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Particle Transport and Diffusion

M. Barkhudarov and J.L. Ditter
Flow Science, Inc.
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1. Introduction

Discrete particles are very useful for the modeling of pollution dispersal, certain types of two-phase flow, the mixing of materials and tracking selected regions of fluid. In the following sections a brief description of the particle model in Version 6.0 of *FLOW-3D*® is presented together with some examples of particle motion.

2. The Main Equation

The motion of a particle is governed by equation

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

where $\mathbf{u}_p$ and ρ are the particle mean velocity and density, respectively, **g** includes gravity and other body forces, **u** and P are fluid velocity and pressure, respectively, and α and β are the drag coefficients divided by the mass m of the particle. The drag coefficients characterize the interaction between the particle and surrounding fluid. Note that both α and β vary with the mass of the particle. At present the influence of the particle motion on the fluid is neglected.

Particle diffusion is described by the diffusion velocity $\mathbf{u}_{diff}$ which is calculated by Monte Carlo technique and added to the mean velocity. Each of the three components of the diffusion velocity is computed in terms of the inverse error function as

$$u_{diff} = \sqrt{\frac{4\lambda}{\Delta t}}\, erf^{-1}(y)$$

where y is a random number between zero and one, λ the particle diffusion coefficient and Δt is the time-step size in the numerical scheme. The sign of $\mathbf{u}_{diff}$ is also chosen randomly. In this form the diffusion velocity is mathematically equivalent to the one given by the Sklarew technique[1]

$$\mathbf{u}_{diff} = -\lambda \frac{\nabla(m \cdot C)}{m \cdot C}$$

with C denoting the particle concentration. It can be shown that if many particles are placed at a point, this Monte Carlo technique will produce a Gaussian distribution of mass about the point. The statistical method employing random numbers proves to be a better approximation of the particle diffusion process in highly distorted flows and/or coarse meshes when the gradient $\nabla(m \cdot C)$ cannot be resolved accurately.

In the above formulation, diffusion is caused by turbulence in the fluid. If there are no forces acting between a particle and the fluid ($\alpha,\beta=0$), then the particle does not diffuse. In terms of FLOW-3D input parameters, particle diffusion is specified by either or both of the two variables: NUP and RMPART. The first one is a constant particle diffusion coefficient, while the second is the inverse Schmidt number. If ν is the fluid kinematic viscosity, the total particle diffusion coefficient is

$$\lambda = NUP + \nu \cdot RMPART$$

Note that ν can vary in space and time due to the presence of turbulence in the fluid.

The influence of the particle mass comes through the values of the drag coefficients. The heavier a particle the smaller are the values of α and β, hence, the smaller the influence of the fluid on the particle. The mass of the particle is defined by the two input variables: particle volume, PVOL, and density, PRHO. If a zero (default) value of PVOL is used, the particle becomes a simple marker particle which follows the mean fluid flow plus diffusion, effectively meaning an infinite drag coefficient.

Reflection from a rigid boundary is controlled by a coefficient of restitution, PCRST. When PCRST=1.0, the reflection is specular, while PCRST=0.0 results in no reflection, *i.e.,* sticking. The value of PCRST can be set to any value between 1.0 and 0.0. For example, PCRST=0.3 will result in a reflected velocity equal to 0.3 times the incident velocity.

At present only one particle species can be described at a time. Those can be introduced either by specifying a particle point source with a constant rate (particles per unit time) and velocity or by initializing a brick-shaped block of particles at the beginning of simulation, or by a combination of both.

3. Particle Mean Motion

The ability of FLOW-3D to calculate the mean motion of mass particles can be tested by injecting a single particle into a uniform stream of air. If the particle is small (< 5 microns), then the flow about the particle can be assumed to be Stokes flow. Stokes flow is encountered when the Reynolds number based on particle diameter is much less than 1 so that inertia effects can be neglected. This is true for sand particles whose diameter is less than 0.006cm and water droplets whose diameter is less than 0.004cm[2].

