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Constitutive modelling of phase transition in granular materials

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ABSTRACT

The goal of this contribution is to briefly present the recent advances in the formulation of a new constitutive approach capable of capturing the response of granular materials from quasi-static to dynamic conditions, when the materials experiences a solid-to-fluid phase transition.
Model predictions have been compared with numerical results under either simple shear conditions or true triaxial conditions.

KEY WORDS: granular flows; solid-fluid transition; constitutive modelling; granular temperature; critical state.

INTRODUCTION

Dry or saturated granular flows are encountered either in a large number of natural phenomena or in different industrial processes. To model granular flows in the framework of continuum mechanics, a key issue is the formulation of a suitable constitutive model, capable of capturing the complex rheological behaviour of the granular material in a wide range of strain rates and concentrations and reproducing the transition from solid- to fluid-like regimes.
In this paper, the recent advances in the formulation of a new constitutive approach, capable of capturing the response of granular materials from solid- to fluid-like regimes, will be briefly presented.
The original model assumes that: (i) the granular material can be either dry or saturated by water, (ii) grains are frictional, deformable and uncrushable.
A parallel scheme is assumed according to which the stress tensor is computed as the sum of a liquid contribution and a granular contribution. The former is calculated by considering the liquid phase as an incompressible Newtonian fluid, with viscosity function of the void ratio. This contribution is nil in dry granular flows. The latter is in turn calculated as the sum of two components: the quasi static stress and the collisional stress. The quasi static stress, accounting for the response of the granular material as a solid-like continuum, is associated with long elapsing frictional contacts among grains involved in force chains and it is computed by assuming an elasto-plastic constitutive relationship including the critical state concept. The collisional contribution, associated with inelastic collisions among grains, is calculated according to kinetic theories of granular gases (Garzo&Dufty, 1999) accounting for frictional and deformable particles that can undergo multiple interactions (Berzi& Jenkins, 2015).When strain rates are small, the quasi-static contribution prevails and the material behaves like a solid (quasi-static regime). On the other hand, when the medium is dilute and deformations are rapid, the material response can be assimilated to that of a fluid.
The energy of the system can be stored by the medium as either elastic or kinetic, increasing this latter with the material agitation, and can be dissipated by means of either force chains or grain inelastic collisions. When saturated granular mixtures are considered, a third dissipation mechanism is introduced, in order to reproduce the interaction between grains and liquid phase.
The transition from solid- to fluid-like conditions is assumed to be governed by the granular temperature and the void ratio, the unique state variables of the model.
The originality of the approach proposed derives from the interpretation of the critical state as a peculiar steady state occurring when the granular temperature tends to zero (Vescovi et al., 2013, Redaelliand di Prisco, 2018).

STATE OF THE ART

The constitutive model for dry granular materials has been formulated under steady simple shear conditions by Vescovi et al.,(2013). According to their formulation, the collisional contribution was calculated by employing the kinetic theory of granular gases (Garzò&Dufty, 1999), whereas, the quasi-static contribution, according to the critical state theory. Redaelli et al.,(2016) extended the formulation to unsteady simple shear conditions. In this case, the quasi-static contribution is calculated by assuming a perfect elasto-plastic constitutive model, based on the critical state concept. A further improvement of the unsteady model, in which strain-hardening plasticity is introduced in the expression of the quasi-static stress, has been proposed by Redaelli (2015).
The limit of the constitutive relationship described by Vescovi et al., (2013) and Redaelli et al., (2016) is that the collisional stresses become singular when the void ratio approaches a critical void ratio. In order to avoid this singularity, Berzi and Jenkins (2015) have suggested to incorporate in the collisional contribution a measure of the duration of particle interaction. Redaelli (2015) and Redaelli and di Prisco, (2018) extended the theoretical framework to three dimensional conditions. Finally, the model has been formulated for saturated granular flows under steady simple shear conditions by Marveggio,(2018).

