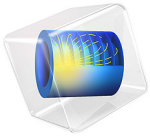

Brownian Motion

Introduction

Particle tracing offers an attractive alternative to continuum-based numerical methods, such as the finite element method, for modeling species transport in strongly convecting flows because the particle tracing method is insensitive to the magnitude of the Péclet number. In most real systems, species transport has both a convective and diffusive component. Particle tracing can be used to solve purely convective motion, purely diffusive motion and anything in-between. Thus using a particle-based approach the entire spectrum of Péclet numbers can be handled without encountering the numerical instabilities associated with the continuum approach.

In this example the agreement between the continuum and particle-based numerical methods is verified in the case of purely diffusive motion.

Model Definition

The diffusion equation is solved in two different ways. First, the species concentration is computed using the Transport of Diluted Species interface, which uses a continuum model in which the concentration is discretized using a finite element mesh in the modeling domain. The equation governing the evolution of the concentration c (SI unit: $\mathrm{mol/m^3}$) in a stagnant background fluid ($\mathbf{u} = \mathbf{0}$) is:

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) = 0$$

where the diffusion coefficient D (SI unit: $\mathrm{m^2/s}$) is defined as

$$D = \frac{k_\mathrm{B} T}{6\pi\mu r_\mathrm{p}}$$

where

- $k_\mathrm{B} = 1.3806488 \times 10^{-23}$ J/K is Boltzmann's constant,
- T (SI unit: K) is the absolute fluid temperature,
- μ (SI unit: $\mathrm{Pa\ s}$) is the fluid viscosity, and
- r_p (SI unit: m) is the particle radius.

The initial concentration is given by a Dirac delta function at the origin,

$$c_0 = \delta(0, 0)$$

That is, the initial concentration is infinitely large at the origin and zero everywhere else, such that the surface integral over any region containing the origin is unity. Because an initial condition that is infinitely large at a point is impractical to model, the initial concentration is instead given a very large finite value in a small area surrounding the origin.

The model geometry consists of two concentric circles as shown in Figure 1. The initial concentration diffuses from the origin radially outward in all directions. After 100 seconds, some of the initial concentration has diffused from the inner circular domain to the outer domain. The transmission probability for diffusion from the inner domain to the outer domain is defined as:

$$\alpha = \frac{\int_O c\,dS}{\int_I c\,dS + \int_O c\,dS}$$

where I denotes the inner domain and O the outer domain.

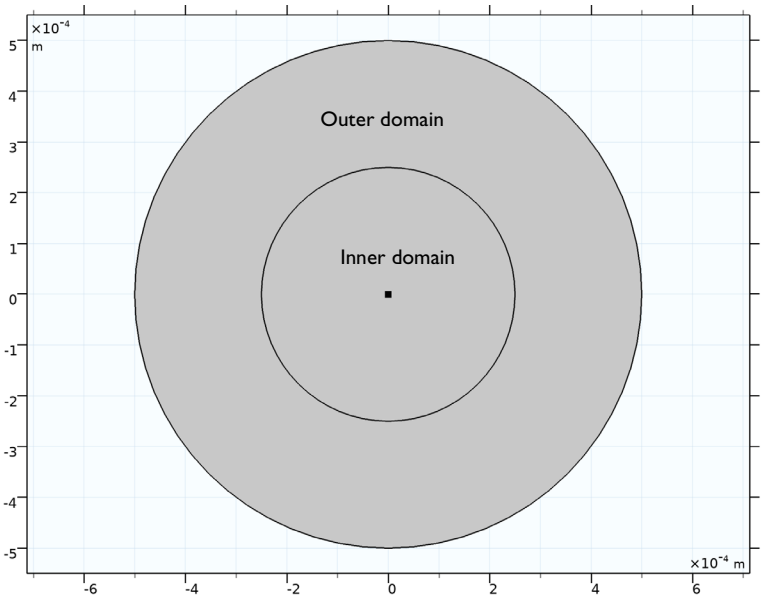

Figure 1: Model geometry. The concentration is initially a delta function at (0,0) and the particles are all released at (0,0) with an initial velocity of zero.