The drag force on a micron-sized spherical particle can be found from Stoke's law for resistance to a moving sphere[2]. According to this law, the drag force acting parallel to the particle's velocity U is

$$D = 6\pi a \mu U$$

where the parameter a is the particle's radius and μ is the viscosity of the mean flow. Under the assumption of Stokes flow, the acceleration of the particle in the x-direction is given by:

$$\frac{du}{dt} = K(u_0 - u)$$

where u is the instantaneous velocity of the particle, u_0 is the x-component of the mean flow velocity, and K is the drag coefficient on the particle divided by its mass. The coefficient K is then expressed as

$$K = \frac{6\pi a \mu}{Particle\ Volume * Particle\ Density}$$

Integrating the relation for particle acceleration once gives

$$\ln|u_0 - u| = -Kt + c_0$$

Assuming that the particle was injected with only a vertical velocity component, the initial condition would be u=0 at t=0 so we get $c_0 = \ln u_0$. The relation for the x-component of velocity is then

$$u = u_0\left(1 - e^{-Kt}\right).$$

Integrating once again and applying the initial condition x=0 at t=0 we get

$$x = u_0\left(t + \frac{e^{-Kt} - 1}{K}\right) \tag{1}$$

which represents the x-coordinate of the particle position with time. In the y-direction the boundary condition is $v = V_0$ at t=0 since the particle is injected into the stream with only a vertical component V_0. The relation for the y-coordinate of the particle position is then

$$y = -\frac{V_0}{K}\left(e^{-Kt} - 1\right). \tag{2}$$

An example which can be used to test FLOW-3D's ability to compute the trajectory of a mass particle could be one in which a 5μm particle is injected with a vertical velocity of 2500cm/s into uniform stream of air moving at 250 cm/s (See Figure 1). The particle is injected into the stream at the point x=0, y=0. Assume for simplicity that the particle has the density of water, 1 gm/cc. The viscosity of air is 0.01 gm/cm-s. Computing K from these parameters gives

$$K = 7.2 * 10^5$$

To simplify the solution, FLOW-3D can be set to skip the computation of the flow field and instead to use a defined flow field to compute the particle trajectories. This is done by specifying the parameter IPONLY=1. The complete input for this file is shown in Appendix A. Since the flow field is steady, the pathlines of the particles can be represented by releasing a series of

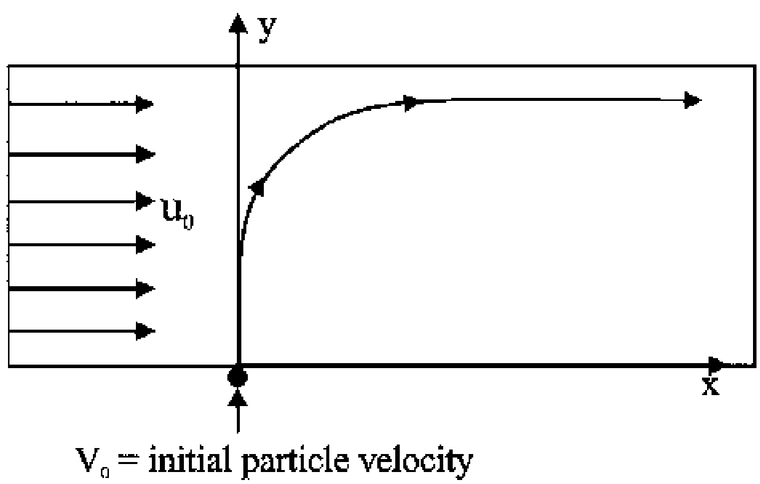


Figure 1. Single particle with mass injected into a uniform stream of air.

particles from a source at (0,0) and plotting their positions at some point in time.

The theoretical prediction of the particle trajectory given by equations 1 and 2 can be integrated numerically and compared to the results of FLOW-3D. The results of this are shown in Figure 2. The results are nearly identical, indicating that FLOW-3D very accurately computes the mass particle trajectory.