DRY GRANULAR FLOWS

In this section, the basic concepts of the model conceived for dry granular flows are presented. For further details, the reader is remanded to the suggested references. Moreover, theoretical models predictions are compared with DEM numerical results in order to highlight the features and the potentialities of the constitutive approach.

A REV composed of identical spheres of diameter *d* and density ρ_p is considered. The stress tensor$\boldsymbol{\sigma}$ is evaluated as the sum of a quasi-static contribution $\boldsymbol{\sigma}_q$, assumed to be associated with long elapsing frictional contacts among grains involved in force chains, and a collisional contribution $\boldsymbol{\sigma}_c$, associated with inelastic collisions:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_q + \boldsymbol{\sigma}_c \tag{1}$$

where subscripts *q* and *c* denote the quasi-static and the collisional contribution, respectively.

Evolving conditions

In case of a REV, for which diffusive terms are nil, the energy produced by the work of the internal stresses $\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}$ is equal to the sum of the stored kinetic fluctuating energy $\dot{E}_{k,f}$, the variation of the elastically stored energy $\dot{E}_{el}$ and the dissipated energy Γ:

$$\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}} = \dot{E}_{k,f} + \dot{E}_{el} + \Gamma . \tag{2}$$

The strain rate tensor is assumed to be calculated as the sum of an elastic reversible and a plastic irreversible component, $\dot{\boldsymbol{\varepsilon}}^e$ and $\dot{\boldsymbol{\varepsilon}}^e$, respectively:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^p . \tag{3}$$

$\dot{E}_{k,f}$ is associated with the agitation of the material and, according to the kinetic theories of granular gases (Garzò and Dufty, 1999), it is given by

$$\dot{E}_{k,f} = \frac{3}{2}\rho_p \frac{1}{1+e}\dot{T} , \tag{4}$$

whereas $\dot{E}_{el}$ is equal to

$$\dot{E}_{el} = \boldsymbol{\sigma}_q : \dot{\boldsymbol{\varepsilon}}^e . \tag{5}$$

According to the parallel scheme, also the dissipated energy can be decomposed into a collisional and a quasi-static contribution:

$$\Gamma = \Gamma_q + \Gamma_c \tag{6}$$

where Γ_q represents the energy dissipated by force chains

$$\Gamma_q = \boldsymbol{\sigma}_q : \dot{\boldsymbol{\varepsilon}}^p \tag{7}$$

and Γ_c the energy dissipated by inelastic collisions.Substituting Equations 3-7 into Equation 2, the following balance of the kinetic fluctuating energy is obtained:

$$\boldsymbol{\sigma}_c : \dot{\boldsymbol{\varepsilon}} = \frac{3}{2} \rho_p \frac{1}{1+e} \dot{T} + \Gamma_c . \tag{8}$$

Under evolving conditions, the constitutive model for the quasi-static contribution is based on perfect-elasto-plasticity incorporating the critical state concept (Jefferies, 1993, Dafalias and Manzari, 2004, Redaelli et al., 2016, Redaelli, 2015)
The collisional stress tensoris modelled according to the kinetic theories of granular gases, conceived for frictional and deformable particles (Jenkins and Berzi, 2015). The collisional dissipated energy Γ_c is calculated by taking into account the role of correlated motion between particles (Jenkins, 2007),and according to the expression proposed by Redaelli (2016) and Redaelli and di Prisco (2018), it is a function of void ratio *e*, granular temperature *T*, deviatoric strain rate tensor $\dot{\mathbf{e}}$ and stress Lode angle ϑ_σ :

$$\Gamma_c = \Gamma_c(e, T, \dot{\mathbf{e}}, \vartheta_\sigma) . \tag{9}$$

By summing the quasi-static and the collisional contribution, avisco-elasto-plastic constitutive relationship is obtained, which takes the following form (Redaelli et al., 2017a):

$$\boldsymbol{\sigma} = \mathbf{D}^{evp} : \boldsymbol{\varepsilon} + \mathbf{c} , \tag{10}$$

where $\mathbf{D}^{evp}(\boldsymbol{\sigma}_q, e, T)$ is the visco-elasto-plastic fourth order tensor, and $\mathbf{D}^{evp}(\boldsymbol{\sigma}_q, e, T)$ is a second order tensor. They are both functions of void ratio, granular temperature and quasi-static stress tensor. The derivation of $\mathbf{D}^{evp}(\boldsymbol{\sigma}_q, e, T)$ and $\mathbf{c}(\boldsymbol{\sigma}_q, e, T)$ is detailed in Redaelli et al. (2015) and Redaelli (2016).

