A novel multiphase DNS framework for the simulation of nano-particulate flows

Ananda Subramani Kannan,
Department of Mechanics and Maritime Sciences, Division of fluid dynamics, Chalmers University of Technology, Göteborg, 412 96, Sweden. @chalmers.se
Background

• General outline of the problem

“Study the motion of a particle with mass $M$ and length scale close to the mean free path of the molecules of the surrounding fluid”

Langevin Equation:

$$\frac{dv(t)}{dt} = -\frac{\gamma}{m} v(t) + \frac{1}{m} \xi(t)$$

Drag on the particle

Stochastic forcing

A typical application: Diesel particulate filters

Figure adapted from DieselNet.com
Background

• Need for a continuum based ‘DNS’ framework

• Breakdown of the ‘point-particle’ assumption

• Complete resolution of the flow around the PM including resulting boundary layers is needed

• Continuum based methods can handle ‘complex’ pore shapes

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Background

• Objectives

The primary objective of the current work is to showcase a numerical method that –

✓ Accounts for “non-continuum effects” on particle motion in disperse gas-particle (weakly rarefied) flows

✓ Accurately resolves the meandering trajectories undertaken by PM in such flow systems due to Brownian motion
### Numerical method

The gas is treated as a **continuum** while the particles are handled in a **Lagrangian** manner.

- **Continuum treatment** (Mirroring immersed boundary method: MIBM*)

\[
\frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{v}_f) = 0
\]

\[
\frac{\partial \rho_f \mathbf{v}_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{v}_f \mathbf{v}_f) = -\nabla P + \mu \nabla^2 (\mathbf{v}_f) + \mathbf{f}_i
\]

*Mark and van Wachem (Journal of Computational Physics, 2008)
Numerical method

- Lagrangian treatment (Langevin equation of motion)

\[
m_i \frac{du_j}{dt} = \frac{\text{Total fluid force}}{C_c} + m_i n_i(t)
\]

Corrected fluid force on particle

Stochastic forcing

\( n_i(t) \) is modelled as a Gaussian white noise random process (Li and Ahmadi*)

\[
n_i(t) = G \sqrt{\frac{\pi S_o}{\Delta t}}
\]

*Li and Ahmadi (Aerosol science and technology, 1992)

→ IB-Lagrangian coupled framework solved using IPS IBOFlow®
Results

• Framework validation (Settling sphere)

Validation case setup

<table>
<thead>
<tr>
<th>Particulate phase</th>
<th>Glass bead</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter</td>
<td>0.5 mm</td>
</tr>
<tr>
<td>Grid resolution (cells/diameter)</td>
<td>10</td>
</tr>
<tr>
<td>Density (kg/m$^3$)</td>
<td>2560</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Fluid phase</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m$^3$)</td>
<td>1000</td>
</tr>
<tr>
<td>Viscosity (pa. s)</td>
<td>0.001</td>
</tr>
<tr>
<td>Time step (s)</td>
<td>1/35th of particle response time</td>
</tr>
</tbody>
</table>

Schematic of the simulation domain
Results

- Framework validation (Settling sphere): Rep = 50

Temporal evolution of particle velocity (comparison between experiments* and simulation)

<table>
<thead>
<tr>
<th></th>
<th>Simulation</th>
<th>Experimental data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-dimensional terminal velocity</td>
<td>0.991</td>
<td>1.0</td>
</tr>
</tbody>
</table>

*All comparisons are with data from Mordant et.al (The European Physical Journal B - Condensed Matter and Complex Systems, 2000)
### Results

- **Diffusion of a 400 nm particle in a micro-channel**

<table>
<thead>
<tr>
<th>Diffusion in a micro-channel</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>System size (l x w x h), µm</strong></td>
<td>10.0 x 10.0 x 10.0</td>
</tr>
<tr>
<td><strong>Particulate phase</strong></td>
<td><strong>Glass bead</strong></td>
</tr>
<tr>
<td>Diameter</td>
<td>400 nm</td>
</tr>
<tr>
<td>Grid resolution (cells/diameter)</td>
<td>24</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>2000, 1000, 500</td>
</tr>
<tr>
<td><strong>Fluid phase</strong></td>
<td><strong>Air</strong></td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>1.0</td>
</tr>
<tr>
<td>Viscosity (pa. s)</td>
<td>1.725 x 10⁻⁵</td>
</tr>
<tr>
<td>Time step (s)</td>
<td>1/35th particle response time</td>
</tr>
</tbody>
</table>

