Clarkson University

Brownian Motion

When a small particle is suspended in a fluid, it subjected to the impact gas or liquid molecules. For ultra fine particles (colloids), the instantaneous momentum imparted to the particle varies random which causes the particle to move on an erotic path now known as Brownian motion. Figure 1 illustrates the Brownian motion process.

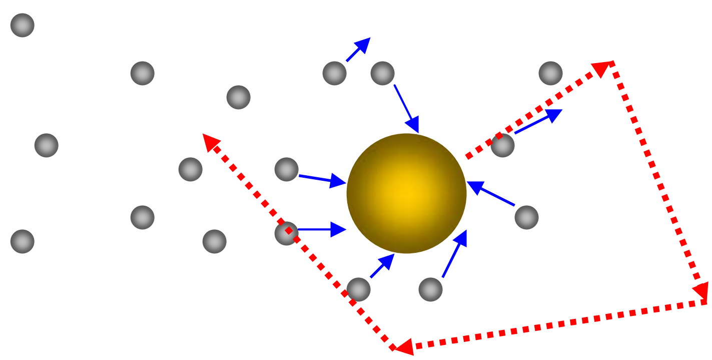


Figure 1. Schematics of a Brownian motion process.

The Brownian motion of a small particle in a stationary fluid in x-direction is governed by the following Langevin equation,

$$\frac{du}{dt} + \beta u = n(t), \tag{1}$$

where u is the velocity of the particle,

$$\beta = 3\pi\mu d / C_c m = 1/\tau \tag{2}$$

and n(t) is a white noise excitation due to the impact of fluid molecules on the particle. The intensity of noise is specified by its spectral intensity given as

$$S_{nn} = \frac{2kT\beta}{\pi m} \tag{3}$$

where $k = 1.38 \times 10^{-16}\, erg / K$ is the Boltzmann constant and T is the temperature. It should be emphasized that the Brown motion occurs in three dimensions and Equation (1) applies only to the x-component of the motion.

For the stochastic equation given by (1), using the standard linear system analysis, it follows that

$$S_{uu}(\omega) = |H(\omega)|^2 S_{nn}(\omega), \tag{4}$$

where $S_{uu}(\omega)$ is the power spectrum of the velocity of the Brownian particle, and $H(\omega)$ is the system function given by

$$H(\omega) = \frac{1}{i\omega + \beta}. \tag{5}$$

Hence,

$$S_{uu}(\omega) = \frac{2kT\beta/\pi m}{\omega^2 + \beta^2} \tag{6}$$

The autocorrelation of the particle velocity field defined as $R(\tau) = \overline{u(t+\tau)u(t)}$ (with a bar standing for the expected value) is the inverse Fourier transform of the power spectrum function. i.e.,

$$R_{uu}(\tau) = \frac{1}{2}\int_{-\infty}^{+\infty} e^{i\omega\tau} S_{uu}(\omega) d\omega \tag{7}$$

Hence

$$S_{uu}(\omega) = \frac{1}{\pi}\int_{-\infty}^{+\infty} e^{-i\omega\tau} R_{uu}(\tau) d\tau \tag{8}$$

From (6) and (7) it follows that

$$R_{uu}(\tau) = \frac{kT}{m} e^{-\beta|\tau|} \tag{9}$$

The mass diffusivity is defined as

$$D = \frac{1}{2}\frac{d}{dt}\overline{x^2}(t) \qquad \text{for large t,} \tag{10}$$

where $x(t)$ is the position of particle given by

$$x(t) = \int_0^t u(t_1) dt_1 \tag{11}$$

Using (11), one finds

$$\overline{x^2(t)} = \int_0^t \int_0^t R_{uu}(\tau_1 - \tau_2) d\tau_1 d\tau_2 \tag{12}$$