4. Particle Diffusion

Next, examples are given of particle motion with diffusion in straight and curved (180^0 turn) ducts. The influence of the particle mass and the level of turbulence in the fluid (through the fluid turbulent viscosity) are shown.

a) Diffusion from a Point Source

In this test simulation 2000 marker particles are initiated at t=0.0 *s* at a point in a quiescent flow and diffuse in the *x*-direction. The diffusion coefficient is 0.1 cm^2/s. In Figure 3, *a,b* shows the distribution of the particle concentration, normalized by the total particle number, with distance. The theoretical Gaussian distribution is also plotted for comparison. It can be seen that the accuracy of the Monte Carlo technique is sufficient to describe particle diffusion, especially if a large number of particles is involved.

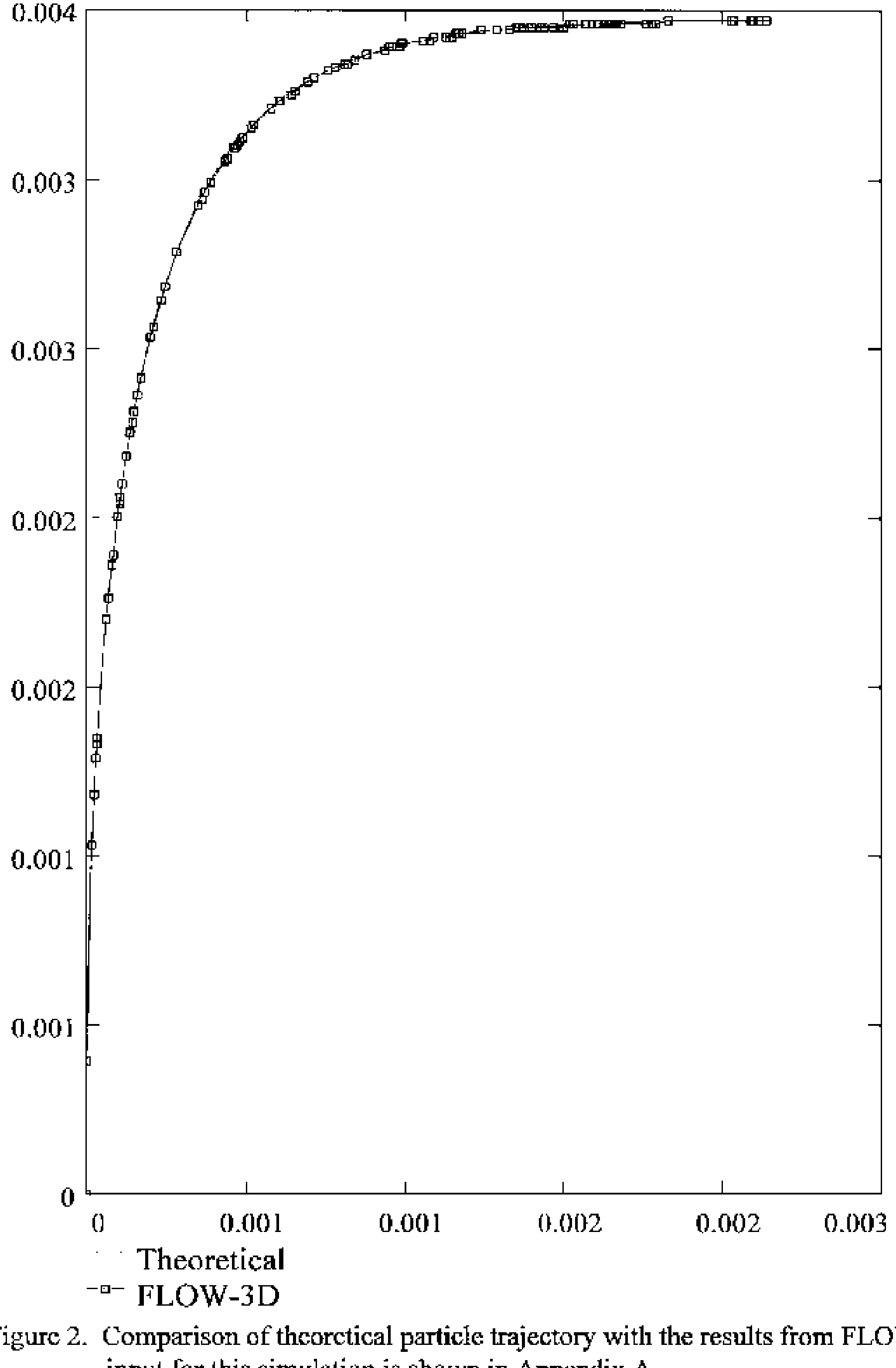
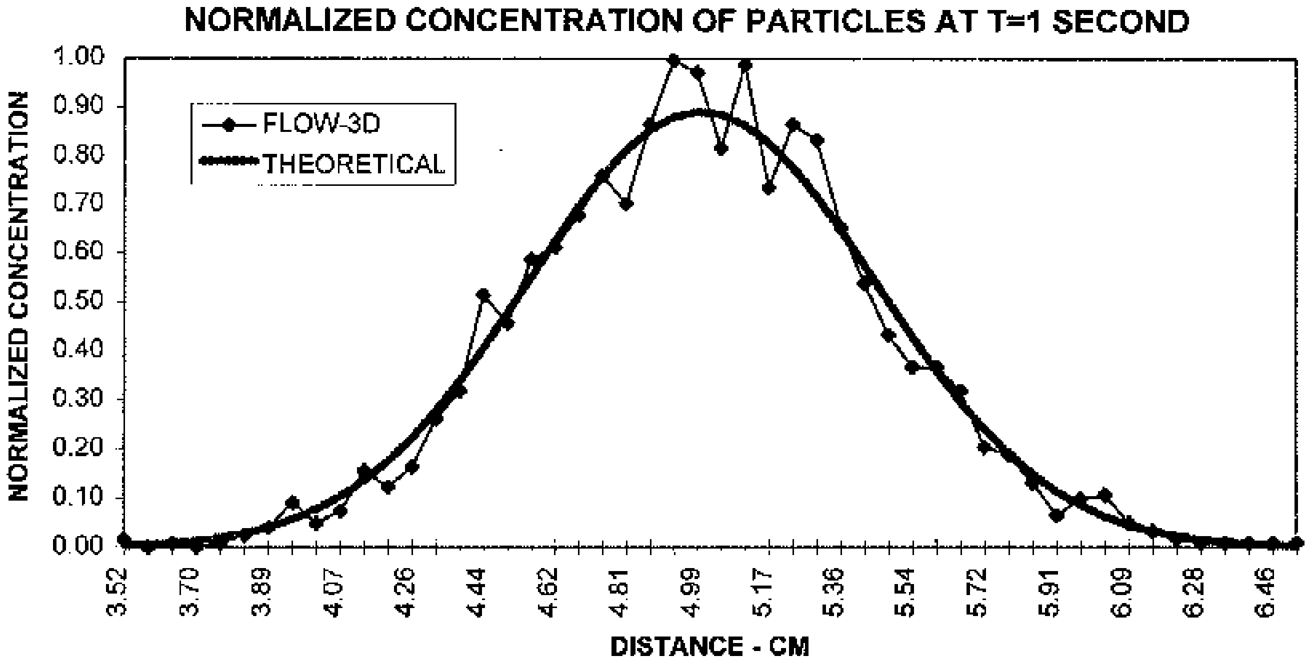


