The Effect of Model Parameters of the Soft-Sphere Scheme on Particle-Particle Collisions

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Outline

• Rationale
• The Importance of the RDPM/IBM
• Soft-Sphere Model
• How to determine $k_n$ and $\eta_n$
• Effects on Drafting Kissing and Tumbling
• Conclusions
Rationale

• Eulerian and Lagrangian systems need a scheme to model particle-particle or particle-wall collisions.

• The soft-sphere scheme is the most common. How do we choose the spring stiffness and damping coefficient in a soft-sphere collision model?

• How do the collision parameters affect the particle dynamics when particles collide?
Resolved Discrete Particle Method (RDPM with IBM)

- Existing collision models are:
  - Hard sphere
    - event driven → one collision at a time
  - Soft sphere
    - time driven → multiple collisions at a time
  - Repulsive force
  - Lubrication force

- The Discrete particle method (DPM) a.k.a. DNS has the capability of handling particle-particle/wall collisions unlike MFIX and DEM

- The RPDM/IBM approach is advantageous because:
  - it effectively handles overlap
  - No regridding is required for moving particles.

Courtesy: A combined soft-sphere collision / IBM for Resolved simulations of particulate flows Wim-Paul Breugem Laboratory for Aero & Hydrodynamics
Soft-Sphere collision model

- Its simplest form is the **linear spring-dashpot model**
- Allows particles to slightly overlap ($<0.5\% \, d$).

For two particles $i$ and $j$, the force balance for collisions in the normal direction is:

$$f_{ij}^n = -k_n \delta_{ij}^n - \eta_n v_{ij}^n$$
Soft-Sphere Model Parameters

\( \delta_{ij}^n \): normal overlap displacement
\( k_n \): normal Spring Stiffness
\( \eta_n \): normal damping coefficient
\( v_{ij}^n \): normal relative velocity

The reduced mass is given as:

\[
m_{ij} = \left( \frac{1}{m_i} + \frac{1}{m_j} \right)^{-1}
\]

\[
f_{ij}^n = -k_n \delta_{ij}^n - \eta_n v_{ij}^n
\]

\[
v_{ij}^n = (v_{ij} \cdot n_{ij}) n_{ij}
\]

We can do same for collisions in the tangential direction
For dry collisions (in air) the following analytical solution is obtained, Hoomans et al. [1]

\[ \eta_n = \begin{cases} 
-\frac{2 \ln(e_n)}{\sqrt{\pi^2 + \ln^2(e_n)}} \sqrt{m_{ij} k_n} & \text{if } e_n \neq 0 \\
\frac{\pi^2}{\ln(e_n)} 2 \sqrt{m_{ij} k_n} & \text{if } e_n = 0
\end{cases} \]

\[ e_n: \text{the normal coefficient of restitution} \]

\[ \eta_n: \text{in terms of } k_n \text{ and } e_n \]

the normal contact time is expressed as:

\[ t_{con,n} = \sqrt{m_{ij} \frac{\pi^2 + \ln^2(e_n)}{k_n}} = N_c \delta t \]

\[ N_c: \text{the number of computational time steps with } N_c > 1 \]

\[ \delta t: \text{time step with } \delta t < t_{con,n} \]

Soft Sphere Collision Parameters $N_c$ and $e_n$

$$k_n = m_{ij} \frac{\pi^2 + \ln^2(e_n)}{(N_c \delta t)^2}$$

In **dry collisions** the contact force dominates the drag force and so can be neglected.

$$\eta_n = - \frac{2m_{ij} \ln(e_n)}{N_c \delta t}$$

**Dry collisions** can be used to approximate collisions in a viscous fluid.

$N_c$ and $e_n$ are now the inputs that link $\eta_n$ and $k_n$. 
How to determine $k_n$ and $\eta_n$ for a collision process

• Experimental methods, Muller et al. [2]
  
  $k_n = 3 \times 10^5 \sim 10^6$ dyn/cm
  - gives a very wide range of results for $k_n$
  - Uses $k_n$ and $e_n$ graphically to find $\eta_n$

• Trial and Error methods, Xu and Yu [3]
  - less elegant

• Method being introduced:
  Using $N_c$ and $e_n$ with $\delta t$ given to find $k_n$ and $\eta_n$
  - (more elegant)

### Experimental/Graphical Approach

<table>
<thead>
<tr>
<th>$k_n$ (dyn/cm)</th>
<th>$\eta_n(e_n=0)$ (dyn s/cm)</th>
<th>$\eta_n(e_n=0.8)$ (dyn s/cm)</th>
<th>$t_{cont,n}$ (s)</th>
<th>$\delta t=0.25\times10^{-3}$</th>
<th>$\delta t=0.5\times10^{-3}$</th>
<th>$\delta t=1\times10^{-3}$</th>
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<td>0.99</td>
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</table>
$\eta_n$ is obtained graphically from $k_n$ and $e_n$ ($0 \sim 0.9$)

