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Additions to the Particle Transport and Diffusion Model for *FLOW-3D*

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1. Introduction

Discrete particles are very useful for the modeling of pollution dispersal, certain types of two-phase flow, mixing of materials, and tracking selected regions of fluid. A brief description of the particle model in Version 6 of *FLOW-3D* can be found in Flow Science Technical Note No. 39 [1]. In this model, particle motion is semi-coupled to the fluid flow in a way that particles do not influence fluid velocity around them, nor do they displace any volume of fluid.

In the sections below the following additions to the basic particle transport model are presented:

- capability of modeling multiple mass particle species
- new fluid-particle drag model
- volumetric particle sources

Species include particles with the same property, density or diamater. These additions and modification do not alter the original (Version 6) particle setup, so that in most cases users should be able to run their old problems without adjusting the input decks.

Sections 2 to 5 contain a brief description of the additions to the particle model and additional plotting features. Changes that may affect simulation results using old input decks (written for Version 6) are outlined in Section 6. The results of a number of calculations demonstrating the new features are given in Section 7.

2. Multiple Mass Particle Species

The capability of handling multiple species is useful for modeling, for example, the efficiency of dust separators or the behavior of foreign inclusions in molten metals. The particle transport model of Version 6 of *FLOW-3D* only allows the user to have a single type of particle in the flow: either marker particles (*i.e.*, particles with zero mass) or mass particles with fixed density, PRHO, and volume, PVOL.

The multiple species model allows the user to have an unlimited number of different species bound only by the total number of particles in the flow. The following is a brief description of the model.

- In a simulation, particles can be either of two types: constant density and variable size or constant size and variable density; marker particles can be used in either case as a species.
- As before, particles can be generated as an initial block of particles and/or at a number of locations in the fluid. The initial block and each of the sources can have independent species setup, but either density or diameter must be constant for *all* particles in the flow.
- At every source the particle density or diameter varies by a constant increment derived from the user-specified total number of species and the range of the variation of the parameter. For example, if ρ_1 and ρ_2 are the bottom and top limits for the particle density, respectively, and N_p is the total number of particle species, then the density between different species will vary by a multiple of $\Delta\rho = \frac{\rho_2 - \rho_1}{N_p - 1}$
- The distribution of species populations is uniform. The actual number of particles in a species can vary between species since the code employs a random number generator to populate species with particles.

3. Fluid-Particle Drag Force

A drag force is imposed on a particle when it moves in a fluid . This force is only applied to mass particles (the drag is effectively infinite for marker particles) but not to the fluid. The equation that governs particle motion has the following form

$$\frac{d\mathbf{u}_p}{dt} = \mathbf{g} - \frac{1}{\rho_p}\nabla P + \alpha \cdot (\mathbf{u} - \mathbf{u}') + \beta \cdot (\mathbf{u} - \mathbf{u}') \cdot |\mathbf{u} - \mathbf{u}'|$$

where $\mathbf{u}_p$ and ρ_p are the particle mean velocity and density, respectively, $\mathbf{g}$ includes gravity and other body forces, $\mathbf{u}$ and P are fluid velocity and pressure, respectively, $\mathbf{u}'$ is the full particle velocity, which is the sum of $\mathbf{u}_p$ and the diffusion velocity [1], and α and β are the drag coefficients. Since the drag coefficients are specified by the user and are constant, the model does not describe accurately the variation of the drag force with particle size.

An additional drag force, $\mathbf{F}_D$, has now been added to take into account the variation in particle size. The additional drag force model is based on an empirically derived function that ties the value of the drag coefficient, $C_D = \frac{8|\mathbf{F}_D|}{\rho U^2 \pi d^2}$, to the Reynolds number in the flow around the particle, $Re = \frac{d\rho U}{\mu}$. For a steady flow around a sphere this coefficient is [2]:

$$C_D = \frac{24}{Re} + \frac{6}{1+\sqrt{Re}} + 0.4 \qquad (1)$$

where

$$\mathbf{F}_D = C_D \cdot \frac{\rho U \pi d^2}{8} \cdot (\mathbf{u} - \mathbf{u}') \qquad (2)$$

is the drag force, $U = |\mathbf{u} - \mathbf{u}'|$, d is the particle diameter and μ is the fluid dynamic viscosity coefficient. Equation (1) is a good approximation for the drag force in a range of Re values from 0 to 10^5 as shown in Fig. 1. For small Reynolds numbers the drag force approaches the Stokes analytical solution for a viscous laminar flow around a sphere without separation.