Changing variables, after some algebra it follows that

$$\overline{x^2(t)} = 2\int_0^t (t-\tau) R_{uu}(\tau) d\tau \tag{13}$$

Thus

$$D = \int_0^\infty R_{uu}(\tau) d\tau \tag{14}$$

Using (6) or (9) in (14), we find

$$D = \frac{kT}{\beta m} = \frac{kTC_c}{3\pi\mu d} \tag{15}$$

Fokker-Planck Approach

An alternative approach is to make use of the Fokker-Planck equation associated with the Langevin Equation given by (1). That is

$$\frac{\partial f}{\partial t} - \frac{\partial}{\partial u}(\beta u f) = \frac{kT\beta}{m}\frac{\partial^2 f}{\partial u^2} \tag{16}$$

The stationary solution to the Fokker-Planck equation given by (16) is given as

$$f = \frac{1}{\sqrt{2\pi kT/m}} e^{-\frac{mu^2}{2kT}}, \tag{17}$$

with $m\overline{u^2} = kT$.

Brownian Motion in a Force Field

Consider the following Langevin equation:

$$\ddot{x} + \beta\dot{x} - \frac{F(x)}{m} = n(t) \tag{18}$$

where

$$F(x) = -\frac{\partial V(x)}{\partial x} \tag{19}$$

is a conservative force field. The corresponding Fokker-Planet equation for the transition probability density function is given as:

$$\frac{\partial f}{\partial t} = -\frac{\partial(\dot{x}f)}{\partial x} + \frac{\partial}{\partial \dot{x}}[(\beta\dot{x} - \frac{1}{m}F(x))f] + \frac{kT\beta}{m}\frac{\partial^2 f}{\partial \dot{x}^2} \tag{20}$$

The stationary solution to (20) is given by

$$f = C_0 \exp\{-\frac{m}{kT}[\frac{\dot{x}^2}{2} - \int_0^x \frac{F(x_1)dx}{m}]\} \tag{21}$$

Using (19), we find

$$f = C_0 \exp\{-\frac{1}{kT}[\frac{m\dot{x}^2}{2} + V(x)]\} \tag{22}$$

For a gravitational force field,

$$V(x) = mg(x - x_0) \tag{23}$$

and

$$f = C_0 e^{-\frac{m\dot{x}^2}{2kT}} e^{-\frac{mg(x-x_0)}{kT}} \tag{24}$$

Computer Simulation Procedure

As noted before, the Brownian force n(t) may be modeled as a white noise stochastic process. White noise is a zero mean Gaussian random process with a constant power spectrum given Equation (3). Thus,

$$\overline{n(t)} = 0 \qquad \overline{n(t_1)n(t_2)} = 2\pi S_{nn}\delta(t_1 - t_2) \tag{25}$$

The following procedure was used by Ounis and Ahmadi (1992) and Li and Ahmadi (1993).

- Choose a time step Δt. (The time step should much smaller than the particle relaxation time.
- Generate a sequence of uniform random numbers U_i (between 0 and 1).
- Transform pairs of uniform random numbers to pairs of unit variance zero mean Gaussian random numbers. The can be done using the following transformations:

$$G_1 = \sqrt{-2\ln U_1}\cos 2\pi U_2 \tag{26}$$
$$G_2 = \sqrt{-2\ln U_1}\sin 2\pi U_2 \tag{27}$$

- Amplitude of the Brownian force then is given by

$$n(t_i) = G_i\sqrt{\frac{\pi S_{nn}}{\Delta t}} \tag{28}$$

- The entire generated sample of Brownian force need to be shifted by $U\Delta t$, where U is a uniform random number between zero and one.