**Schematic of simulation domain**

Un-Bounded channel

A novel multiphase DNS framework for the simulation of particulate flows in a micro-channel
Results

• Diffusion of a 400 nm particle in a micro-channel: Lagrangian treatment (one-way coupled)

Basis –

\[ m_i \frac{du_i}{dt} = \left( \frac{v_f - u_i}{\tau_p C_c} \right) + (m_i n_i(t)) \]

Corrected Stokes drag \hspace{1cm} \text{Stochastic forcing}

\[ MSD = \frac{1}{N} \sum_{n=1}^{N} (x(t + dt) - x(dt))^2 \]

\[ MSD_{\text{analytical}} = 2.0 \times D_{\text{phi}} \times T \text{ (in 1D)} \]

Where –

\[ dt \text{ is a ‘pre-determined’ lag interval} \]

Effect of particle/fluid density ratio on non-dimensional MSD

A novel multiphase DNS framework for the simulation of particulate flows in a micro-channel
Results

- Diffusion of a 400 nm particle in a micro-channel: MIBM based DNS framework (two-way coupled)

Basis –

\[ m_i \frac{du_i}{dt} = \left( \frac{\text{Total fluid force}}{C_c} \right) + m_i n_i(t) \]

Corrected fluid force on particle

Stochastic forcing

- Deviation noted between MIBM and Lagrangian treatments

- Transition from ballistic to diffusive behavior

\[ a D_{phi} = \frac{kT C_c}{3\pi \mu_f d_p} \]

\[ b \tau_p = \frac{m_p C_c}{3\pi \mu_f d_p} \]

Effect of particle/fluid density ratio on non-dimensional MSD

**Figure:**

1. MSD* = \( \frac{MSD}{a D_{phi} \tau_p} \)
2. Non-dimensional time (T*)

A novel multiphase DNS framework for the simulation of particulate flows in a micro-channel
Conclusions

✓ A coupled Lagrangian-IB framework has been formulated in this work that has –

- Acceptable resolution of the flow physics dealing with particles settling in a fluid (appreciable two-way coupling)
- Capability to resolve “Brownian motion”
  - Current models (Li-Ahmadi) need to be corrected prior to DNS

✓ Challenging phenomenon to simulate with all the necessary coupling
  - Smaller length scales mean that these simulations are on the ‘limit’
  - Deeper investigation into the coupling between the fluid and nano-particles
Thank you for listening!

Ananda Subramani Kannan
Doktorand | Doctoral student
Institutionen för Mekanik och maritima vetenskaper | Department of Mechanics and Maritime Sciences
Avdelningen för strömningslära | Division of Fluid Dynamics
email: ananda@chalmers.se

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Numerical method

A novel multiphase DNS framework for the simulation of particulate flows in a micro-channel

Mirroring Immersed Boundary method (Continuum) → Cunningham correction for rarefaction → Corrected force on particle → Updated position of the Immersed Boundary → Semi-implicit method for particle motion (Lagrangian)
Results

• Diffusion of a 400 nm particle in a micro-channel: RMS Velocities

Basis –

\[ V_{rms}(Analytical) = \sqrt{\frac{k_B T}{m}} \]

• Inverse dependence on density

• General trend captured

• Deviations merit an investigation

Effect of particle/fluid density ratio on root mean squared velocity (Vrms)
Results

• Diffusion of a 400 nm particle in a micro-channel: Positions

  • General trajectory captured
    • Some minor differences that need to be investigated
      - Fully resolved fluid force used in solving Langevin equation
      - Includes more effects than just steady drag

Effect of particle/fluid density ratio on particle positions
Ongoing work…

Reactor

- To study diffusion of inert particles in a micro-channel under weakly rarefied flow conditions

Cross section of holes (nominal 1.8µm, 1.4µm, 1.0µm, and 0.6µm diameter with 5µm pitch) etched into Si
What is IBM?

✓ **Immersed boundary**: Fundamental Idea

- The IB represented through some means such as a **surface grid**

- The Cartesian **volume grid** generated with no regard to this surface grid

- BC’s incorporated by modifying the equations in the vicinity of the boundary

- Solid body occupies the domain $\Omega_b$, with boundary denoted by $\Gamma_b$

- Fluid occupies the domain $\Omega_f$
Knudsen number

✓ Flow regimes and Kn number

\[ Kn = \frac{\lambda}{d_p} \]

Region of interest
Stokes-Einstein Diffusivity

✓ Statistics before IBM period

For 3D Brownian motion

\[
< (\Delta r^2) > = 6D \Delta t
\]

Mean Squared Distribution \((<\Delta r^2>)\) and the lag time \((\Delta t)\) and is characterized by the diffusion coefficient \(D\) (Einstein diffusivity) given by –

\[
D = \frac{k_b T C_c}{3 \pi \eta d_p}
\]
Some relevant relations (Li – Ahmadi model):

The Li-Ahmadi model assumes that ‘**steady drag**’ is the only dominant hydrodynamic effect for a Brownian - particle diffusing in a quiescent fluid.