The new expression for the drag force takes into account the particle size and mass therefore it is more appropriate for use in simulations with multiple particle species.

4. Volumetric Particle Sources

The capability of introducing point sources for particles has been extended to include volumetric sources. These sources have x_{min}, x_{max}, y_{min}, y_{max}, z_{min}, z_{max} spatial limits within which particles are generated randomly at a given rate. This capability allows a user to specify 2-D or 3-D particle sources, for example, at inlets. All particles generated at a source have the same initial velocity specified by the user.

5. Additional Plotting Capabilities

A number of new particle plotting options have been added to the code to help with visualizing different particles. In addition to the existing capability of color shading the particles according to the value of the third coordinate on a 2-D plot, particles can also be shaded according to the value of the particle density or diameter, the u-, v- or w-velocity components, or the particle velocity magnitude. The new plotting capabilities can be used for both 2-D and 3-D particle plots.

6. Changes That May Affect Simulation Results Using Old (Version 6) Input Decks

A. Particle - Free Surface Interaction

The modeling of the behavior of particles in the vicinity of a free surface has been modified. The old model would either remove a particle if it appeared to be in the void or reflect it from the free surface as if it were a solid wall.

In the modified model, particles are either allowed to leave fluid and enter void regions, in which case their dynamics are described by ballistic trajectories, or they are forced to stay in the fluid. In the latter case, particles that are trying to escape fluid are assumed to be held back by the free surface and their position is adjusted so that they stay at the free surface; they are allowed to move only along the free surface or *into* the fluid.

In either particle behavior mode near the free surface, massless marker particles are not allowed to leave the fluid at all. The actual mode is chosen through input using the variable FSRST. When particles *are* allowed into the void, then sources can also be set in the void regions.

This modification is intended to describe the free surface more like a flexible film that can "catch" small particles due to surface tension effects, rather than a solid wall reflecting them.

B. Drag Force Addition

The new drag force addition introduces an additional input variable which is the third drag coefficient PDRG3. PDRG3 is simply a multiplier for the drag force specified by equation (2). The default value of PDRG3 is 1.0 (and PDRG1=PDRG2=0.0), so that the drag force will be present in the dynamics of mass particles moving in a viscous fluid unless the user sets PDRG3 to zero. If the locally evaluated fluid viscosity is equal to zero (*e.g.*, in a void region), then a drag force will not be computed.

C. Defaults

The default values of the particle point source coordinates are changed to be outside the mesh rather than at the origin of the coordinate system as they were in the original (Version 6) model.

7. Test Simulations

The sections below contain brief descriptions and results of simulations that are designed to test and demonstrate the new particle model capabilities. In all of these simulations, particle diffusion effects are not included.

A. Drag Model Test 1

In this simulation, three particle point sources are specified in a quiescent fluid of density 1.0 g/cm^3 and viscosity 1.0 cm^2/s. Particles of variable density (IPTYPE=2) are generated at each source at a rate 5 s^{-1} with an initial velocity of 0.04 *cm/s* and a diameter of 10 *cm*. Each source generates a single particle species of density 0.2, 2.0 and 20.0 g/cm^3. In this case the maximum Reynolds number in the flow around the particles is equal to 0.4 as each particle is emitted. The particle velocity then decreases due to the drag given by equations (1) and (2) and eventually the particle stops.

Figure 2 shows the results of the calculation at 150 seconds. It can be seen that the lighter particles travel the shortest distance before coming to a stop, while the heaviest have enough energy to move all the way across the domain, which is 1 *cm* wide. Since the Reynolds number is small, the drag force is close to the Stokes drag; the maximum difference between the Stokes drag and the one given by equation (1) is less than 7% and the difference decreases quickly as the particle moves away from the source. The analytical solution for the total distance traveled by a particle with density 2.0 *g/cm³* from the source using the Stokes solution is 4/9 *cm*, which is close to the distance seen in Fig. 2 (middle source).

B. Drag Model Test 2

In this simulation, 10 particle species (with density varying from 0.01 to 10.0 *g/cm³* and a diameter of 1.0 *cm*) are injected at a point source with an initial y-velocity of 4 *cm/s* into a fluid (with density 1.0 *g/cm³* and viscosity 0.01 *cm²/s)* moving in the x-direction at a constant uniform speed of 3 *cm/s*. Gravity is absent, so that particle trajectories are affected only by inertia and drag.