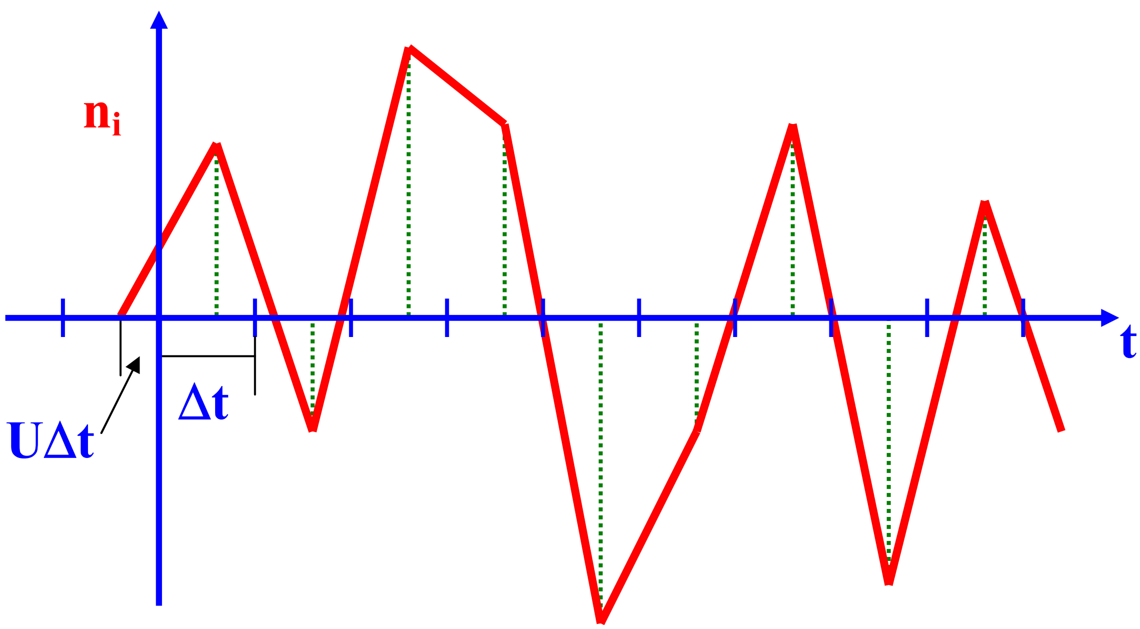


Figure 2. Numerically simulated Brownian force.

Example: Particle Dispersion and Deposition in a Viscous Sublayer

Ounis, Ahmadi and McLaughlin (1991) and Shams and Ahmadi (2000) studied dispersion and deposition of nano- and micro-particles in turbulent boundary layer flows. A sample simulated Brownian force for a 0.01 μm particle is shown in Figure 3. Here the wall units with ν / u^* and ν / u^{*2} being, respectively, the length and the time scales are used. Note that the relevant scales the wall layer including the viscous sublayer are controlled by kinematic viscosity ν and shear velocity u*. The random nature of Brownian for is clearly seen form Figure 3.