Diffusion can also be modeled using a particle-based approach. The combination of the **Brownian Force** and the **Drag Force** results in diffusion of particles from regions of high to low number density. The equations of motion are:

$$\frac{d}{dt}(m_\mathrm{p}\mathbf{v}) = \mathbf{F}_\mathrm{D} + \mathbf{F}_\mathrm{b}$$

$$\mathbf{F}_\mathrm{D} = \left(\frac{1}{\tau_\mathrm{p}}\right) m_\mathrm{p}(\mathbf{u} - \mathbf{v})$$

$$\tau_\mathrm{p} = \frac{\rho_\mathrm{p} d_\mathrm{p}^2}{18\mu}$$

This is the *Stokes* drag law, which is appropriate when the relative Reynolds number of the particles in the fluid is small. Because the fluid is stagnant and the particle speeds are low, the Stokes drag law is applicable in this example. The Brownian force is given by

$$\mathbf{F}_\mathrm{b} = \zeta\sqrt{\frac{12\pi k_\mathrm{B}\mu T r_\mathrm{p}}{\Delta t}}$$

- m_p (SI unit: kg) is the particle mass,
- d_p (SI unit: m) is the particle diameter,
- τ_p (SI unit: s) is the particle velocity response time,
- $\mathbf{v}$ (SI unit: m/s) is the velocity of the particle,
- $\mathbf{u}$ (SI unit: m/s) is the fluid velocity, which in this example is set to zero representing a stagnant background fluid,
- Δt (SI unit: s) is the size of the time step taken by the solver, and
- ζ (dimensionless) is a vector of independent, normally distributed random numbers with zero mean and unit standard deviation.

As explained in Ref. 1, independent values are chosen for all components of ζ. A different value of ζ is created for each particle, at each time step for each component of the Brownian force. The Brownian force leads to spreading of particles from regions of high particle density to low density.

Initially, 5000 particles are released from the origin with initial velocity components all zero. The transmission probability from the inner to the outer domain is computed by counting the number of particles in the outer domain and dividing it by the total number of particles.

Results and Discussion

The computed transmission probability for the two different methods is shown in Table 1. Since the Brownian force uses pseudorandom number generators, the problem is solved five times, each time with a different seed. In each case the transmission probability is slightly different but all cases agree with the result from solving the diffusion equation.

TABLE 1: TABLE OF RESULTS FOR THE COMPUTED TRANSMISSION PROBABILITY.

METHOD	TRANSMISSION PROBABILITY
Diffusion Equation	0.23645
Particle Tracing 1	0.24460
Particle Tracing 2	0.23080
Particle Tracing 3	0.24860
Particle Tracing 4	0.23760
Particle Tracing 5	0.23840

Figure 2 plots the location of the particles at the final solution time for 4 different runs.

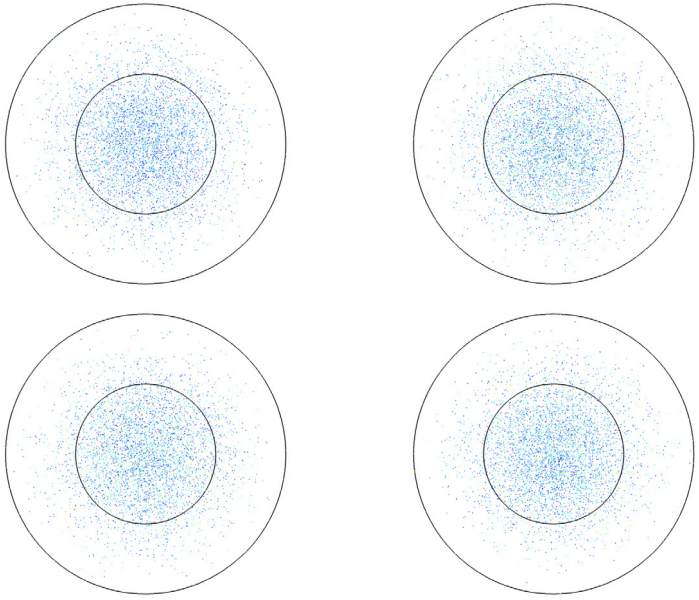

Figure 2: Plot of the particle location after 100 seconds. For each run, different random numbers were generated.

It is clear from these results that diffusive processes can be modeled using a particle-based approach. Furthermore, if a significant nonzero background fluid velocity were applied, the particle based approach would remain numerically stable.

