

# Supplemental Information

## 1 DEM particle force models

### 1.1 Fluid-particle coupling forces

The fluid-particle coupling forces considered in the current LES-DEM model are listed in equation 1:

$$\mathbf{F}_{pf} = \mathbf{F}_d + \mathbf{F}_{\nabla p} + \mathbf{F}_{\nabla \cdot \tau} + \mathbf{F}_{bg} + \mathbf{F}_{am} + \mathbf{F}_L + \mathbf{F}_B \quad (1)$$

Here, the forces include drag force  $\mathbf{F}_d$ , pressure gradient force  $\mathbf{F}_{\nabla p}$ , fluid viscous force  $\mathbf{F}_{\nabla \cdot \tau}$ , buoyancy and gravity force  $\mathbf{F}_{bg}$ , added mass force  $\mathbf{F}_{am}$ , lift force  $\mathbf{F}_L$ , and Basset history force  $\mathbf{F}_B$ . With the consideration of all possible forces, the model has the capability to describe the full picture of the particle saltation process.

Among all the forces, the drag force  $\mathbf{F}_d$  is the most important. The classic Schiller-Naumann drag force model proposed in Schiller & Naumann (1935) is used in this research:

$$\mathbf{F}_d = \frac{1}{8} \pi \rho_f C_d D^2 |\mathbf{U}_f - \mathbf{u}_{p,i}| (\mathbf{U}_f - \mathbf{u}_{p,i}) \quad (2)$$

where  $D$  is the particle diameter,  $\rho_p$  is the particle density, and  $C_d$  is the drag coefficient calculated as:

$$C_d = \max \left[ 0.44, \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}) \right] \quad (3)$$

Here,  $Re_p$  is the particle Reynolds number defined as:

$$Re_p = \frac{|\mathbf{U}_f - \mathbf{u}_{p,i}| D}{\nu} \quad (4)$$

where  $\nu$  is the fluid viscosity.

The drag force represents skin friction and form drag arising from small scale distortions of the fluid streamlines in the neighborhood of the particle (Anderson & Jackson, 1967). The force on the particle due to large scale pressure gradients is represented by the pressure gradient force, which has the form of:

$$\mathbf{F}_{\nabla p} = -V_p \nabla p \quad (5)$$

where  $p$  is the fluid pressure and  $V_p$  is the volume of particle.

The fluid viscous force is due to the shearing of surrounding fluid, which is evaluated as:

$$\mathbf{F}_{\nabla \cdot \boldsymbol{\tau}} = -V_p \nabla \cdot \boldsymbol{\tau} \quad (6)$$

where  $\boldsymbol{\tau}$  is the fluid shear stress tensor.

The pressure gradient force and fluid viscous force do not contribute significantly to the motion of a particle in gas-particle flows where the density ratio between gas and particle is generally in the order of  $10^{-3}$ . However, they are important in liquid-solid flows, which is the case in this paper and the material density ratio is not far from unity (Crowe, 2012).

The gravitational and buoyancy forces on a particle can be combined into one as:

$$\mathbf{F}_{bg} = -V_p(\rho_s - \rho_f)\mathbf{g} \quad (7)$$

where  $\mathbf{g}$  is the gravitational acceleration.

Another important particle force is the lift force due to particle rotation, which is driven by fluid shearing and particle contact with a surface (Crowe, 2012). The lift force can be divided into the Saffman lift force (Saffman, 1965) and the Magnus lift force (Rubinow & Keller, 1961), both of which are considered in this research. The lift force model proposed in Loth & Dorgan (2009) is used. It combines the two lift forces with a unified formula:

$$\mathbf{F}_L = \frac{\pi}{8} C_L \rho_f D^2 (\mathbf{U}_f - \mathbf{u}_{p,i}) \cdot (\mathbf{U}_f - \mathbf{u}_{p,i}) \quad (8)$$

where  $C_L$  is the coefficient of lift force.  $C_L$  is comprised of two parts:

$$C_L = J(\epsilon) \frac{12.92}{\pi} \sqrt{\frac{\omega^*}{Re_p}} + \Omega_{p,eq}^* C_{L,\Omega} \quad (9)$$