Figure 3 shows the particle trajectories; the lightest particles behave like marker particles and move with the flow, while the heaviest particles protrude the farthest into the fluid.

C. Flow in a Curved Duct: Point Source

In this simulation a single point source of 10 particle species is located at the entrance to a 180 degree bend (10.0 *cm* $<r<$ 20.0 *cm)* in which there is a steady flow of fluid with density 1.0 *g/cm³*, viscosity 0.01 *cm²/s*, and angular velocity of 0.3 *rad/s*. All particles have a fixed diameter of 1.0 *cm* and density varying between 0.01 and 10.0 *g/cm³* and velocity at the source of 4 *cm/s*. All particles are assumed to reflect without loss of energy at the duct walls (PCRST=1.0).

Figure 4 shows the steady state solution for particle trajectories for the case when a constant drag coefficient, α, is used by specifying PDRG3=0.0 and PDRG1=0.001. The difference in particle motion occurs only because of the buoyancy effects; the lightest particles (density 0.01 *g/cm³*), for example, are pushed towards the inward wall of the duct due to the pressure gradient in the positive radial direction.

Figure 5 shows the steady state particle trajectories when equation (1) is used for the drag force coefficient. Particle motion is more diverse in this case due to variation of the drag coefficient as well as the particle mass. The trajectories of heavier particles are closer to straight lines than the trajectories of lighter particles.

D. Flow in a Curved Duct: Distributed Source

In this simulation the duct dimensions are ten times larger than in the previous case (Section C) and the fluid density is 0.001 *g/cm³*, which is much smaller than that of the particles, minimizing the buoyancy effects on particle motion. The fluid has a viscosity of 10^{-5} *cm²/s* and moves at a constant angular velocity of 0.3 *rad/s*. Two particle species are introduced at a distributed source at the inlet at a rate of 100 particles per second with an initial velocity of 45 *cm/s* in the azimuthal direction. The source has zero thickness in the θ-direction and extends across the whole area of the inlet. The particle densities are 0.01 and 10.0 *g/cm*^{3} and the diameter is 1 *cm*. The Re-dependent drag coefficient is used in the simulation.

Figure 6 shows the distribution of the particles in the flow after 40 seconds of simulation time. The lighter particles (light shading) collect at the outer wall of the duct, while the heavier particles are scattered around due to reflection off the walls. There are two regions near the inner wall with no particles in them: at $\theta=60°$ and at $\theta=180°$.

E. Buoyant Particles

In this test a number of particles of three species are introduced into a fluid as an initial block of particles (Fig. 7a). The fluid of density 1.0 *g/cm*^{3} is quiescent with a hydrostatic pressure distribution in the z-direction. The particle densities are 0.5, 1.0 and 1.5 *g/cm*^{3} so that the lighter particles should float upwards, the heavier ones should sink, and particles of the same density as the fluid should not move at all. Particle diameter here is 0.001 *cm* and the Re-dependent drag coefficient is used in the simulation.

Figures 7b and c show the distribution of particles at 28.2 and 35.2 seconds after the start of the simulation. The results are as expected.

F. Particle Behavior in Voids

In this simulation, pressure distribution in the fluid is hydrostatic, fluid density is 1.0 *g/cm*^{3}, and viscosity is 0.01 *cm*^{2}*/s*. Particles have a fixed density of 1.0 *g/cm*^{3} and diameter 1.0 *cm*. They are generated at a point source at a rate of 300 particles per second. In both cases the Re-dependent drag coefficient is used, and particles are allowed to move into void (FSRST=1.0).

The source is placed outside the fluid, 8.0 *cm* above the free surface, and the initial velocity has a horizontal component of 10.0 *cm/s*. As can be seen in Fig. 8, after leaving the source and before reaching the free surface, particles follow a parabolic trajectory. On entering the fluid the particles move along a straight line since the buoyancy force balances gravity. The drag force slows the particles until they come to a complete stop.

G. Particle Behavior at a Free Surface

In this simulation a particle point source is placed in a fluid with the same properties as in the previous calculation (Section F). Particles here cannot penetrate the free surface (FSRST=0.0). The particle density is 1.008 *g/cm*^{3} (slightly heavier than the fluid), and at the source the velocity has components in the x-direction, 25.0 *cm/s*, and the z-direction, 100.0 *cm/s*. The fluid moves downward at a constant velocity of 2 *cm/s* with a hydrostatic distribution of pressure in the z-direction. The drag coefficient is Re-dependent.

