Verification and validation study of continuum granular frictional flow theories using a discrete technique and experimental data*

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Introduction

Two frictional flow theories are evaluated for dense granular flows. We assume, similar to Johnson and Jackson,[2] that the total stresses acting on a granular assembly are the sum of stresses due to instantaneous binary collisions derived from kinetic theory and frictional stresses due to enduring contact between layers of particles. We describe a frictional model,[3,4] which has been traditionally used in the MFIX computer code (www.mfix.org). We also use another frictional model developed by Srivastava and Sundaresan,[5] who implemented it in the MFIX code and conducted validation studies of bin discharge. A simplified version of this model is described here. By implicitly expressing the divergence of solids velocity in this model, it is no longer necessary to relax the stresses by solving an additional transport equation for the ratio of frictional to critical pressure. The frictional stresses in this model affect the granular assembly at solids concentration lower than packing as proposed by Johnson and Jackson.[2]
Validation studies of dense frictional flow theories are available in the literature.[8,9] Such studies include other complications in the flow physics, such as interstitial fluid, complex geometries, and cohesive particles. In contrast, this study focuses only on dense frictional flows in a vacuum, so no effect of the fluid is introduced in the model equations. Furthermore, we only study relatively simple systems such as bin discharge, similar to Srivastava and Sundaresan,[5] and compare results of the discharge rate to the Beverloo et al.[10] correlation. For a detailed quantitative comparison of the dense frictional models, we use further simplifications by studying a gravity-free granular shear flow between two parallel plates. Computer data generated using a discrete particle method with a soft-sphere contact model (DEM) are used for comparison with continuum models. Discrete techniques using both soft-sphere and hard-sphere contact models are powerful tools for validating continuum models, as shown by many studies in the literature.[11-13] Although most of these studies are aimed at validating granular kinetic theories, discrete techniques are also useful to study dense frictional flows and are used here to validate two frictional flow theories commonly used in continuum modeling.

Granular flow model

The granular kinetic theory model used in this study is essentially the same as that derived by Lun et al.[1] This includes conservation equations for flow of solids in a vacuum and the constitutive relations for the solids stresses based on granular kinetic theory. In this study, the total stress of the granular assembly is assumed to be the sum of collisional (derived from granular kinetic theory) and frictional stresses.[2]
Conservation of mass for constant solids density:

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$$\rho_s\left[\frac{\partial \varepsilon_s}{\partial t}+\nabla\cdot\left(\varepsilon_s \mathbf{v_s}\right)\right]=0 \tag{1}$$

Conservation of linear momentum:

$$\rho_s\left[\frac{\partial \varepsilon_s \mathbf{v_s}}{\partial t}+\nabla\cdot\left(\varepsilon_s\, \mathbf{v_s}\mathbf{v_s}\right)\right]=\nabla\cdot\left(\boldsymbol{\tau}_\mathbf{k}+\boldsymbol{\tau}_\mathbf{f}\right)+\varepsilon_s\rho_s\,\mathbf{g} \tag{2}$$

Translational granular energy conservation equation:

$$\frac{3}{2}\rho_s\left[\frac{\partial \varepsilon_s\Theta_s}{\partial t}+\nabla\cdot\left(\varepsilon_s\Theta_s \mathbf{v_s}\right)\right]=-\nabla\cdot\mathbf{q}+\boldsymbol{\tau}_\mathbf{k}:\nabla\mathbf{v_s}-\rho_s J_s \tag{3}$$

Solids kinetic-collisional and frictional stress terms:

$$\boldsymbol{\tau}_\mathbf{k}=\left[-P_s+\eta\mu_b\nabla\cdot\mathbf{v_s}\right]\mathbf{I}+2\mu_s\mathbf{S_s} \tag{4}$$

$$\boldsymbol{\tau}_\mathbf{f}=-P_f\,\mathbf{I}+2\mu_f\mathbf{S_s} \tag{5}$$

$$\mathbf{S_s}=\frac{1}{2}\left(\nabla\mathbf{v_s}+\left(\nabla\mathbf{v_s}\right)^T\right)-\frac{1}{3}\nabla\cdot\mathbf{v_s}\,\mathbf{I} \tag{6}$$