Figure 2. Comparison of theoretical particle trajectory with the results from FLOW-3D. The input for this simulation is shown in Appendix A.



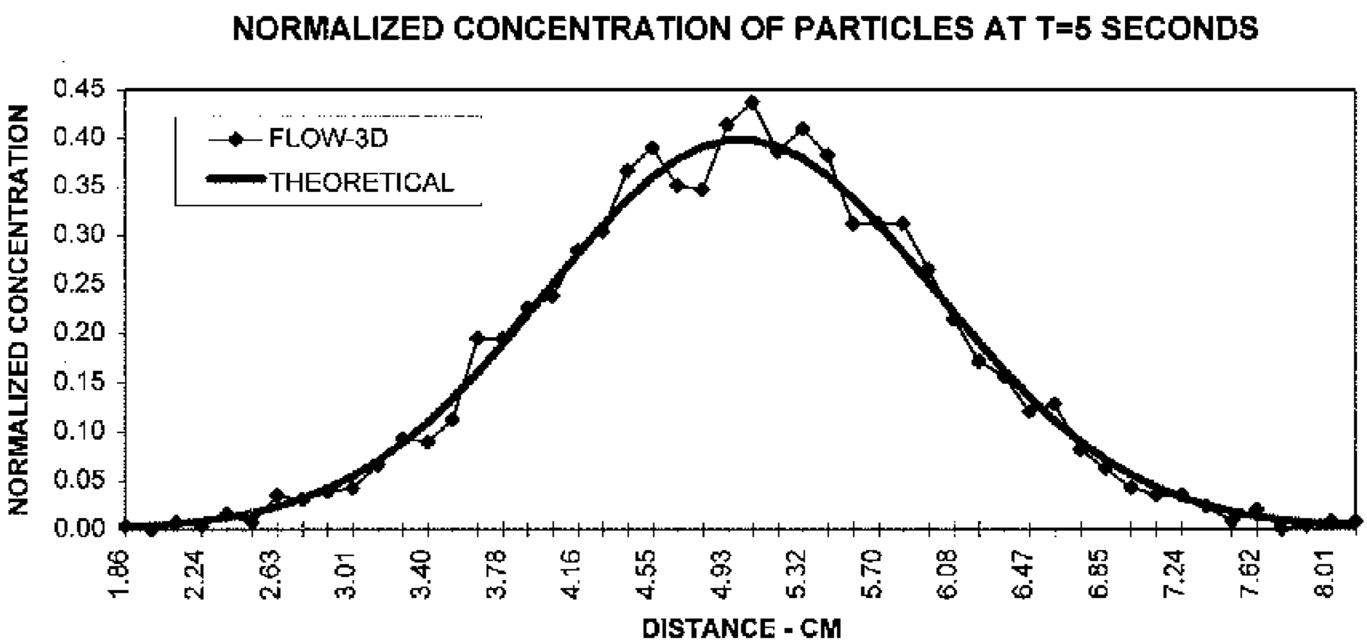


Figure 3. Normalized particle distribution in the problem of 1-D diffusion from a point source at (a) t=1.0 s and (b) t=5.0s as compared to the theoretical curve.

b) Flow in a Straight Duct

In this 2-D simulation, the fluid (water) moves along a straight, 10 *cm* wide channel at a constant, uniform velocity of u_0=2 *cm/s*. There is no gravity and the channel length is 20 *cm*. A particle source is located near the right (inlet) mesh boundary. The source rate is 100 particles per second with the particle velocity at the source equal to the fluid velocity. The Schmidt number is assumed to be equal to 1.0, while NUP is set to zero.

The particle volume is 6.55e-11 cm^3 corresponding to the spherical radius of 2.5 μm. The quadratic drag coefficient is β=0 for all simulations. The fluid velocity is assumed to be constant and uniform throughout the simulation so that the solution of the flow equations can be skipped and only the particle dynamics are solved. This is done by setting IPONLY=1.