Reference

1. M. Kim and A.L. Zydney, "Effect of Electrostatic, Hydrodynamic, and Brownian Forces on Particle Trajectories and Sieving in Normal Flow Filtration", *J. Colloid and Interface Science*, vol. 269, pp. 425–431, 2004.

Application Library path: `Particle_Tracing_Module/Tutorials/brownian_motion`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

2 In the **Select Physics** tree, select **Chemical Species Transport> Transport of Diluted Species (tds)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Time Dependent**.

6 Click **Done**.

GEOMETRY 1

Start by adding some definitions for the geometry and physical properties of the background fluid.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
router	0.0005	5E-4	Outer radius
rinner	0.00025	2.5E-4	Inner radius
rp	1E-7[m]	1E-7 m	Particle radius
T	300[K]	300 K	Temperature
eta	2E-5[Pa*s]	2E-5 Pa·s	Fluid viscosity
D	k_B_const*T/(6*pi*eta*rp)	1.0987E-10 m²/s	Diffusivity
ds	1	1	Input to random number generator

GEOMETRY 1

Circle 1 (c1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Geometry 1** node.

2 Right-click **Geometry 1** and choose **Circle**.

3 In the **Settings** window for **Circle**, locate the **Size and Shape** section.

4 In the **Radius** text field, type router.

Circle 2 (c2)

1 In the **Geometry** toolbar, click **Circle**.

2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.

3 In the **Radius** text field, type rinner.

Point 1 (pt1)

1 In the **Geometry** toolbar, click **Point**.

2 In the **Settings** window for **Point**, click **Build All Objects**.

3 Click the **Zoom Extents** button in the **Graphics** toolbar. The geometry should look like Figure 1.

DEFINITIONS

Construct an expression for the initial concentration, which is a smoothed delta function.

Variables 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node.

2 Right-click **Definitions** and choose **Local Variables**.

3 In the **Settings** window for **Variables**, locate the **Variables** section.

4 In the table, enter the following settings:

Name	Expression	Unit	Description
smooth	2E-7		Smoothing distance
xd	x[1/m]		x coordinate
yd	y[1/m]		y coordinate
c0	1		Peak initial concentration
c_init	2*c0*(1-flc2hs(xd^2+yd^2-smooth^2,5e-11))		Initial concentration

Define a pair of **Integration** component couplings so that the fraction of the concentration that diffuses from the inner domain to the outer domain can be computed.

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 Select Domain 1 only.

Integration 2 (intop2)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 Select Domain 2 only.

TRANSPORT OF DILUTED SPECIES (TDS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Diluted Species (tds)**.

2 In the **Settings** window for **Transport of Diluted Species**, locate the **Transport Mechanisms** section.

3 Clear the **Convection** check box.

Concentration 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Concentration**.

2 Select Boundaries 1, 2, 5, and 8 only.

3 In the **Settings** window for **Concentration**, locate the **Concentration** section.

4 Select the **Species c** check box.

Transport Properties 1

1 In the **Model Builder** window, click **Transport Properties 1**.

2 In the **Settings** window for **Transport Properties**, locate the **Diffusion** section.

3 In the D_c text field, type `D`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the *c* text field, type `c_init`.

MESH 1

Use a very fine mesh at the point (0, 0).

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Extra fine**.

Scale 1

1 In the **Mesh** toolbar, click **Modify** and choose **Mesh>Scale**.

2 In the **Settings** window for **Scale**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Point**.

4 Select Point 5 only.

5 Locate the **Scale** section. In the **Element size scale** text field, type `0.05`.

Free Triangular 1

1 In the **Mesh** toolbar, click **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click **Build All**.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `0 100`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `1E-4`.

6 In the **Home** toolbar, click **Compute**.

RESULTS

Use the **Global Evaluation** feature to compute the fraction of the total concentration that diffused from the inner domain to the outer domain.

Global Evaluation 1

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Time selection** list, choose **Last**.

4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
`intop1(c)/(intop1(c)+intop2(c))`	1	

5 Click next to **Evaluate**, then choose **New Table**.

COMPONENT 1 (COMP1)

Now solve the same problem using a particle-based approach.

ADD PHYSICS

1 In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Fluid Flow>Particle Tracing>Particle Tracing for Fluid Flow (fpt)**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Study 1**.