The range of $k_n$ that is of interest is $(10^5 \sim 10^6)$ dyn/cm
Relationship between $\delta t$ and $k_n$

$t_{\text{cont},n}$ vs. $k_n$

$\delta t$ vs. $k_n$
Finding $\eta_n$ and $k_n$ from $N_c$, $e_n$

1. Predictions from the **non-linear Hertz contact theory** are used to get the **lower limit** of the contact time $(N_c \delta t \sim 10^{-9}s)$

$$K = \frac{8E}{15(1-\sigma^2)} \sqrt{\frac{R_i R_j}{R_i + R_j}} \quad t_{con,n} = 2.94 \left[ \frac{m_{ij}}{K^2 v_{n,ij}^n} \right]^{\frac{1}{5}} = N_c \delta t$$

$E$ is the Young’s modulus and $\sigma$ is the Poisson's ratio

2. From the discussion of Van der Hoef et al. [4]

- Choose $(N_c \delta t)$ **not too large** to allow severe overlapping between particles
- Choose $(N_c \delta t)$ **not too small** to accurately resolve collision in time (inaccuracy)

First, we use stability/convergence tests to find a value for $\delta t$

We vary $N_c$ to find a range that satisfies the above limits

Relationship between $\eta_n/k_n$ and $N_c$ for different time steps

$k_n$ vs $N_c$

$\eta_n$ vs $N_c$
Relationship between $\eta_n / k_n$ and $e_n$ for different $N_c$'s

$k_n$ vs $e_n$

$\eta_n$ vs $e_n$
Effects of the Collision scheme on Drafting Kissing and Tumbling (DKT)

What is DKT?

During Sedimentation particles experience DKT

- Drafting ⇒ Attraction due to low pressure
- Kissing ⇒ Repeated collisions
- Tumbling ⇒ Rolling on each other

Effect of Collision Parameters on DKT

To study $k_n$ and DKT we use:

- $k_n = 1000, \ 5 \times 10^4, \ 5 \times 10^5$ dyn/cm
- $\eta_n = 100$ dyn s/cm

To study $\eta_n$ and DKT we use:

- $\eta_n = 0, \ 50, \ 100$ dyn s/cm
- $k_n = 50000$ dyn/cm

The results show that as $k_n$ and $\eta_n$ decrease the softer the collisions get and the longer the kissing process.

$\rho_p = 1120$ kg/m$^3$

$\rho_f = 962$ kg/m$^3$

$\mu = 0.913$ Ns/m$^2$

$d_p = 15$ mm
Results: Settling velocity and DKT

Particle settling velocity for different $k_n$

Particle settling velocity for different $\eta_n$
Results: Settling Trajectory and DKT

Particle settling trajectory at different $k_n$

Particle settling trajectory for different $\eta_n$
Spring Stiffness and DKT-video

\[ k_n = 1000 \]  \hspace{1cm} \[ k_n = 50000 \]  \hspace{1cm} \[ k_n = 500000 \]
Damping Coefficient and DKT-video

\[ \eta_n = 0 \]  
\[ \eta_n = 50 \]  
\[ \eta_n = 100 \]
Refining the range of $k_n$

We could by trial and error find the range:

$$5000 \leq k_n \leq 10^5 \text{ dyn/cm}$$

for $\eta_n = 150 \text{ dyn s/cm}$

The change in DKT with $k_n$ was insignificant

Particle settling velocity for

$$5000 \leq k_n \leq 100,000$$
Overlap and Contact time in DKT: refining range with $N_c$

Periodic kissing increases with $k_n$

For very small $N_c$ (large $k_n$) the model approaches a hard sphere scheme with no overlap.

The choice of $N_c$ is in the range: $8 < N_c < 15$ since for this range

Overlap $= \%$diameter $< 0.5\%$ of diameter

<table>
<thead>
<tr>
<th>$N_c$</th>
<th>$k_n$</th>
<th>$\eta_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>160142.35</td>
<td>171.60</td>
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<td>10</td>
<td>102491.10</td>
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<tr>
<td>12</td>
<td>71174.37</td>
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</tbody>
</table>

There is a great degree of agreement with the range that was used in trial and error: $5000 \leq k_n \leq 10^5$ dyn/cm for $\eta_n = 150$ dyn s/cm
Conclusions

• $k_n$ and $\eta_n$ decrease with the time step $\delta t$

• Increasing $k_n$ (decreasing $N_c$) increases the kissing process

• A graphical approach gives a foreknowledge of the range without experiments

• Two main approaches to choose the soft-sphere collision parameters:
  1. given $k_n$ and $e_n$ to find $N_c$ and $\delta t$
  2. given $\delta t$ we can use $N_c$ to find $k_n$ and $\eta_n$ which is more elegant
Questions?