Solids pressure:

$$P_s=\varepsilon_s\rho_s\Theta_s\left[1+4\eta\varepsilon_s g_0\right] \tag{7}$$

The compressibility factor (Z) derived by Carnahan and Starling[15] can be used to express the radial distribution function at contact (g_0):

$$g_0=\frac{1-0.5\varepsilon_s}{\left(1-\varepsilon_s\right)^3} \tag{8}$$

Solids viscosity model:

$$\mu_s=\left(\frac{2+\alpha}{3}\right)\left[\frac{\mu}{g_0\eta(2-\eta)}\left(1+\frac{8}{5}\eta\varepsilon_s g_0\right)\left(1+\frac{8}{5}\eta(3\eta-2)\varepsilon_s g_0\right)+\frac{3}{5}\eta\mu_b\right] \tag{9}$$

$$\mu=\frac{5}{96}\rho_s d_p\sqrt{\pi\Theta_s}\ ,\ \ \mu_b=\frac{256}{5\pi}\mu\varepsilon_s^2 g_0 \tag{10}$$

Granular energy flux and conductivity:

$$\mathbf{q}=-\kappa_s\,\nabla\Theta_s \tag{11}$$

$$\kappa_s=\left(\frac{\kappa}{g_0}\right)\left[\left(1+\frac{12}{5}\eta\varepsilon_s g_0\right)\left(1+\frac{12}{5}\eta^2(4\eta-3)\varepsilon_s g_0\right)+\frac{64}{25\pi}(41-33\eta)\eta^2\left(\varepsilon_s g_0\right)^2\right] \tag{12}$$

$$\kappa=\frac{75\rho_s d_p\sqrt{\pi\Theta_s}}{48\eta(41-33\eta)} \tag{13}$$

Collisional dissipation of granular energy:

$$J_s=\frac{48}{\sqrt{\pi}}\eta(1-\eta)\frac{\varepsilon_s^2 g_0}{d_p}\Theta_s^{3/2} \tag{14}$$

Frictional-collisional wall boundary condition:[2]

$$\frac{\mathbf{v_{sl}}}{\left|\mathbf{v_{sl}}\right|}\cdot\left(\boldsymbol{\tau}_\mathbf{k}+\boldsymbol{\tau}_\mathbf{f}\right)\cdot\mathbf{n}+\frac{\phi\pi\,\rho_s\varepsilon_s g_0\sqrt{\Theta_s}}{2\sqrt{3}\varepsilon_s^{\max}}\mathbf{v_{sl}}+\left(\mathbf{n}\cdot\boldsymbol{\tau}_\mathbf{f}\cdot\mathbf{n}\right)\tan\delta=0 \tag{15}$$

$$\mathbf{n}\cdot\mathbf{q} = \frac{\phi\pi\left|\mathbf{v_{sl}}\right|^2 \rho_s \varepsilon_s g_0 \sqrt{\Theta_s}}{2\sqrt{3}\varepsilon_s^{\max}} - \frac{\sqrt{3}\pi\,\rho_s \varepsilon_s g_0 \left(1-e_w^2\right)\sqrt{\Theta_s}}{4\varepsilon_s^{\max}}\Theta_s \qquad (16)$$

Syamlal et al. (S-R-O) frictional model

This model has been traditionally used in the MFIX code and was described in detail by Syamlal et al.[4] The model equations as presented in this study were first written by Schaeffer,[3] who described the plastic flow of a granular material and related the shear stress to the normal stress. The Syamlal et al.[4] (S-R-O) model expresses the frictional stresses by the following equations:

$$P_f = P_c = \begin{cases} 10^{25}\left(\varepsilon_s - \varepsilon_s^{\max}\right)^{10} & \varepsilon_s > \varepsilon_s^{\max} \\ 0 & \varepsilon_s \le \varepsilon_s^{\max} \end{cases} \qquad (17)$$

$$\mu_f = \begin{cases} \dfrac{P_c \sin(\delta)}{2\sqrt{I_{2D}}} & \varepsilon_s > \varepsilon_s^{\max} \\ 0 & \varepsilon_s \le \varepsilon_s^{\max} \end{cases} \qquad (18)$$

In this case, the critical solids pressure is a power law function[4] of the solids volume fraction that allows for some compressibility near the packing limit similar to other plastic flow theories.[7,17,18]