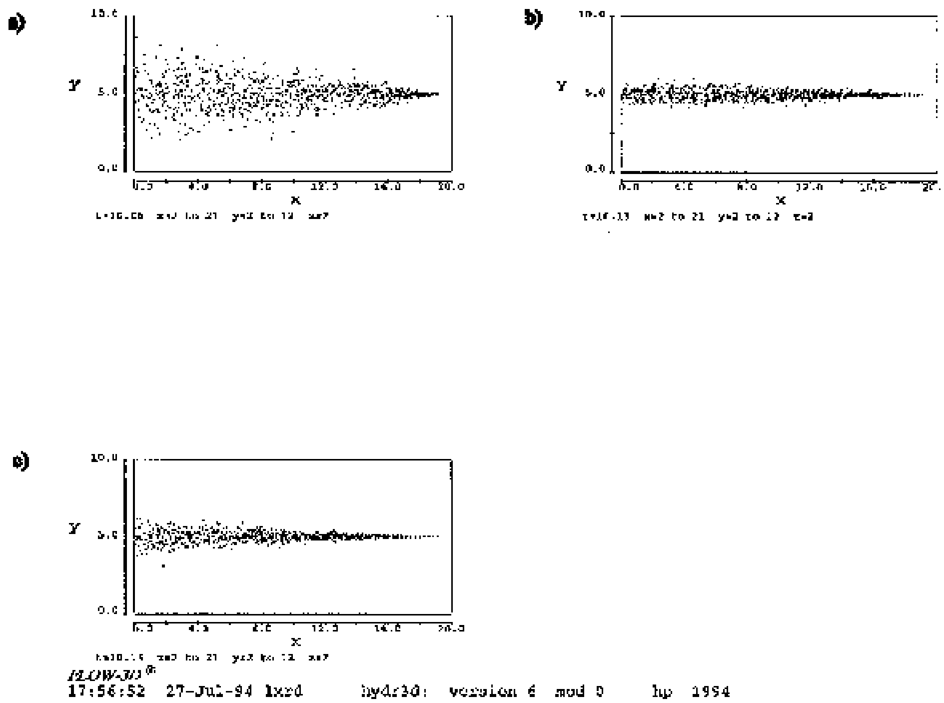


Figure 4. Particle transport from a point source in a uniform flow.

The three parameters that are varied are α, ρ and μ. The linear drag coefficient varies with the density according to $\alpha \propto 1/\rho$. For the three plots shown in Figure 4 these parameters are:

a) light particles, high turbulence: $\rho = 100\ g/cm^3$, $\alpha = 1.0\ s^{-1}$, $\mu = 0.1\ \frac{g}{cm \cdot s}$;

b) light particles, low turbulence: $\rho = 100\ g/cm^3$, $\alpha = 1.0\ s^{-1}$, $\mu = 0.01\ \frac{g}{cm \cdot s}$;

c) heavy particles, high turbulence: $\rho = 1000\ g/cm^3$, $\alpha = 0.1\ s^{-1}$, $\mu = 0.1\ \frac{g}{cm \cdot s}$.

For a constant value of the Schmidt number the particle diffusion coefficient is linearly proportional to ν. As can be seen in Figure 4, the largest particle diffusion occurs in the first case where the particles are relatively light and the turbulence in the fluid is large. When the fluid turbulence is decreased by a factor of 10 (case *b*) or the particle mass increases by the same factor (case *c*), the particle diffusion is reduced.

Since the pressure gradient in the fluid and gravity are zero, cases *b* and *c* are equivalent in the sense of the average particle motion. The actual positions of the corresponding particles in the two cases are different since random quantities are involved in the solution.