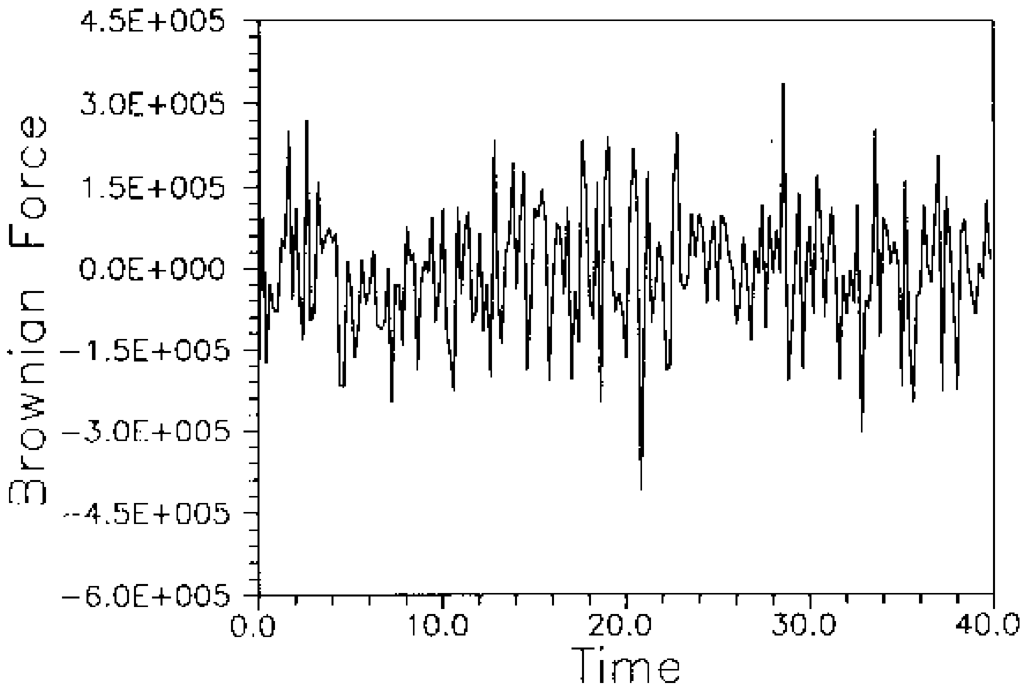


Figure 3. Sample simulated Brownian force.

Using the definition of particle diffusivity, D, as given by (10), the variance of the particle position is given by

$$\overline{x^2}(t) = 2Dt \tag{29}$$

Thus, for a given diffusivity, the variance of the spreading rate of particles may be evaluated from Equation (29).

To verify the Brownian dynamic simulation procedure, Ounis et al (1991) studied that special case of a point source in a uniform flow with $U^+ = U/u^* = 1$. For different particle diameters, Figure 4 displays the time variation of their simulated root mean square particle position. Here, for each particle size, 500 sample trajectories were evaluated, compiled and statistically analyzed. The corresponding exact solutions given by Equation (29) are also shown in this figure for comparison. It is seen that small nano-meter sized particles spread much faster by the action of the Browning motion when compared with the larger micrometer sized particles. Figure 4 also shows that the Brownian dynamic simulation results for the mean square displacement are in good agreement with the exact solutions.