Srivastava-Sundaresan (S-S) frictional model

The frictional model used in this study was proposed by Srivastava and Sundaresan[5] who gave expressions of the frictional stresses for a compressible granular assembly. This model is expressed by the following equations:

$$P_c = \begin{cases} 10^{25}\left(\varepsilon_s - \varepsilon_s^{\max}\right)^{10} & \varepsilon_s > \varepsilon_s^{\max} \\ Fr\dfrac{\left(\varepsilon_s - \varepsilon_s^{\min}\right)^r}{\left(\varepsilon_s^{\max} - \varepsilon_s\right)^s} & \varepsilon_s^{\max} \ge \varepsilon_s > \varepsilon_s^{\min} \\ 0 & \varepsilon_s \le \varepsilon_s^{\min} \end{cases} \qquad (19)$$

$$\frac{P_f}{P_c} = \left(1 - \frac{\nabla\cdot\mathbf{v_s}}{n\sqrt{2}\sin(\delta)\sqrt{\mathbf{S_s}:\mathbf{S_s} + \Theta_s / d_p^2}}\right)^{n-1} \qquad (20)$$

$$\mu_f = \frac{\sin(\delta)}{\sqrt{2}}\frac{P_f}{\sqrt{\mathbf{S_s}:\mathbf{S_s} + \Theta_s / d_p^2}}\left\{n - (n-1)\left(\frac{P_f}{P_c}\right)^{\frac{1}{n-1}}\right\} \qquad (21)$$

Application of the frictional models to a discharge of 1 mm particles from a 2D bin

The first application of the frictional models presented in this study is to a 2D bin discharge. This is the same example that was studied by Srivastava and Sundaresan:[5] a 2D rectangular bin 8 cm wide and 100 cm high with an open top and an orifice centered at the bottom. Two issues were reported by Srivastava and Sundaresan[5] that are addressed in this section: First, the cause of the grid-scale flutter in the solids volume fraction observed initially in the simulation was determined and eliminated in this study, and second, lower discharge rates were computed in this study, which resulted in better agreement with the Beverloo correlation.

Temporal profiles of discharge rate

Figure 1 shows the temporal variation of the discharge rates for the four orifice diameters of 1.4, 1.6, 1.8 and 2 cm.

A comparison of the discharge rate for the case of a bin with an orifice diameter of 1.4 cm with the simulation results of Srivastava and Sundaresan[5] (see their figure 4) shows that our computed discharge rate (shown in figure 2) was lower. The reason for the disagreement could be a limitation in the frictional viscosity. The current model does not set any limit for computed values of the frictional viscosity for either S-S or S-R-O models. In the previous publication, Srivastava and Sundaresan[5] may have used an upper limit to the frictional viscosity, which value is not known. This is suspected because in one simulation using the S-S model, we limited the frictional viscosity to100 poise, which resulted in almost double the discharge mass flow rate.

Figure 1 shows that lower values of discharge rate are computed using the Syamlal et al.[4] (S-R-O) frictional model as compared to the S-S predictions. This is due to a fundamental difference between these two frictional models: the S-S model friction starts at a lower solids volume fraction ($\varepsilon_s^{\min}$) so that the computed normal and shear stresses are lower than those computed using the S-R-O model where friction starts at maximum packing.

Verification of Beverloo correlation

Numerical data obtained using the S-S and S-R-O frictional models were compared to the Beverloo et al.[10] correlation for estimating the discharge rate from hoppers and bins, which was written by Srivastava and Sundaresan[5] for a 2D bin discharge as:

$$W = C\,\rho_B\, g^{0.5} D_o^{1.5} H \tag{23}$$

Figure 2 shows that the discharge rate is a function of $D_o^{1.4}$ and $D_o^{1.9}$ for the S-S and S-R-O models, respectively. This is in agreement with the results of Srivastava and Sundaresan,[5] who found that the discharge rate scales as $D_o^{1.4}$ using their frictional model. The S-R-O frictional model over-predicts the value for the exponent of the orifice width.

According to Figure 2, the computed value of *C* (the empirical constant in the Beverloo correlation) was calculated as 1.08 and 0.61 for the S-S and S-R-O models, respectively. Srivastava and Sundaresan[5] computed a larger value *C* = 1.6, due to their larger computed discharge rate. This current study, however, found the value of *C* to be closer to the experimental measurements using the S-S model. The S-R-O frictional model predicted

lower discharge rates for all widths of the orifice and, thus, a value of *C* that is in better agreement with the Beverloo correlation.
The next section is proposed to help us highlight more accurately the distinctions between these two frictional continuum models.

