the

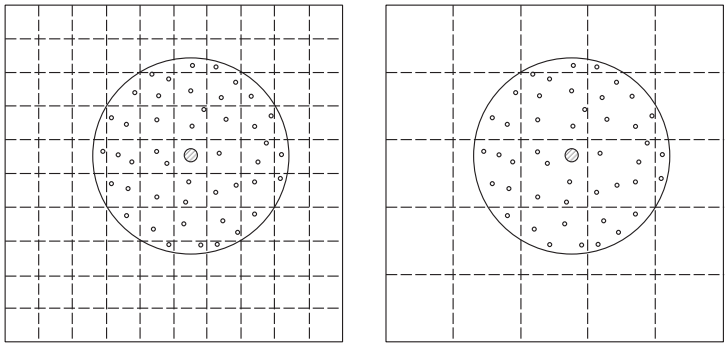

Figure 1 New treatment of drop parcel: drop number density in the parcel is grid independent. Large shaded circle denotes the representative drop in the parcel

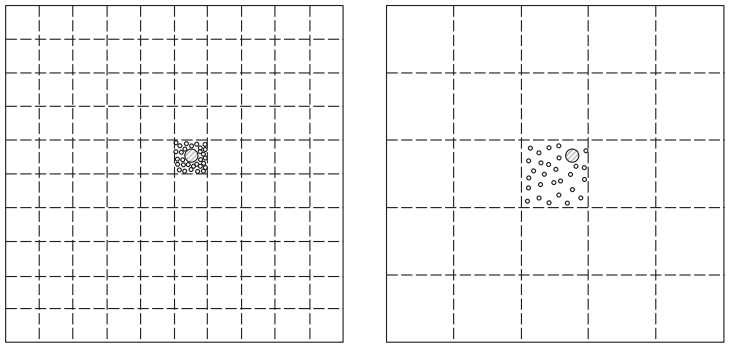

Figure 2 Standard treatment of drop parcel: drop number density in the parcel is grid dependent. Large shaded circle denotes the representative drop in the parcel

grid size, the worse is the model performance at a fixed number of drops in the parcel (drop number density tends to infinity).

According to Fig. 1, the interaction between a parcel and gas is no more concentrated in the computational cell where the representative drop is located. Within the new parcel model, all neighboring cells containing parcel drops should experience the effects of interphase mass, momentum, and energy exchange.

For adequate distributing mass, momentum, and energy fluxes among neighboring cells containing parcel drops, the following procedure is suggested. It is assumed that the effect of parcel on the gas state in a given computational cell is proportional to parcel volume in the cell. For calculating the volume (or surface area) of a complex object, one can use the random number approach. First, the region occupied by the parcel is filled with a certain number of random points with the uniform isotropic spectrum. Then, the relative number of points in each computational cell occupied by the parcel is determined. Thereafter, mass, momentum, and energy fluxes for the representative drop are calculated using gas parameters in the cell where it is located. At last, the integral fluxes of mass, momentum, and energy are distributed among neighboring computational cells proportionally to a relative number of

random points in each cell. This procedure guarantees that the parcel interacts with the same volume of gas regardless the grid cell size.

The parcel size can change in time due to various physical processes. For example, when emanating through the injector nozzle, a parcel can be as small as a dense pack of fuel drops, whereas in the course of time, its size increases due to drop collisions, spray expansion, turbulent dispersion, etc. At conditions of variable pressure (e.g., in Diesel engine), the parcel size can vary due to compression/expansion of the medium. For evaluating the rate of parcel growth, the problem of particles dispersion in the finite-volume cloud placed in the field of steady-state homogeneous isotropic turbulence was solved. As expected, the rate of parcel growth was found to be constant at fixed turbulence conditions and depended on turbulence intensity and frequency, drop size and mass, as well as ambient gas viscosity. As a result of systematic calculations, a simple correlation was derived which approximates the parcel growth rate as a function of all governing parameters.

Validation

The procedure outlined above was implemented into AVL FIRE code [1]. Discussed below are the results of different test calculations demonstrating advantages of the new model.