5 Click **Add to Component 1** in the window toolbar.

6 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Transport of Diluted Species (tds)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

5 Click **Add Study** in the window toolbar.

6 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

ROOT

1 Click the **Show More Options** button in the **Model Builder** toolbar.

2 In the **Show More Options** dialog box, in the tree, select the check box for the node **Physics>Advanced Physics Options**.

3 Click **OK**.

PARTICLE TRACING FOR FLUID FLOW (FPT)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Particle Tracing for Fluid Flow (fpt)**.

2 In the **Settings** window for **Particle Tracing for Fluid Flow**, click to expand the **Advanced Settings** section.

3 From the **Wall accuracy order** list, choose **1**.

4 From the **Arguments for random number generation** list, choose **User defined**.

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Particle Tracing for Fluid Flow (fpt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Particle Properties** section.

3 In the d_p text field, type `2*rp`.

4 From the ρ_p list, choose **User defined**.

Drag Force 1

1 In the **Physics** toolbar, click **Domains** and choose **Drag Force**.

2 In the **Settings** window for **Drag Force**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Drag Force** section. From the μ list, choose **User defined**. In the associated text field, type `eta`.

Brownian Force 1

1 In the **Physics** toolbar, click **Domains** and choose **Brownian Force**.

2 In the **Settings** window for **Brownian Force**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Model Input** section. In the T text field, type `T`.

5 Locate the **Brownian Force** section. From the μ list, choose **User defined**. In the associated text field, type `eta`.

6 Locate the **Advanced Settings** section. In the i text field, type `ds`.

Release from Grid 1

Release 5000 particles at the origin with an initial velocity of zero.

1 In the **Physics** toolbar, click **Global** and choose **Release from Grid**.

2 In the **Settings** window for **Release from Grid**, locate the **Initial Velocity** section.

3 From the **Initial velocity** list, choose **Constant speed, spherical**.

4 In the v_0 text field, type `0`.

5 In the N_{vel} text field, type `5000`.

Particle Counter 1

1 In the **Physics** toolbar, click **Domains** and choose **Particle Counter**.

2 Select Domain 1 only.

3 In the **Settings** window for **Particle Counter**, locate the **Particle Counter** section.

4 From the **Release feature** list, choose **Release from Grid 1**.

The Brownian force depends on the time step taken by the solver. The default tolerances are very strict for the particle tracing interfaces. When including forces with random components such as the Brownian force the tolerances need to be relaxed, otherwise the solver will take very small time steps and the model will take a long time to solve.

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 2** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `0 100`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `1E-2`.

6 In the **Home** toolbar, click **Compute**.

RESULTS

Global Evaluation 2

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

4 From the **Time selection** list, choose **Last**.

5 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)>Particle Tracing for Fluid Flow>Particle Counter 1> fpt.pcnt1.alpha - Transmission probability**.

6 Click **Evaluate**.

ROOT

Finally, add another study and solve the same problem 4 times, with different random numbers generated for each run. A **Parametric Sweep** over the parameter `ds` is used to create unique random numbers for each run.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Transport of Diluted Species (tds)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

5 Click **Add Study** in the window toolbar.

6 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 3

Step 1: Time Dependent

1 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

2 In the **Output times** text field, type `0 100`.

3 From the **Tolerance** list, choose **User controlled**.

4 In the **Relative tolerance** text field, type `1E-2`.

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
ds (Input to random number generator)	2 3 4 5	

5 In the **Study** toolbar, click **Compute**.

RESULTS

Global Evaluation 3

1 In the **Model Builder** window, expand the **Results>Datasets** node.

2 Right-click **Derived Values** and choose **Global Evaluation**.

3 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

4 From the **Dataset** list, choose **Study 3/Parametric Solutions 1 (sol4)**.

5 From the **Time selection** list, choose **Last**.

6 From the **Table columns** list, choose **Time**.

7 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)>Particle Tracing for Fluid Flow>Particle Counter 1> fpt.pcnt1.alpha - Transmission probability**.

8 Click the arrow next to the **Evaluate** button and select **New table**.

Particle Trajectories (fpt) 1

1 In the **Model Builder** window, click **Particle Trajectories (fpt) 1**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Parameter value (ds)** list, choose **2**.

4 In the **Particle Trajectories (fpt) 1** toolbar, click **Plot**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.

View the particle trajectories for other parameter values by selecting different options from the **Parameter value (ds)** list. Note that the distributions all look similar but that the particle positions are distinct in each plot. Four such plots are shown in Figure 2.