Validation of the frictional models for 1D granular Couette flow
We applied the frictional flow theories discussed previously to model a gravity-free granular flow (in a vacuum) in a Couette shear cell. To conduct the validation study, we generated computer data of the granular flow using the soft-sphere discrete element method[20] (DEM) available in MFIX. In this study, the mass, *m*, of a particle is equal one. The normal and tangential spring constants were equal, with a value of $k/m = 8\times10^{10}$ s^{-2}. The same value for particle-particle and particle-wall friction coefficients was used in this study: $\mu_p = \mu_w = 0.5$. Other physical parameters such as restitution coefficients ($e = e_w = 0.8$), were the same as those used in the study of Karion and Hunt.[21]
Figure 3 shows a snapshot (after 20 sec) of particle position and velocity in the periodic shear cell. Particles with high velocity are observed at the top and bottom walls due to friction with the moving walls. Near the walls, a relatively dilute flow is observed due to the high energy particles that tend to push nearby particles toward the center of the channel where the flow is clearly denser. Layering of particles is observed at the center of the channel, although some pockets of void can also be seen—perhaps due to large shear (and energy) applied at the frictional walls.
Figure 4 shows a comparison of time-averaged DEM data and the results obtained using the continuum frictional flow theories discussed in this study. Although we used the transient continuum models, the numerical simulations quickly reached a steady-state after only few seconds of simulation. It was expected that transient continuum gas-solids simulations reach steady-state for flows with no gravity as demonstrated by Benyahia et al.,[22] who verified that the frequency of oscillations scales with $\sqrt{g}$. Furthermore, we found identical results in both 1D and 2D periodic geometries, and therefore, only 1D continuum simulation results are reported in this study. Figure 4 shows that both the continuum collisional-frictional models used in this study are able to reproduce the qualitative trends computed using DEM. Due to the high granular temperature gradient between the walls and center of the channel, solids moves to the center in order to balance the collisional pressure. This migration of solids to the center can be limited with frictional pressure, which, in the case of S-R-O model, does not occur until maximum packing is reached. This is the reason why this model predicts packed regions ($\nu_s^{\max} = 0.9$) at the center of the channel. This is not the case with the S-S model where friction starts at $\nu_s^{\min} = 0.6$ so that a better agreement is obtained at the center. The continuum models predict a more dilute flow near the walls due to the large values of granular temperature computed in that region because of wall boundary conditions. We should mention that one parameter, the specularity coefficient ϕ in the granular boundary condition proposed by Johnson and Jackson,[2] was adjusted in order to fit the near-wall velocity data obtained using the S-S model. A value of $\phi = 0.052$ is used to obtain the continuum data shown in figure 4. It is possible that the cause of the disagreement observed for the granular temperature profiles is mainly due to the fact that we are only

solving for the translational granular energy, and, thus, a good agreement is not expected in the dilute regions of this highly frictional flow. Nevertheless, it is clear from figure 4 that a better quantitative agreement with DEM data is obtained using Srivastava-Sundaresan (S-S) frictional model.

Conclusion

We present in this study a granular kinetic theory model derived by Lun et al.,[1] and conduct a comparative study of two frictional flow theories, one proposed by Syamlal et al.,[4] and one by Srivastava and Sundaresan.[5] These two continuum frictional flow theories are validated for a granular bin discharge with an empirical correlation developed by Beverloo et al.[10] and show reasonable agreement for both the Srivastava-Sundaresan (S-S) and Syamlal et al.[4] models. A more detailed comparison of the two continuum frictional models is conducted in the second part of this study. We validate these two theories with computer simulation data obtained using a discrete element method (DEM) for a granular Couette flow. Both frictional continuum theories show similar trends as DEM data. The solids area fraction was lower at the walls due to the higher granular temperature generated from friction with the moving walls. Overall, the S-S frictional model shows better agreement with DEM data.