Hence a Brownian force that can counteract the effect of this drag is formulated thus -

$$F_{bi} = g \sqrt{\left(\frac{\pi S_{nn}}{\Delta t}\right)}$$

where:

- $g$: Random number with zero mean and unit variance

$$S_{nn} = \frac{2kT\beta}{\pi m_p}$$

**Power spectrum of the random process**

$$\beta = \frac{3\pi \mu d_p}{C_cm_p}$$

**Inverse of particle response time**

Note that we provide a diffusivity to this model, formulated as -

$$D = \frac{kT}{\beta m_p} = \frac{kTC_c}{3\pi \mu_f d_p}$$

And hope to obtain the necessary Brownian behavior.

A novel multiphase DNS framework for the simulation of particulate flows in a micro-channel
Some relevant relations (Li – Ahmadi model):

Further, the Cunningham correction (Cc) defined as –

$$C_c = 1.0 + \frac{2\lambda}{d_p} \left( 1.257 + 0.4e^{\frac{1.1d_p}{2\lambda}} \right) \quad \lambda \text{ is the mean free path of the fluid}$$

Is used to correct the particle motion for rarefaction noted in these systems (the Knudsen numbers are typically greater than 0.1)

We can re-write the diffusivity as –

$$D = \frac{kT C_c}{3\pi \mu_f d_p}$$

Clearly $D$ is dependent on $d_p$ (both through $d_p$ and $Cc$)
Some scaling relations (Li – Ahmadi model):

Let us first scale at a constant particle diameter ($d_p$) under different particle/fluid density ratios.

We can scale all the cases using the **diffusional length scale** ($\sqrt{D_0 \tau_p}$) with –

$$ D_0 = \frac{kT C_c}{3\pi \mu_f d_p} \quad \tau_p = \frac{m_p C_c}{3\pi \mu_f d_p} $$

Clearly $D$ is independent of particle ‘density’; and hence its value remains unchanged across various particle/fluid density ratios (see fig.). The relevant hydrodynamic time scale of the system is defined as –

$$ \tau_0^v = \frac{d_p^2}{v_f} \quad \text{(time it takes for the generated fluid momentum to diffuse a particle radius)} $$

This shows that a Brownian particle will persist in a given direction of motion until the fluid momentum generated by the particle diffuses away.
Some scaling relations (Li – Ahmadi model):

Let us next scale at a constant particle/fluid density ratios for different particle diameters ($d_p$).

We can scale all this once again using the diffusional length scale ($\sqrt{D_0 \tau_p}$) with –

\[
D_0 = \frac{kT C_c}{3\pi \mu_f d_p} \quad \tau_p = \frac{m_p C_c}{3\pi \mu_f d_p}
\]

Clearly $D$ is dependent on the particle on particle diameter (both through $d_p$ and $C_c$).
Results

- Diffusion of a 400 nm particle in a micro-channel: Trajectories

Notably higher “dispersion”

Trajectories of a particle with density 1000 kg/m³ after 500 particle response times
Grid convergence study

✓ Settling nanoparticle under ‘fictitious’ gravity

10 microns

→ No Brownian effects
→ No Gravity or buoyancy
→ Fictitious force along $-ve \ z$ direction
Grid convergence study

✓ Choosing the ‘appropriate’ z-Force (PySim)

Particle settling under ‘fictitious’ gravity representing Vrms from the Li-Ahmadi diffusion (PySim)

\[ \text{fictG} = 1e-12 \text{ N} \]

→ Force calculated so as to get the Vrms from a representative Li-Ahmadi diffusion

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Particle settling under fictitious gravity representing Vrms from the Li-Ahmadi diffusion (PySim)
Grid convergence study

✓ Effect of grid size: Settling nanoparticle (@ fixed dt of $\tau_P/200$)

Grid convergence (left) and corresponding courant number plots (right)
Timestep convergence

✓ Effect of time step size: Settling nanoparticle

Time convergence at a 24 cells/dp grid resolution