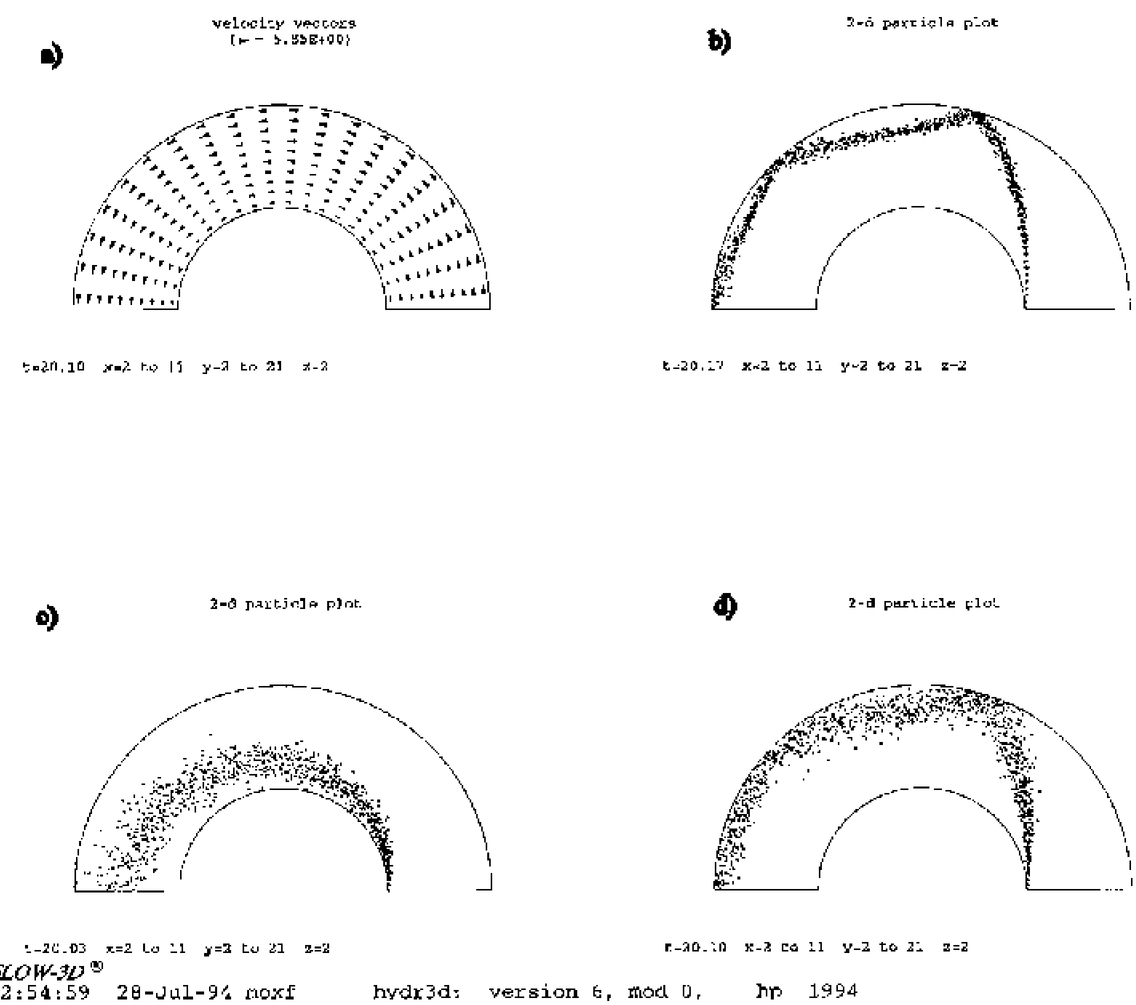


Figure 5. Particle separation in a curved duct.

c) Flow In a Curved Duct

In this 2-D simulation the flow occurs in a constant radius duct which extends 180^0 in the azimuthal direction. The inner radius is 10 *cm* and the outer one 20 *cm*. This or similar designs are used for dust or other particle separation from air. Since dust particles are usually significantly heavier than the air, the centrifugal force drives them to the outer wall of the duct where they can be collected. However, lighter particles are separated less efficiently, and turbulence in the flow may diffuse the particles preventing their accumulation at the outer wall.

First, a fluid flow simulation is made to obtain a steady state flow in the duct in which the velocity varies linearly with radius, corresponding to a constant angular velocity of 0.3 *rad/s* (Figure 5, *a*). Gravity is absent for simplicity. Then, a restart calculation is made with a particle source introduced in the flow near the inlet at the inner radius wall. The fluid flow calculations can be skipped at this stage.