In order to evaluate the stress tensor, it is necessary to give the evolution laws for the state variables. In particular, the evolution of the void ratio is governed by the mass balance for the REV as

$$\frac{e}{1+e} = -\dot{I}_{1\varepsilon} , \tag{11}$$

being $\dot{I}_{1\varepsilon} = Tr(\dot{\boldsymbol{\varepsilon}})$ is the volumetric strain rate (compression is positive), whereas the evolution of *T* is obtained by the balance of fluctuating energy for the REV (Equation 8).

Under simple shear conditions, Redaelli(2015) extended the model by employing an elasto-strain hardening plasticity for evaluating the quasi-static contribution.

Steady state conditions

Under steady state conditions, the energy produced by the work of internal stresses is purely deviatoric and it is equal to the dissipated energy Γ.
Equation 2 simply reduces to

$$\mathbf{s}_c : \dot{\mathbf{e}} = \Gamma_c , \tag{12}$$

being $\mathbf{s}_c$ the collisional deviatoric stress tensor.

At steady state, the quasi-static contribution coincides with critical state locus equation. Its expression has been determined by means of 3D-DEM numerical quasi-static simulations (Sun and Sundaresan, 2011, Xiao et al., 2015, Zhao and Guo, 2013).
The formulation of the steady state locus is used in the definition of evolving constitutive relationships as an attractor locus (Redaelli et al., 2016).According to this model, the well known critical state locus can be interpreted as a peculiar steady state occurring when the granular temperature (or analogously for the deviatoric strain rate) approaches a zero value (Vescovi et al 2013, Redaelli et al 2016).

Constitutive parameters

To define the constitutive relationship, 10 parameters have been introduced: 5 are micro-mechanical and refer to the single particle and 5 are macro-mechanical. The micro-mechanical parameters are particle density ρ_p and diameter d, particle young modulus E_p, interparticle friction coefficient μ_p and normal coefficient of restitution e_n (Redaelli and di Prisco, 2018). Among the 5 macro-mechanical parameters 2 are employed to define the Gibbs elastic energy, 1 to define the yield locus, 1 for the plastic potential and 1 for the collisional contribution (Redaelli et al., 2017b).

Comparison with DEM results

In this section, model predictions (lines) are compared with DEM true triaxial tests results (markers).
The DEM simulations have been performed by Redaelli and di Prisco (2018) on periodic cells by imposing the deviatoric strain rate $\dot{J}_e = \sqrt{\dot{\mathbf{e}} : \dot{\mathbf{e}}}$, the confining pressure $I_{1\sigma} = Tr(\boldsymbol{\sigma})$ and the stress Lode angle θ_σ. Details of the DEM model are in Redaelli and di Prisco (2018).
The micro-mechanical parameters employed in the DEM simulations are listed in Table 1.
In Figure 1, the sensitivity of the material response on the inertial number I at steady state is illustrated. The inertial number (Jop et al., 2006) is in fact a very convenient measure of the system dynamicity and it is defined as