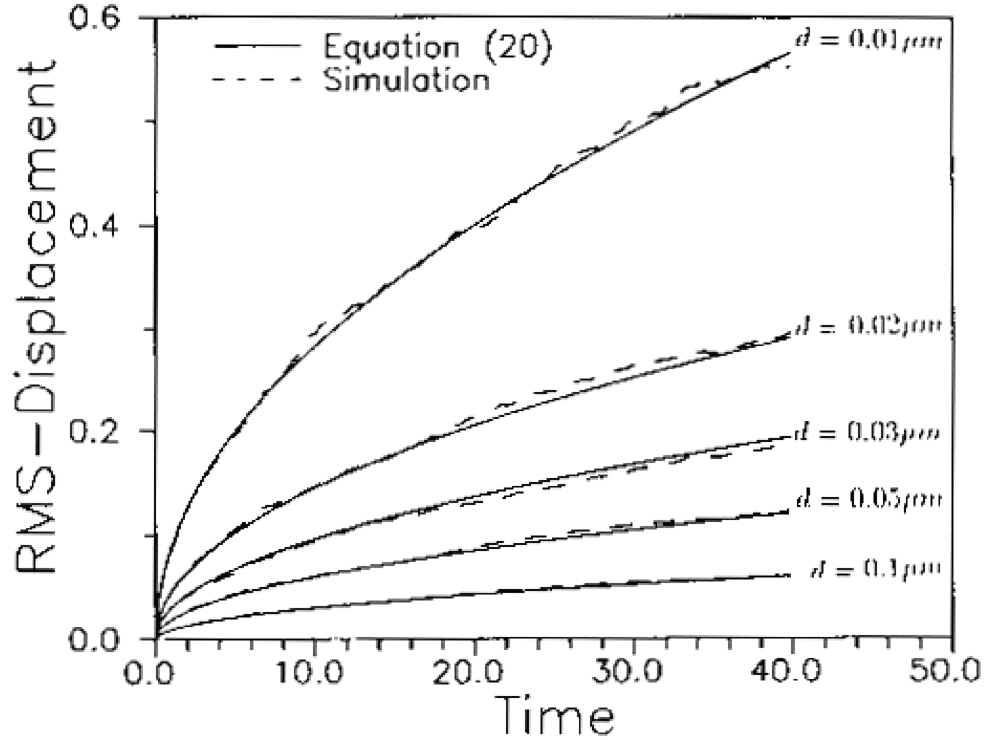


Figure 4. Sample simulated root-mean square displacement for different particles.

Ounis et la. (1991) performed a series of Lagrangian simulation studies for dispersion and deposition of particles emitted from a point source in the viscous sublayer of a turbulent near wall flow. Figures 5, 6 and 7 show time variation of particle trajectory statistics for different diameters, for the case that the point source is at a distance of 0.5 wall units away from the wall. In these simulation it is assumed that when particles touch the wall they will stick to it. At every time step, the particle ordinates are statistically analyzed and the mean, standard deviation and the sample minimum and maximum were evaluated. The points that the minimum curve touches the wall identify the locations of a deposited particle. Figure 5 shows that 0.05 μm particles have a narrow distribution and in the duration of 40 wall units none of these particle are deposited on the wall. As the particle diameter becomes smaller, their spreading due to Brownian diffusion increases and a number of particles reach the wall. For example, Figure s 6 shows that five 0.03 μm particle are deposited on the wall in the duration of 40 wall units, while Figure 7 indicates that 190 0.01 μm particles (out a sample of 500 particles) are deposited on the wall. Figures 5-7 further show that the Brownian diffusion of particles is strongly affected by their size. This is because the power spectral intensity of Brownian force in inversely proportional to the square of diameter.

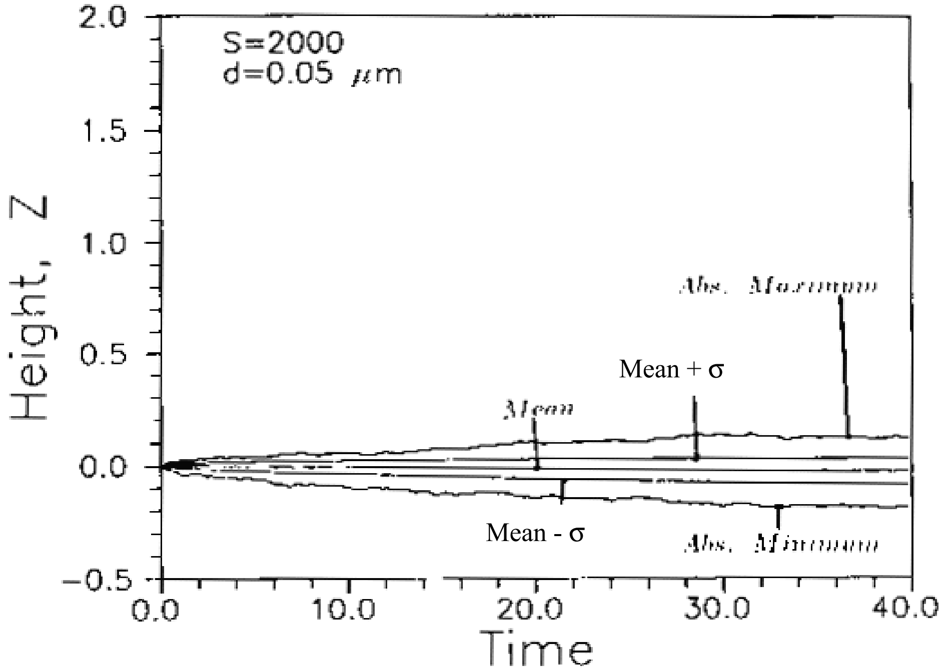


Figure 5. Simulated trajectory statistics for 0.05 μm particles.