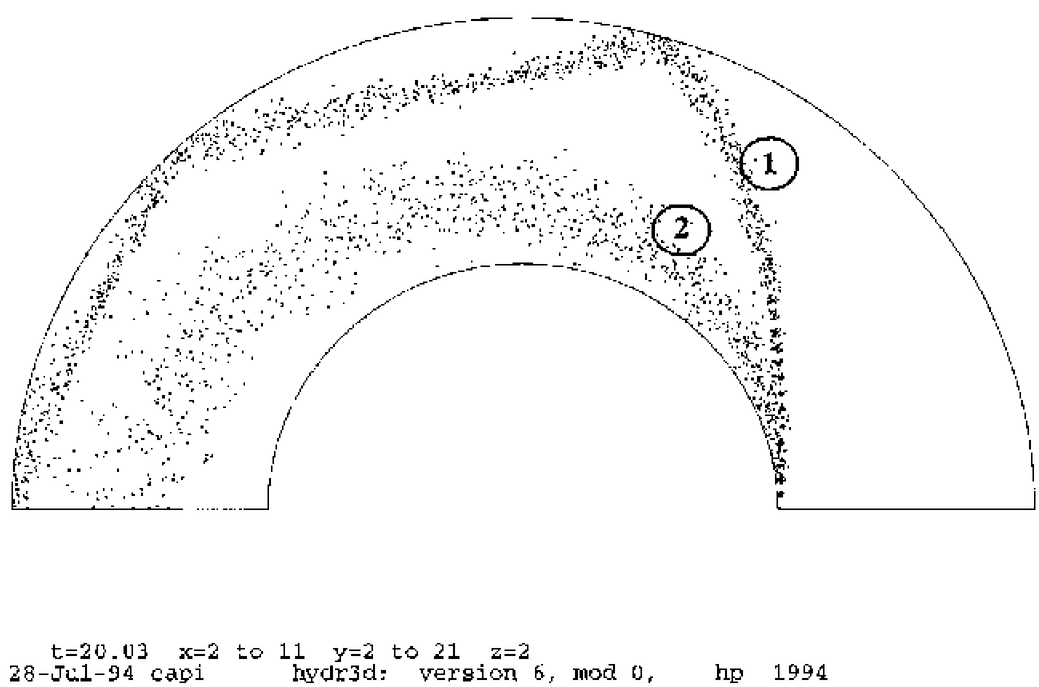


Figure 6. Separation of heavy (1) and light (2) particles in the curved duct.

The same particle input as in the previous case is used except that the particle velocity at the source is equal to 3 *cm/s*, which is the local fluid velocity. As before, three cases are considered, shown in figure 5, *b-d*, respectively:

a) heavy particles, low turbulence: $\rho = 1000\ g/cm^3$, $\alpha = 0.2\ s^{-1}$, $\mu = 0.1\ \frac{g}{cm \cdot s}$;
b) light particles, low turbulence: $\rho = 100\ g/cm^3$, $\alpha = 2.0\ s^{-1}$, $\mu = 0.1\ \frac{g}{cm \cdot s}$;
c) heavy particles, high turbulence: $\rho = 1000\ g/cm^3$, $\alpha = 0.2\ s^{-1}$, $\mu = 1.0\ \frac{g}{cm \cdot s}$.

As can be seen from plots in Figure 5, *c* and *d*, increasing the particle density and decreasing the fluid viscosity by the same factor are no longer equivalent. The density change affects the mean particle motion in such way that lighter particles get carried away by the fluid faster than they separate to the outer wall. The heavier particles separate more efficiently due to higher inertia. Figure 6 shows a simple superimposition of these plots to indicate more clearly the difference in the motion of the two species.

Comparing plots *b* and *d* in Figure 5 shows that higher level of turbulence indeed reduces the efficiency of the separation process.

References

1. R.S.Hotchkiss, C.W.Hirt, "Particulate Transport in Highly Distorted Three-Dimensional Flow Fields," Proceedings of Computer Simulation Conference, San Diego, CA, June 1972.

2. G.K. Batchelor, An Introduction to Fluid Dynamics, Cambridge University Press, 1967.

APPENDIX A

5 micron Water Particle Injected Vertically at (0,0) w/velocity 2500 cm/s
Media is Uniform Stream of Air Moving at 250 cm/s

```
$xput
 remark='units are cgs',
  icolor=1,   epsadj=1.0,     twfin=1.0e-5,    prtdt=1000.0,    ui=250.0,
$end
$limits
  irpr=2, jbkpr=2, ktpr=2,
$end
$props
$end
$bcdata
  wl=6,   ubct(1,1)=250.0,
  wr=6,   ubct(1,2)=250.0,
$end
$mesh
  nxcelt=80,    px(1)=0.0,   px(2)=0.003,
  nycelt=60,    py(1)=0.0,   py(2)=0.004,
  nzcelt=1,     pz(1)=0.0,   pz(2)=0.0003,
$end
$obs
$end
$fl
$end
$bf
$end
$temp
$end
$grafic
 nvplts=1, contpv(1)='p',
 nppltS=1,
$end
$parts
 iponly=1,
  ippkt=1,
  rate(1)=1.0e07,
  vpp(1)=2500.0,
  xpp(1)=0.0,
  ypp(1)=0.0,
  zpp(1)=0.0,
  pvol=6.54498e-11,
  prho=1.0,
  pdrg1=7.2e05,
$end
```