As the particles move upward, they reach the free surface where their vertical velocity is reset to zero while continuing to move in the horizontal direction (Fig. 9a). Since the particles are heavier than the fluid, they start to sink after being stopped at the free surface (Fig. 9b). As soon as the free surface moves below the source, the particles are no longer generated at the exposed source (Fig. 9c).

References

1. M.R.Barkhudarov and J.L.Ditter, "Particle Transport and Diffusion," Flow Science Technical Note #39, August 1994 (FSI-94-TN39).

2. Frank M.White, Viscous Fluid Flow, McGraw-Hill Book Company, New York, 1974.

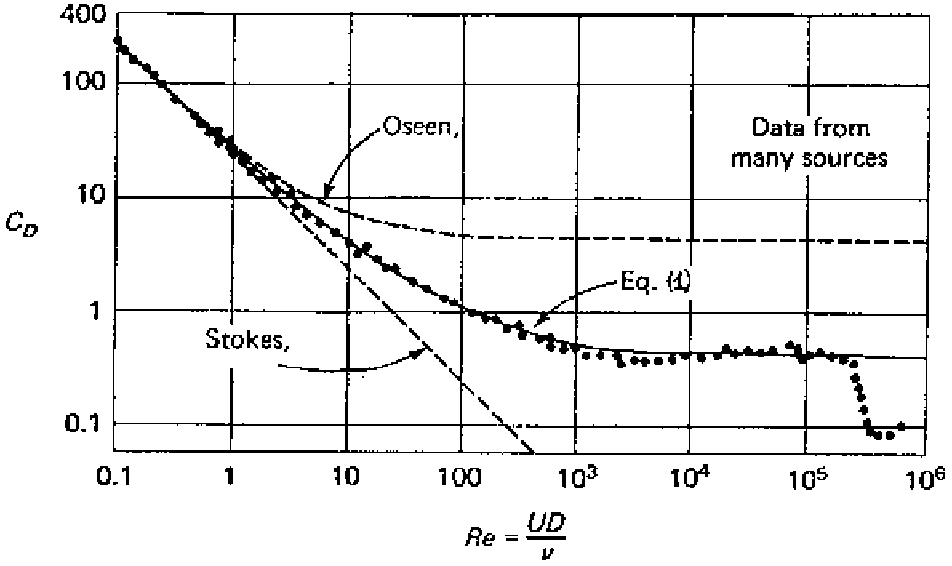

Fig. 1. Comparison of experiment, theory, and the empirical formula given by equation (1) for drag coefficients of a sphere in a steady state viscous flow [2].

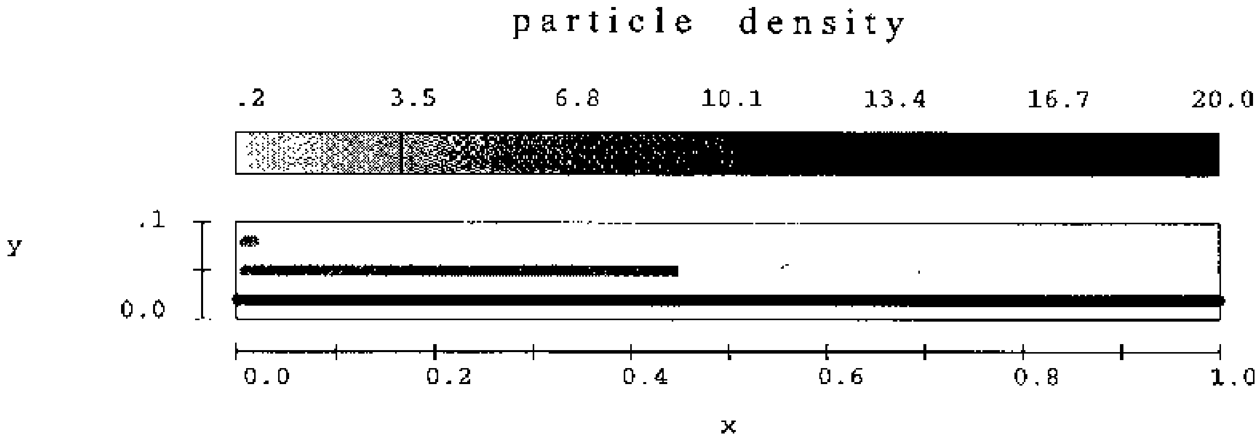

Fig. 2. Comparison of total distances traveled by particles of three different densities from point sources at the left boundary to a complete stop. The drag coefficient is Re-dependent and the fluid is quiescent.