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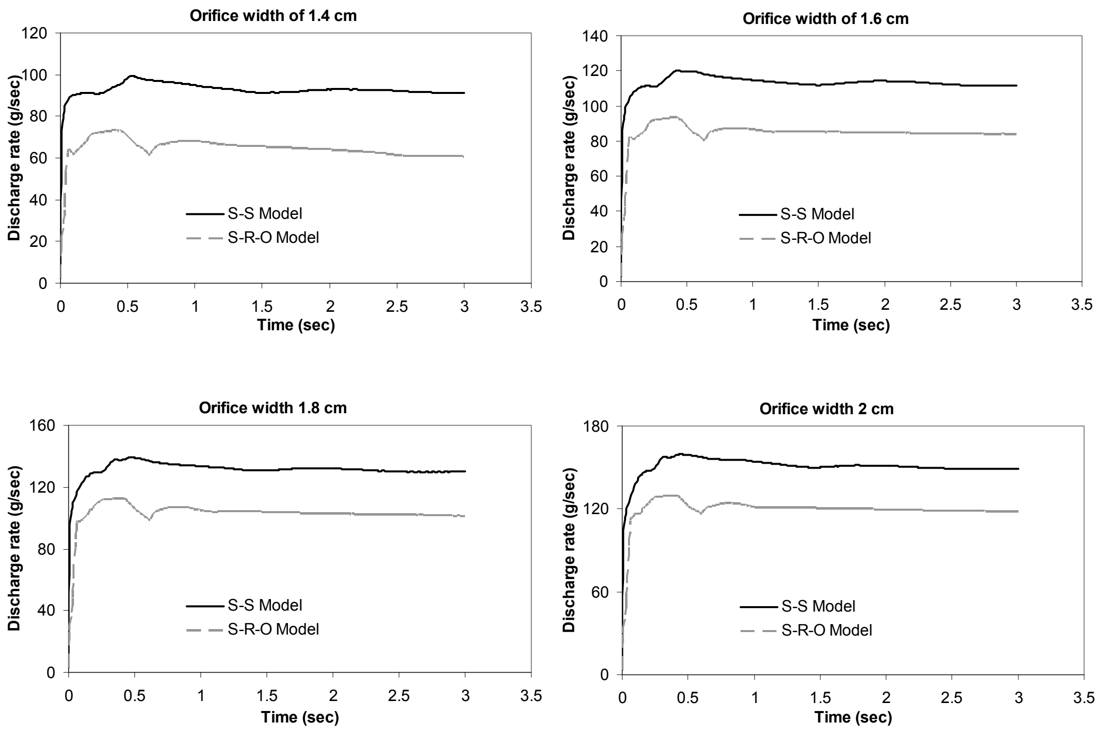

Figure 1: Temporal variation of the solids discharge rate for 4 different orifice widths using the Srivastava and Sundaresan[5] (S-S), and Syamlal et al.[4] (S-R-O) frictional models.

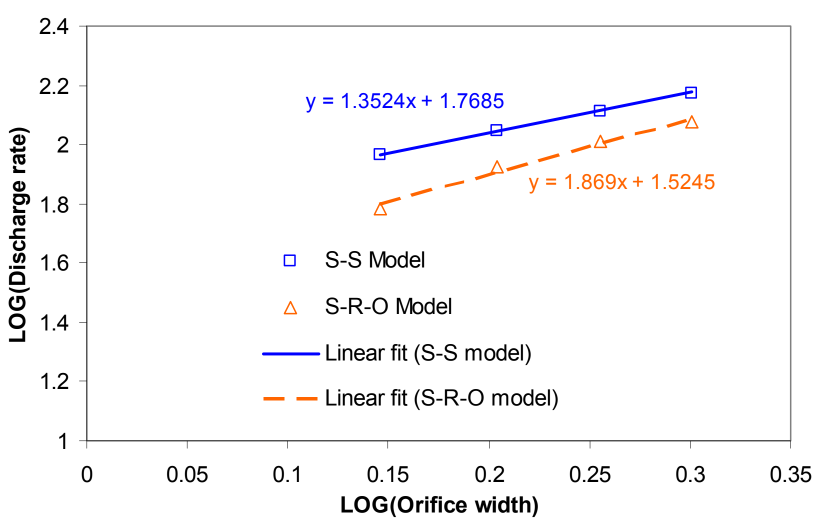

Figure 2: Verification of the Beverloo correlation using both S-S and S-R-O frictional models. The linear best fits of the computed data and the corresponding equations are also plotted.