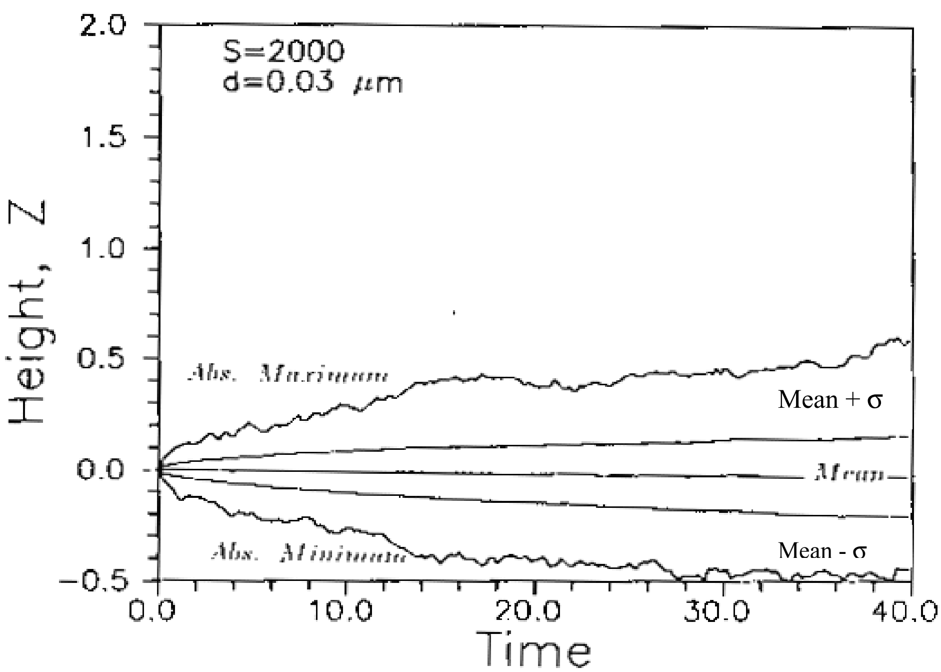


Figure 6. Simulated trajectory statistics for 0.03 μm particles.

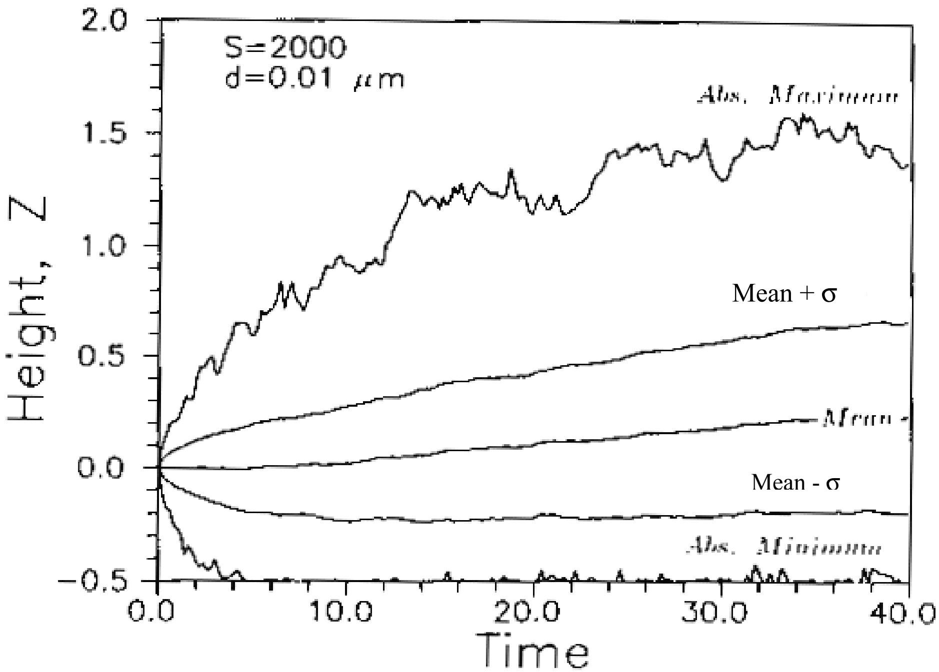


Figure 7. Simulated trajectory statistics for 0.01 μm particles.