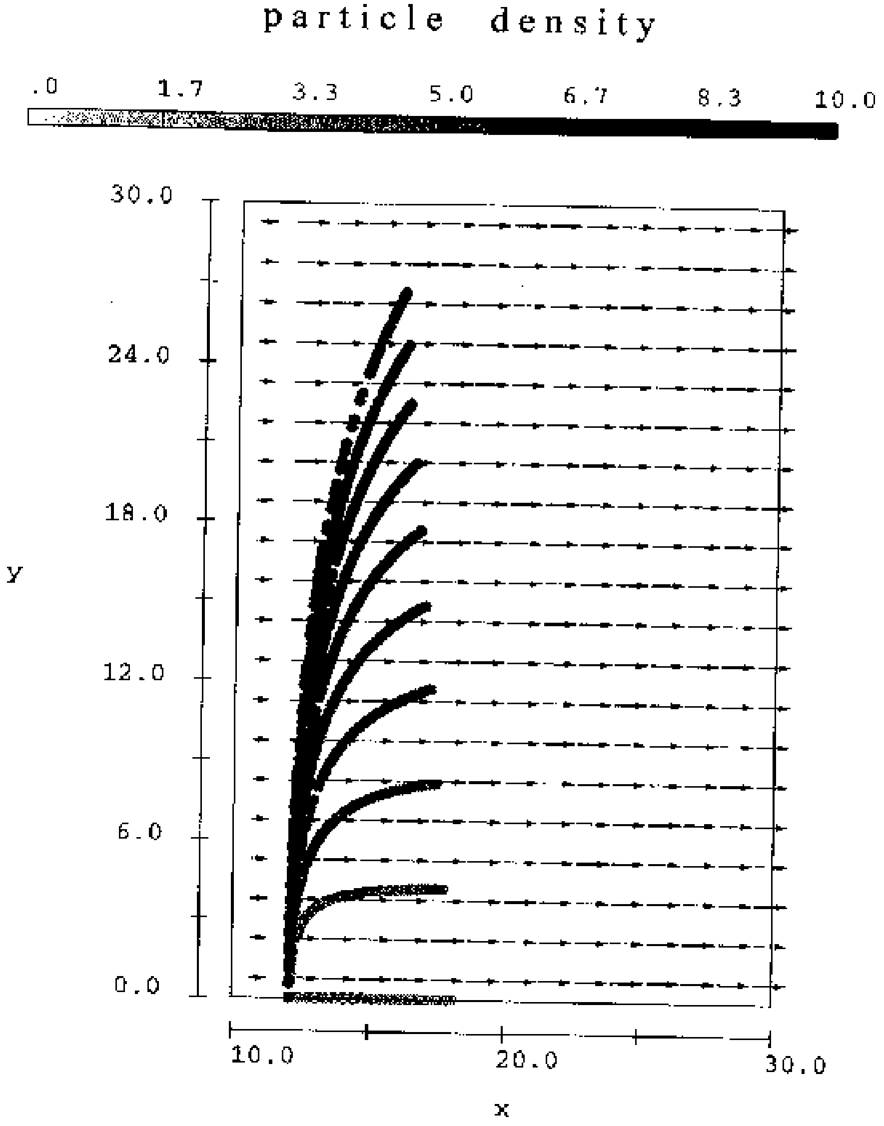

Fig. 3. Trajectories of particles of 10 different densities injected in the vertical direction into a fluid moving horizontally. Re-dependent drag, the time is 20 seconds from the start the simulation.