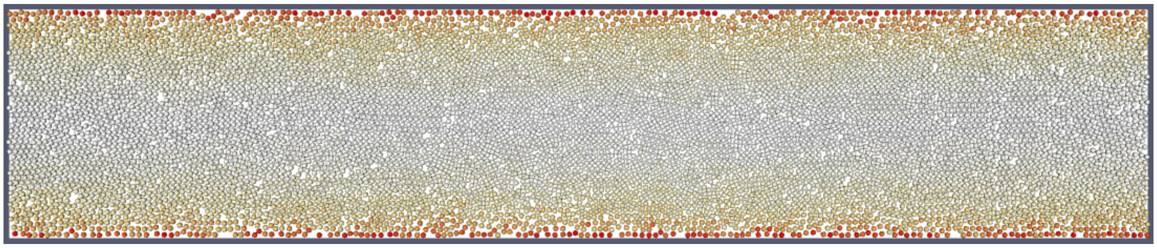

Figure 3: Instantaneous particle position and velocity in the periodic shear cell. Red color indicates higher velocity with maximum of about 9 m/s obtained at the top and bottom moving walls. Periodic boundaries apply to the right and left sides. Particles are monodisperse with an average solids area fraction of ν_s = 0.75 and $h/d_p = 40$.

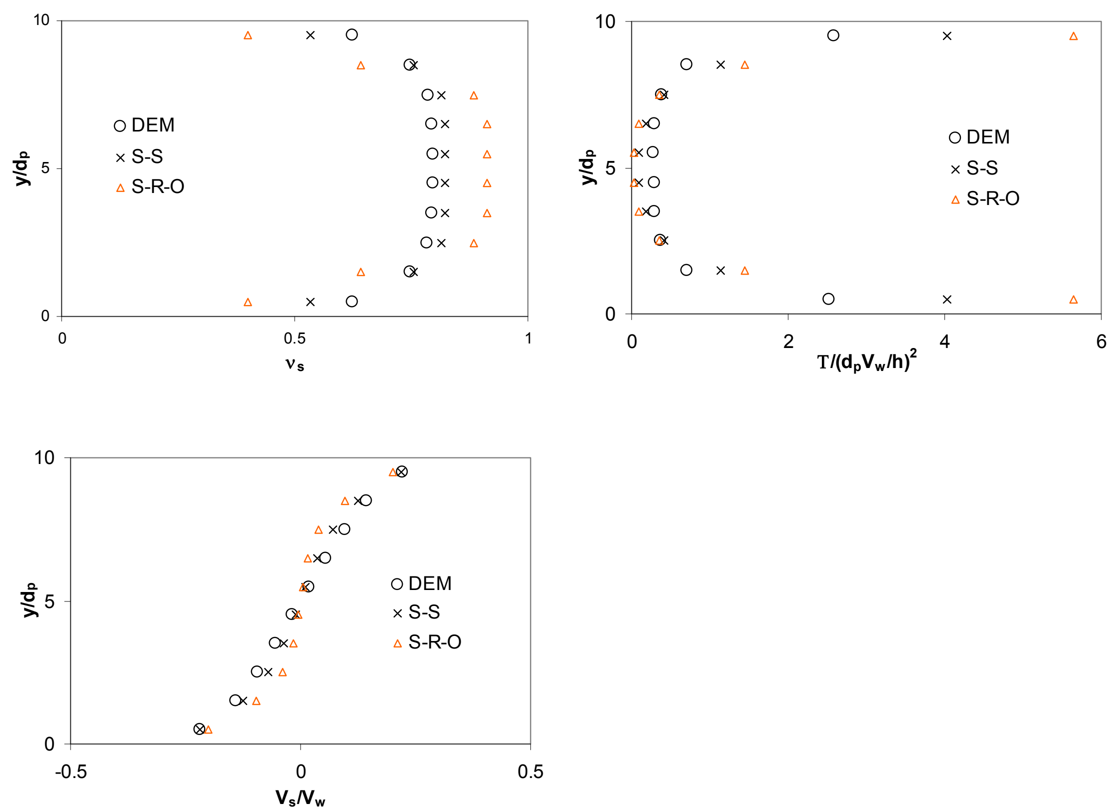

Figure 4: Comparison between the time-averaged DEM results and the steady continuum collisional-frictional models (using S-S and S-R-O frictional models) for the solids area fraction, granular temperature, and velocity.