Figure 8 shows variations of the number of deposited particles, N_t, with time for a point source at a distance of $z_o = 0.5$ wall units from the wall. The solid lines in this figure are the exact solution for a diffusion model given as

$$N_t = N_o \mathrm{erfc}(\frac{z_o}{\sqrt{4Dt}}) \tag{30}$$

It is seen that the Brownian dynamic simulation results and the diffusion equation analysis are in good agreement for the range of particle diameters studied. Figure 8 also shows that as the particle diameter decreases, the number of deposited particles increases sharply. Additional results (not shown here) indicate that the deposition rate decreases as the distance of source from the wall increases. Figures 4-8 show that the Brownian motion process is a significant mechanism for nano-particle diffusion and wall deposition.

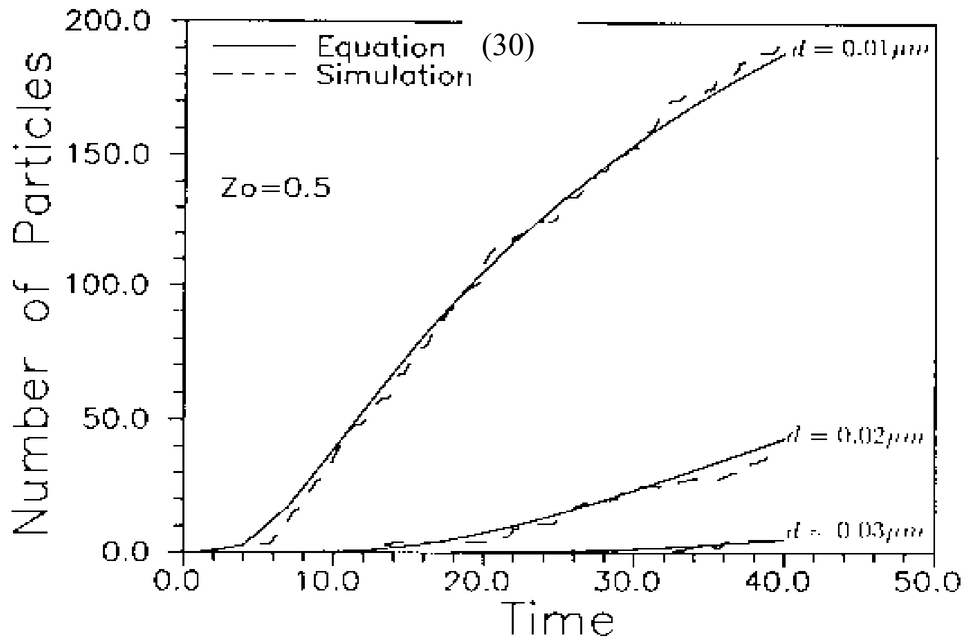


Figure 8. Comparison of the simulated number of deposited particles with the diffusion model given by Equation (30).