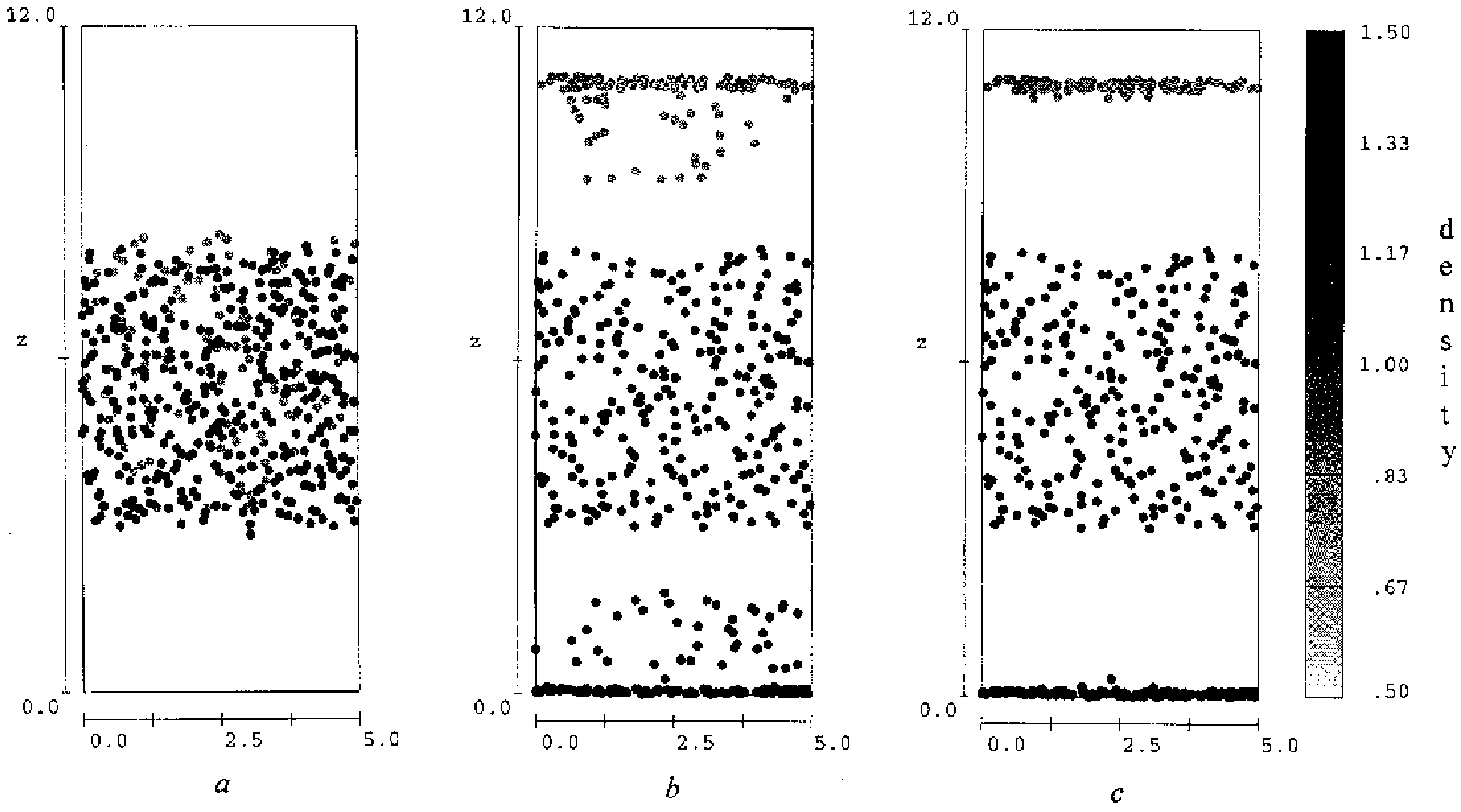

Fig. 7. Three particle species, differing by density, floating in a quiescent fluid with hydrostatic pressure distribution in the z-direction. Initially particles are randomly placed within a fluid region (*a*), then the heaviest particles (black) sink to the bottom, the lightest (light gray) float to the top, and the particles with the density of the fluid (dark gray) remain at the initial locations (*b,c*). Re-dependent drag coefficient.