where the first term is for the Saffman lift force and the second for the Magnus lift force. Here,  $J$  is a function of  $\epsilon$  (McLaughlin, 1991; Mei, 1992):

$$J = \begin{cases} -14.176\pi^2\epsilon^5 \ln(1/\epsilon^2), & \epsilon < 0.1 \\ 0.3 \left\{ 1 + \tanh \left[ \frac{5}{2} (\log_{10} \sqrt{\frac{\omega^*}{Re_p}} + 0.191) \right] \right\} \left\{ \frac{2}{3} + \tanh \left[ 6 \left( \sqrt{\frac{\omega^*}{Re_p}} - 0.32 \right) \right] \right\}, & 0.1 \leq \epsilon \leq 20 \\ 1 - 0.287/\epsilon^2, & \epsilon > 20 \end{cases} \quad (10)$$

where  $\epsilon = \sqrt{2\alpha/Re_p}$ ,  $\alpha = |\boldsymbol{\omega}|D^2$ , and  $\boldsymbol{\omega}$  is the fluid vorticity.  $\omega^*$  and  $\Omega_p^*$  are two dimensionless parameters defined as:

$$\omega^* = \frac{|\boldsymbol{\omega}|D}{|\mathbf{U}_f - \mathbf{u}_{p,i}|}, \quad \Omega_p^* = \frac{|\boldsymbol{\Omega}_p|D}{|\mathbf{U}_f - \mathbf{u}_{p,i}|} \quad (13)$$

where  $\boldsymbol{\Omega}_p$  is the particle angular velocity.

For the Magnus lift force, another two coefficients have to be calculated. The first one is the coefficient of Magnus lift force  $C_{L,\Omega}$  (Rubinow & Keller, 1961), which can be calculated as in Loth & Dorgan (2009):

$$C_{L,\Omega} = 1 - \{0.675 + 0.15(1 + \tanh[0.28(\Omega_p^* - 2)])\} \tanh(0.18Re_p^{1/2}) \quad (14)$$

To evaluate  $\Omega_{p,eq}^*$  in equation 9, the empirical model proposed in Loth & Dorgan (2009) is used:

$$\Omega_{p,eq}^* = \frac{\omega^*}{2}(1 - 0.0075Re_\omega)(1 - 0.062Re_p^{1/2} - 0.001Re_p) \quad (15)$$

where  $Re_\omega = |\omega|D^2/\nu$ . The direction of the lift is defined to be perpendicular to  $(\mathbf{U}_f - \mathbf{u}_{p,i})$  and a positive  $C_L$  is taken in the direction of  $\omega \times (\mathbf{U}_f - \mathbf{u}_{p,i})$  for Saffman lift force and in the direction of  $\Omega_p \times (\mathbf{U}_f - \mathbf{u}_{p,i})$  for Magnus lift force.

The added mass force, due to the acceleration of particles in the fluid, is calculated as:

$$\mathbf{F}_{am} = \frac{1}{2}\rho_f V_p \left( \frac{D\mathbf{U}_f}{Dt} - \frac{d\mathbf{u}_{p,i}}{dt} \right) \quad (16)$$

where  $D/Dt$  is the material derivative (Auton, Hunt, & Prud'Homme, 1988). The Basset history force is due to the temporal delay in boundary layer development when the relative velocity changes with time (Basset, 1888). The Basset history force is defined as:

$$\mathbf{F}_B = \frac{3}{2}D^2\sqrt{\pi\rho_f\mu_f} \int_0^t \frac{\frac{d\mathbf{U}_f}{dt} - \frac{d\mathbf{u}_{p,i}}{dt}}{\sqrt{t-\tau}} d\tau \quad (17)$$