Java Applet for Brownian Motion

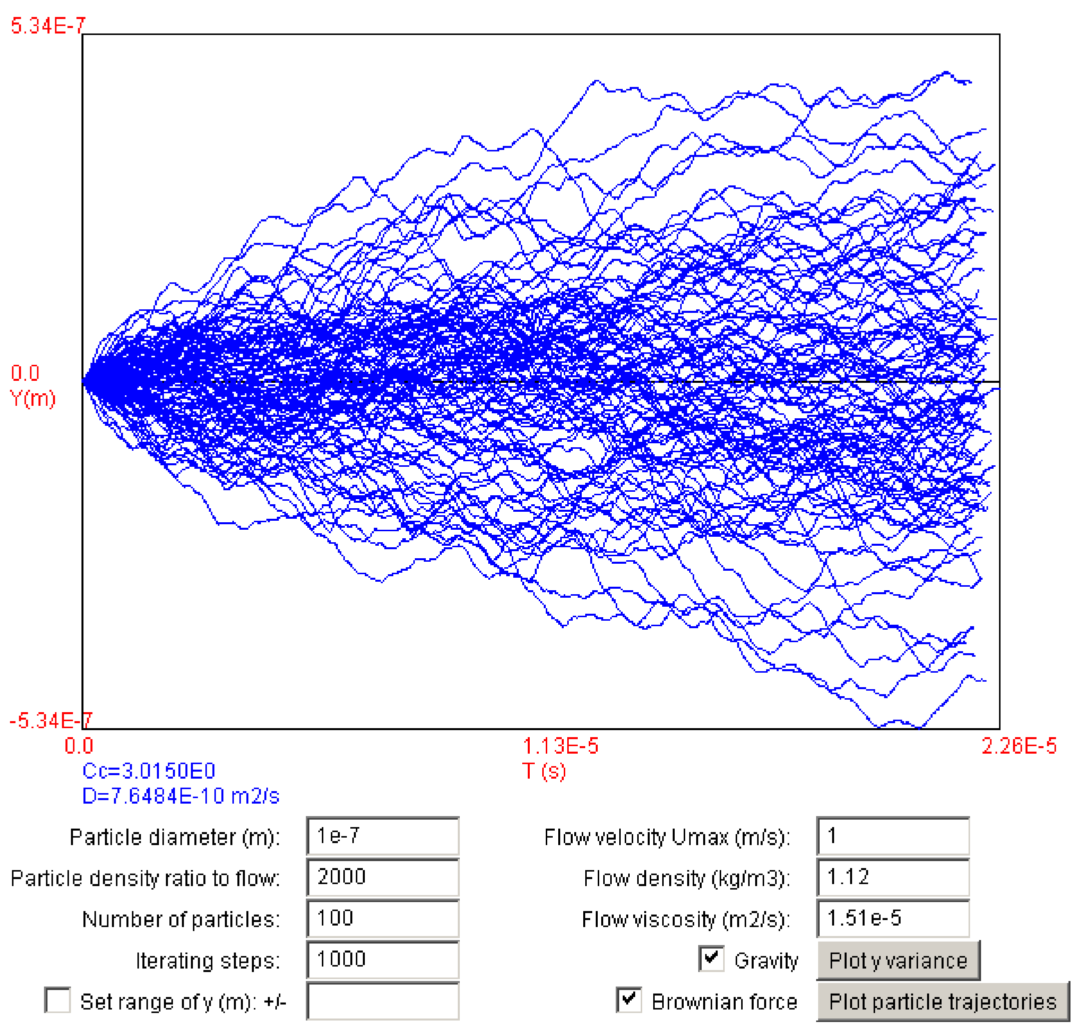
A Java Applet for analyzing Brownian motion of particles in laminar pipe flow is developed which is available at the course web site. The program solves the particle equation of motion including the Brownian excitation

$$\frac{d\mathbf{u}^p}{dt} = \frac{1}{\tau}(\mathbf{u}^f - \mathbf{u}^p) + \mathbf{g} + \mathbf{n}(t) \qquad (31)$$

The Brownian force is simulated as a white noise process with an appropriate power spectral intensity. The flow and particle parameters and time duration and sample size can be specifies. The variance of the particle position is also compared with the exact solution to the diffusion equation given as

$$\sigma_y^2(t) = 2Dt \qquad (32)$$

Java Applet for particle trajectory analysis



Java Applet for comparison of variance of particle position with the exact solution.