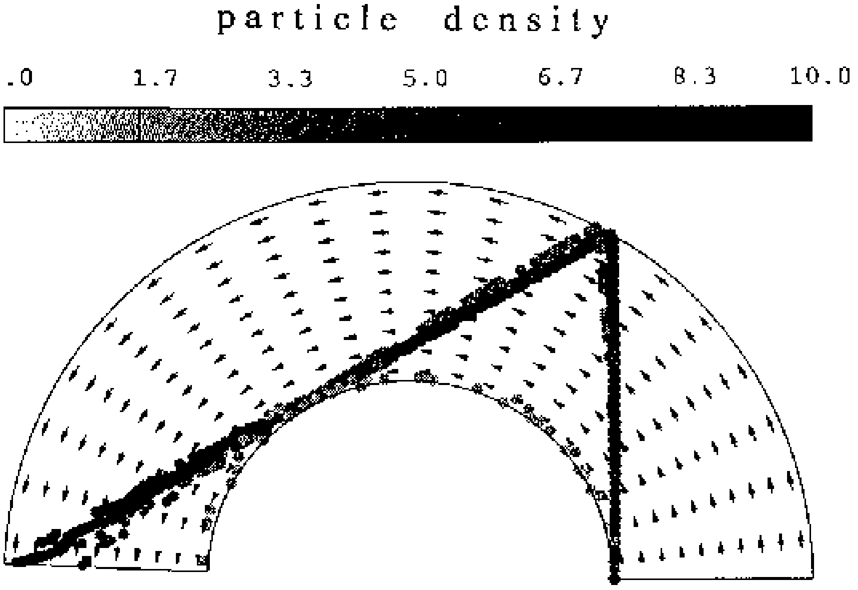

Fig. 4. Trajectories of particles of 10 different densities in a fluid moving at a constant angular velocity in a curved duct. Constant drag coefficient.

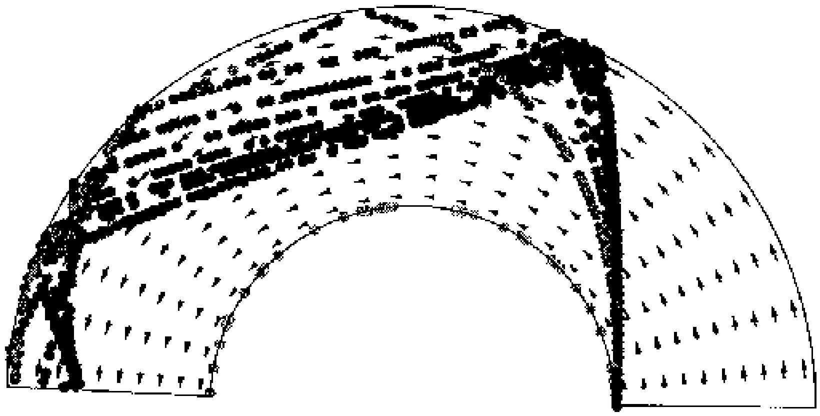

Fig. 5. Same as in Fig. 4 but with the Re-dependent drag coefficient.

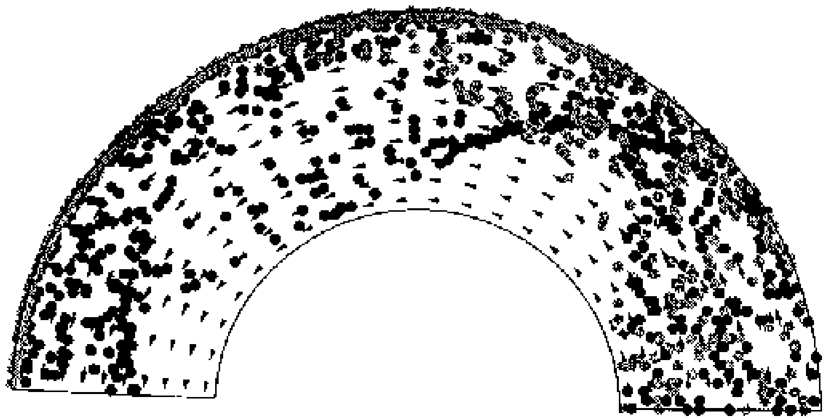

Fig. 6. Trajectories of two particle species with different densities in a fluid moving at a constant angular velocity in a curved duct. Particles originate from a source distributed across the inlet with the heavier particles shaded black. Re-dependent drag coefficient. The duct dimensions are ten times larger than those in Figs. 4 and 5.

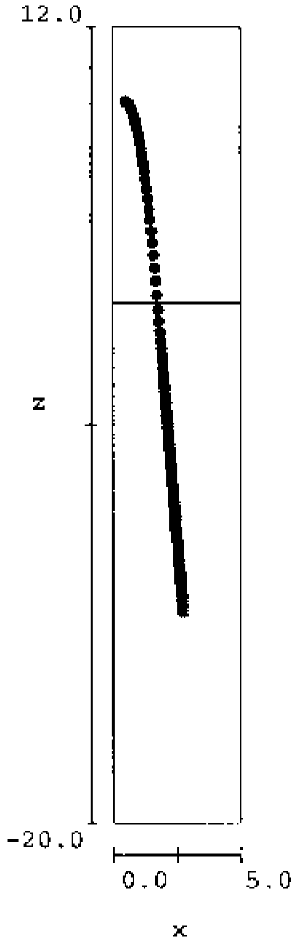

Fig. 8. Trajectory of particles with the same density as the fluid falling from a point source in a void into a quiescent fluid with hydrostatic pressure distribution. Re-dependent drag coefficient.