It is well known that the evaluation of the Basset term is difficult because the denominator in the integrand vanishes when the upper integration limit is approached. To solve this problem, Bombardelli, González, & Niño (2008) proposed a new treatment by using the method in Tatom (1988). Their method calculates the term by the Riemann-Liouville integral as follows:

$$\int_a^t \frac{\frac{d\mathbf{u}_r}{dt}}{\sqrt{t-\tau}} d\tau = \Gamma\left(\frac{1}{2}\right) \frac{d^{-0.5}\left(\frac{d\mathbf{u}_r}{dt}\right)}{[d(t-a)]^{-0.5}} \quad (18)$$

where  $\mathbf{u}_r$  is the relative velocity between fluid and particles,  $\Gamma(\cdot)$  is the Gamma function (Abramowitz & Stegun, 1970),  $a$  is the lower limit of integration ( $=$  to 0 for the Basset history force). For a general function  $f$ , the term can be further evaluated using a series expansion:

$$\frac{d^q f}{[d(t-a)]^q} = \lim_{N \rightarrow \infty} \left[ \left( \frac{t-a}{N} \right)^{-q} \frac{1}{\Gamma(-q)} \sum_{k=0}^{N-1} \frac{\Gamma(k-q)}{\Gamma(k+1)} f\left(t - \frac{k(t-a)}{N}\right) \right] \quad (19)$$

where  $q$  is an arbitrary value ( $= -0.5$  in our case).

However, the method proposed in Bombardelli et al. (2008) could still suffer from data overflow problem. For example, when  $N = 1000$ ,  $\Gamma(1000)$  has a value of  $10^{2564}$ . In order to solve this, an

alternative is sought to find a robust mathematical formula. We propose to use the Stirling equation to approximate the Gamma function:

$$\Gamma(x) \approx \sqrt{2\pi} e^{-x} x^{x-\frac{1}{2}} \quad (20)$$

Then the term which will lead the data overflow can be re-written as:

$$\frac{\Gamma(x + \frac{1}{2})}{\Gamma(x + 1)} = \exp \left[ \frac{1}{2} + x \log(x + \frac{1}{2}) - (x + \frac{1}{2}) \log(x + 1) \right] \quad (21)$$

The use of this equation ensures no data overflow and it is much simpler and more convenient to be implemented in numerical codes. To demonstrate the accuracy, a test case is conducted using  $f(x) = \frac{1}{3}x^3$ ,  $\frac{df(x)}{dx} = x^2$ . As shown in Figure 1, the relative error compared with the analytical solution gradually decreases with an increasing  $N$ . When  $N = 1000$ , the relative error is less than 0.5%.

## 1.2 Particle contact force model

A simplified version of Hertz-Mindlin particle contact model proposed by Zhu, Zhou, Yang, & Yu (2007) is used in this research. This model is widely used in for example Chand, Khaskheli, Qadir, Ge, & Shi (2012), Furbish and Schmeeckle (2013) and Schmeeckle (2014). All the particles were treated as spheres with certain volume. The particle-particle and particle-wall interactions are conceptualized as a spring-dashpot model in both the normal and tangential directions. When there is a normal distance  $\delta_n$  and a tangential distance  $\delta_t$  between two particles, the normal contact force  $F_n$  and the tangential contact force  $F_t$  are given by:

$$F_n = K_n \delta_n - \gamma_n v_n \quad (22)$$

and

$$F_t = K_t \delta_t - \gamma_t v_t \quad (23)$$

where  $v_n$  and  $v_t$  are the relative velocities in the normal and tangential directions, respectively.  $K_n$  and  $K_t$  are the stiffness coefficients.  $\gamma_n$  and  $\gamma_t$  are the damping coefficients. They are calculated as:

$$K_n = \frac{4}{3} Y \sqrt{R \delta_n} \quad (24)$$

$$K_t = 8G \sqrt{R \delta_n} \quad (25)$$

$$\gamma_n = -2\sqrt{5/6} \beta \sqrt{S_n m} \geq 0 \quad (26)$$

$$\gamma_t = -2\sqrt{5/6}\beta\sqrt{S_tm} \geq 0 \quad (27)$$

$S_n$ ,  $S_t$  and  $\beta$  coefficients are given by:

$$S_n = 2Y\sqrt{R\delta_n} \quad (28)$$

$$S_t = 8G\sqrt{R\delta_n} \quad (29)$$

$$\beta = \frac{\ln(e)}{\sqrt{(\ln(e))^2 + \pi^2}} \quad (30)$$

Here,  $e$  is the coefficient of restitution,  $Y$  is the effective Young's modulus,  $G$  is the effective shear modulus,  $\theta$  is the Poisson's ratio,  $R$  is the effective radius, and  $m$  is the effective mass. For sediment particles, the Young's modulus and Poisson's ratio of silicon dioxide are commonly used. For the coefficient of friction, Niño & García (1998a) recommended the value of  $f$  between  $0.73 \sim 0.89$  based on their experimental data. Schmeeckle, Nelson, Pitlick, & Bennett (2001) used a value of 0.9 in their numerical model, which is also used in this research. For the coefficient of restitution  $e$ , the range of its value differs in the literature. For example, Drake & Calantoni (2001) found  $e > 0.8$  for natural sand particles and  $e < 0.1$  for gravels. These values are much different from others. Schmeeckle et al. (2001) and Ruiz-Angulo & Hunt (2010) showed much lower value of  $e$  when particle collision happened in fluid. In this case, the fluid viscous damping effect is lumped into the restitution coefficient. Thus,  $e$  should be called the “wet” restitution coefficient. In our model, since the fluid viscous force has already been explicitly considered, a “dry” restitution coefficient with a value of 0.95 is used. The research of Drake & Calantoni (2001) found that both the restitution coefficient and the coefficient of friction do not significantly influence the integral quantities in sediment transport. Similar treatment can also be found in van Wachem, Yu, & Hsu (2010) and Durán, Andreotti, & Claudin (2012), in which  $e=0.95$  and  $e=0.9$  were used, respectively. The particle density  $\rho_s$  is  $2,650 \text{ kg/m}^3$ . The values of other material parameters for particles used in this research can be found in the main text.

To solve the particle motion equation, the Crank-Nicolson scheme was used for numerical stability:

$$\mathbf{u}_{p,i}'' = \mathbf{u}_{p,i} + \frac{1}{2}K'_{sl}\Delta\mathbf{U} \quad (31)$$

where

$$K'_{sl} = \Delta t |\mathbf{f}_{pf}| / (m_{p,i} |\mathbf{U}_f - \mathbf{u}_{p,i}|) \quad (32)$$

$$\mathbf{u}_{p,i}' = \frac{\mathbf{u}_{p,i} + K'_{sl} [\mathbf{U}_f - (1 - \alpha_{CN})\mathbf{u}_{p,i}]}{1 + K'_{sl}\alpha_{CN}} \quad (33)$$

$$\Delta U = U_f - \left[ (1 - \alpha_{CN}) \mathbf{u}_{p,i} + \alpha_{CN} \mathbf{u}'_{p,i} \right] \quad (34)$$

Here  $\mathbf{u}_{p,i}$  is the velocity of particle  $i$  at the old time step,  $\mathbf{u}'_{p,i}$  is the predicted particle velocity,  $\mathbf{u}''_{p,i}$  is the final updated particle velocity at the current time step.  $\alpha_{CN}$  is the coefficient of the Crank-Nicolson scheme which had a value of 0.5 in this research.

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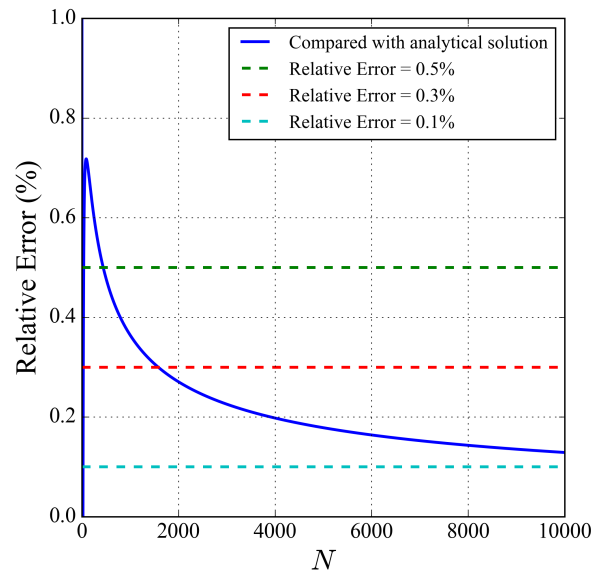


Figure 1: Relative error of the new approximation method for the Basset history force.