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Letter to the Editor
Langrangian Stochastic Particle Tracking

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In response to "Comparison of Three Approaches to Model Particle Penetration Coefficient through a Single Straight Crack in a Building Envelope" by B. Zhao et al. in *Aerosol Science and Technology* 44:405–416, 2010

Dear Editors,

The above article provides useful insights in various analytical and numerical methods in calculating Brownian deposition of fine particles on building wall cracks. However, the authors make a serious error by stating that for fundamental reasons the Lagrangian stochastic force model cannot be used to model Brownian motion correctly. Specifically on page 412, they state that:

> According to Fick's law, Brown diffusion depends on particle concentration gradient. However, the information of particle concentration gradient cannot be obtained when calculating the Brown force by Lagrangian approach. It should be pointed out that the calculation of particle trajectory does NOT depend on the particle concentration gradient, which may make the simulation of Brownian diffusion inaccurate . . .

This statement is contrary to the accepted literature in the field. When modeling Brownian diffusion, the link between Lagrangian and Eulerian approaches can be understood comparing statistical (microscopic) and continuum (macroscopic) mechanics. Consider a total of N_0 particles originally positioned at y-z plane which are allowed to diffuse in the positive and negative x directions (2 dimensional diffusion). Fick's second law predicts how diffusion causes the concentration field to change with time.

$$\frac{\partial N(x,t)}{\partial t} = D\frac{\partial^2 N(x,t)}{\partial x^2} \qquad [1]$$

where N is the number concentration and D is the diffusion coefficient. Certainly, Fick's second law is the more general case and Fick's first law can be derived from it. This equation is written for diffusion in continuum mechanics (macroscopic). By combining statistical and continuum mechanics, it is possible to show that *individual particle positions for an ensemble of particles, themselves, contain the information regarding the concentration field*. Furthermore, it is possible to express D in terms of parameters other than particle concentration.

In the microscopic world, the motion of a particle is described by the Langevin equation (also known as Lagrange equation or Newton's second law).

$$\frac{d\vec{V}}{dt} = -\frac{1}{\tau}\vec{V} + \vec{a} \qquad [2]$$

where $\vec{V}$ is particle velocity, τ is particle relaxation time, and $\vec{a}$ is stochastic acceleration function due to particle collisions. For isotropic Brownian diffusion, Seinfeld and Pandis (2006) derive that

$$\langle x^2 \rangle = \frac{2kTC_C}{3\pi\mu D_P}\, t \qquad [3]$$

stating that the mean-squared-position $\langle x^2 \rangle$ is related to the Boltzmann constant k, absolute temperature T, Cunningham correction factor C_C, continuum phase viscosity μ, and particle diameter D_P. This is also known as the Stokes-Einstein-Sutherland relation.

This is substantial, but we still need to find an expression for coefficient of diffusion as a function of parameters other than particle concentration. We can further multiply the left and right hand side of Equation (1) by x^2 and integrate over the complete x-axis. Seinfeld and Pandis (2006) did this calculation and provide

$$LHS = \int_{-\infty}^{+\infty} x^2 \frac{\partial N(x,t)}{\partial t} dx = N_0 \frac{\partial \langle x^2 \rangle}{\partial t} \qquad [4]$$

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$$RHS = \int_{-\infty}^{+\infty} x^2 D \frac{\partial^2 N(x,t)}{\partial x^2} dx = 2DN_0 \quad [5]$$

Combining Equations (3), (4), and (5), one can express the diffusion coefficient as a function of parameters other than particle concentration.

$$D = \frac{kTC_C}{3\pi\mu D_P} \quad [6]$$

Other authors arrive at similar expressions for diffusion coefficient combining statistical and continuum mechanics. For example, a simplified model by Sonntag and Van Wylen (1966) relates diffusion coefficient to statistical mechanics parameters for a mono-atomic gas.

$$D = \frac{1}{3}\overline{V}\Lambda \quad [7]$$

where $\overline{V}$ is mean molecular velocity and Λ is the mean free path for the continuum phase. They argue that the comparison between experimental and theoretical data for diffusion coefficient is fair. They show that with more sophisticated statistical mechanics models, excellent agreement between theoretical and experimental diffusion coefficients has been achieved.

Li and Ahmadi (1992) provide a version of Lagrangian stochastic force model with a Gaussian white nose forcing function that they apply to the Brownian diffusion of a point source of 500 massless particle trajectories in a stagnant fluid background. Their simulation shows excellent agreement between the stochastic simulation and the solution to the diffusion equation (their Figure 3).

Reynolds (1999) also studies variations of the Lagrangian stochastic forcing model in predicting deposition of Brownian particles at various Reynolds numbers. They also find the model and experimental results in good agreement (their Figure 4). They suggest that, however, various difficulties exist in obtaining correct results using this technique. First, the Reynolds number effects must be taken into consideration correctly. Second, one must account for differences between tracer particles and Brownian particles correctly.

Therefore, contrary to the authors' statements, the definition of Lagrangain stochastic model is physically plausible and representative of non-continuum fluid mechanics without the need to consider particle concentration information. Also, the credible literature confirms that this model, if computed correctly, agrees well with theoretical and experimental results. It is not clear why Zhao et al.'s FLUENT simulation grossly underestimates deposition by Brownian motion.

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