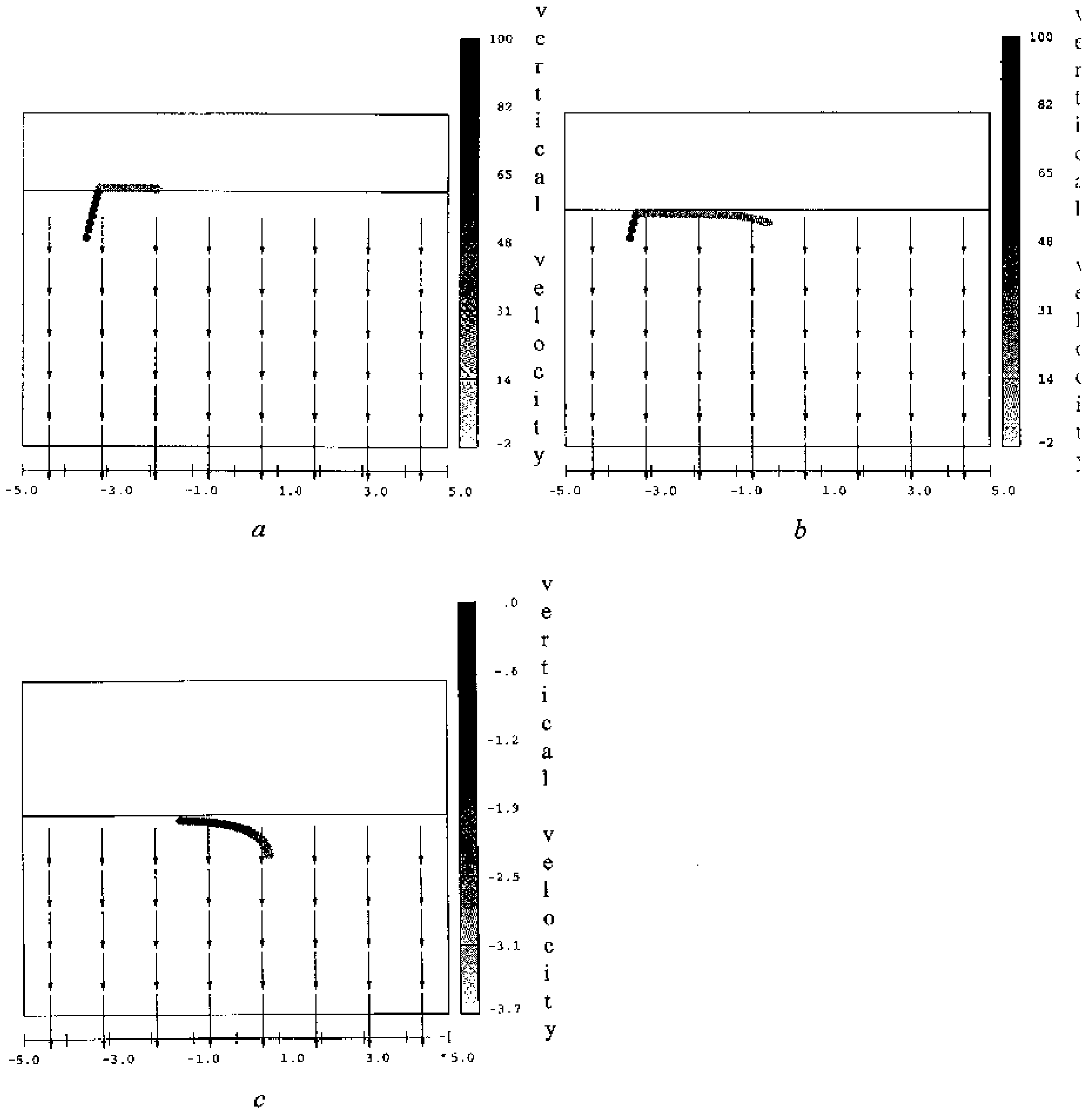

Fig. 9. Particle motion in a case when particles cannot penetrate the free surface. Particles are generated at a source which initially is located in the fluid (*a*). The initial particle velocity at the source has positive horizontal and vertical velocity components. Particle upward motion ceases at the free surface and particles start to sink since they are heavier than the fluid (*b,c*). As the free surface moves downwards and the source appears in the void, particles are no longer generated (*c*).