First, a series of test calculations for nonevaporating sprays in the field of constant turbulence was performed using three computational grids shown in Fig. 3. These grids are referred to as coarse (Fig. 3, left), medium (Fig. 3, middle), and fine (Fig. 3, right). The cell size in the central region of the computational domain in the coarse, medium, and fine grids was 10, 2.5, and 0.6 mm, respectively. The total number of cells in the grids of Fig. 3 was 490, 11,480, and 148,440, respectively. The spray injection direction was opposite to the z-axis in Fig. 3. The characteristic values of turbulent kinetic energy and its dissipation were taken constant and equal to 3000 m^2/s^2 and $7.71 \cdot 10^6$ m^2/s^3, respectively. The initial air temperature was 293 K, the initial pressure was 1 bar. The initial velocity of drop parcels at the exit of injector nozzle was taken equal to 320 m/s. The outer diameter of the nozzle was 0.2 mm, and the nozzle outer half-cone angle was 8°. All calculations were made for 10-micrometer n-dodecane drops.

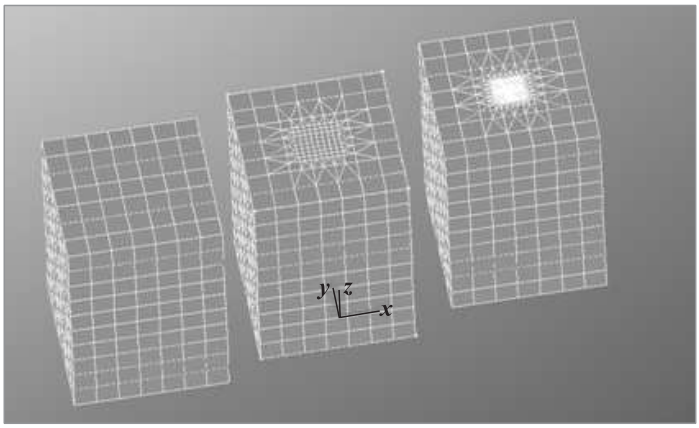

Figure 3 "Coarse" (left), "medium" (middle), and "fine" (right) computational grids used for simulating spray vaporization and penetration with the new and standard parcel models

Figures 4 and 5 show the results of calculations. The parcel size in the new model in this series of test calculations was taken constant. Figure 4 compares the predicted spray penetration lengths obtained with the new parcel model (solid curves) and with the standard parcel model (dashed curves). The new model provides grid independence of spray penetration (the results for coarse and medium grids overlap each other) for the test conditions chosen. Figure 5 shows the corresponding spray images obtained with the new parcel model.

Second, computer simulation of drop vaporization in the parcel was performed with the standard and new parcel models at different computational grids using AVL FIRE. Figure 6 shows the predicted temporal evolution of n-heptane drop diameter in the course of quiescent parcel vaporization in air at 1500 K and 1 bar in the field of homogeneous isotropic turbulence with the initial turbulent kinetic energy 60 m^2/s^2 and integral length scale 7 mm. The parcel was assumed to contain 100 identical 50-micrometer drops. For modeling drop vaporization, a model reported in [2] was used. The calculation was performed for two uniform grids with cells of different size. Curves *1* and *2* correspond to the standard parcel model, whereas curves *3* and *4* correspond to

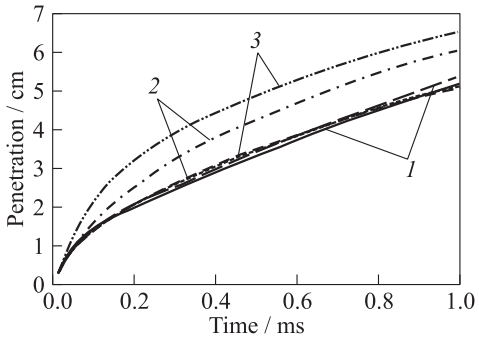

Figure 4 Comparison of predicted spray penetrations obtained with the new parcel model (solid curves) and with the standard parcel model (dashed curves) at coarse (*1*), medium (*2*), and fine (*3*) grids

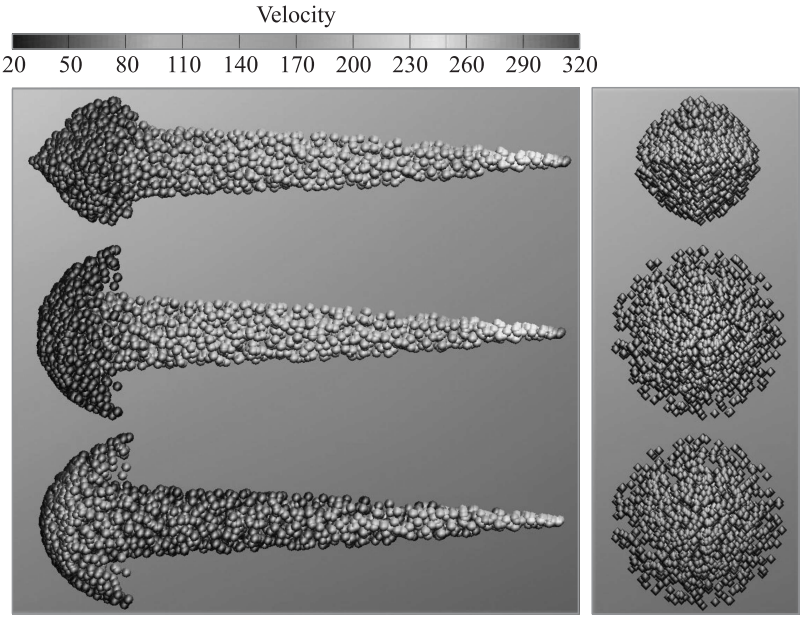

Figure 5 Spray images obtained with the new parcel model with coarse, medium, and fine grids (from top to bottom)

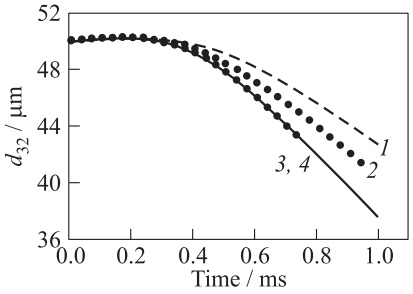

Figure 6 Predicted time histories of n-heptane drop diameter obtained with two uniform computational grids. Standard parcel model with different grid cell size: *1* — 1 mm and *2* — 2 mm; new model: *3* — 1 mm and *4* — 2 mm

the new model. Clearly, the new model provides grid-independence of parcel vaporization history in the special case of quiescent parcel.

Results

The new parcel model was used for predicting the penetration length of an evaporating spray and for comparing the results of calculations with experimental data obtained at AVL LIST GmBH for n-hexadecane spray and vapor penetration at injection pressure 300 bar and ambient air pressure and temperature 60 bar and 884 K, respectively. In the calculations, the spray was modeled without activating a break-up model as monodispersed with all drops possessing mean diameter $d_{32} = 13.3$ μm, with

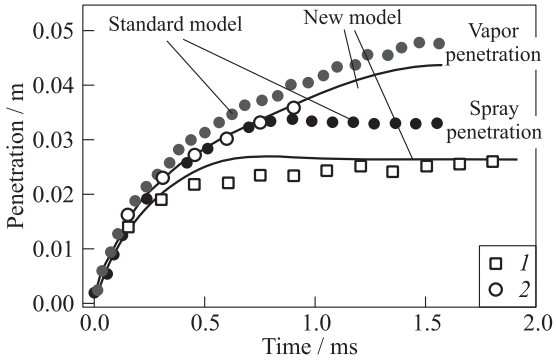

Figure 7 Comparison of measured (open symbols) liquid spray (*1*) and vapor (*2*) penetration lengths with those predicted by standard (closed symbols) and new (curves) parcel model

the spray outer half-cone angle 7°, and injection duration 1.9 ms, all taken from experiment. The drop vaporization model was the model of [2]. No parameter tuning was made. Figure 7 compares calculations with measurements. As is seen, contrary to the standard parcel model, under these simplified conditions, the new model provides the results correlating well with the experimental points.

Concluding Remarks

The new model of drop parcel in the liquid spray has been developed and validated. The model suggests that drop parcels have finite time-variable sizes which keep the local instantaneous drop number density consistent independently of local grid resolution. Test calculations for sprays indicate that the new model is considerably more grid-insensitive than the standard parcel model. More tests will be performed in the future including break-up models and temporal evolution of parcel diameter due to variable turbulence conditions in the computational domain. Then, the new model can be used for simulating Diesel engine operation.

Acknowledgments

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