$$I = d\dot{J}_e \sqrt{\frac{\rho_p}{I_{1\sigma}}} . \tag{13}$$

In particular, in Figure 1a, the stress ratio μ is plotted as a function of the inertial number for triaxial compression (θ_σ=0°) and extension (θ_σ=60°). Whereas, in Figure 1b, the results are reported in the void-ratio-inertial number plane. The empty symbols refer to DEM data characterized by and imposed deviatoric strain rate $\dot{J}_e = 12$ 1/s and different values of the imposed pressure confining pressure $I_{1\sigma}$,whereas, the filled markers refer to the DEM data characterized by $I_{1\sigma} = 150$ kPa and different values of $\dot{J}_e$.
The qualitative and quantitative agreement between DEM numerical results and model predictions is satisfactory both under triaxial compression and extension. The model is capable of capturing the dependence of the numerical response on inertial number, imposed deviatoric strain rate, imposed pressure and loading path. The dependency of the stress ratio on I of the DEM data is in agreement with what predicted by the μ-I rheology (Jop et al., 2006, Midi G.D.R, 2004) and it is well captured by the model. The model is also capable of capturing the bifurcation observed in the void ratio-inertial number plane, for decreasing I values. It is in fact possible to observe that

different values of the void ratio are associated with the same value of inertial number. This response cannot be obtained by employing the well known *e-I* rheology (Jop et al., 2006, Midi G.D.R, 2004).

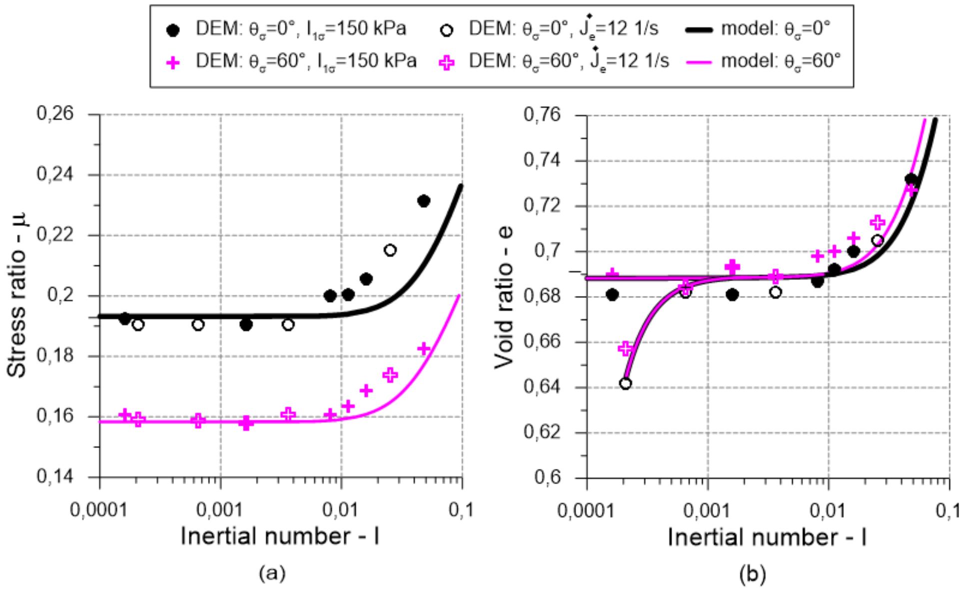

Figure 1 Comparison between DEM simulation results and theoretical model under dry steady triaxial conditions: (a) stress ratio versus inertial number, (b) void ratio versus inertial number

SATURATED GRANULAR FLOWS

In this section, the previously described model, conceived for dry conditions, is extended to take into account the presence of water within the granular material.
Under saturated conditions, the stress tensor $\boldsymbol{\sigma}$isevaluated as the sum of a solid component$\boldsymbol{\sigma_S}$, associated with the solid phase and coinciding with the stress tensor under dry conditions (Equation 1), and a liquid contribution $\boldsymbol{\sigma_L}$, associated with the fluid phase:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_S + \boldsymbol{\sigma}_L \tag{14}$$

where subscripts *S* and *L* denote the solid and the liquid contribution, respectively.
As the liquid phase is assumed to be Newtonian and incompressible, the liquid stress tensor can be written as:

$$\boldsymbol{\sigma}_L = pI + 2\eta\dot{\mathbf{e}} \tag{15}$$

being *p* the hydrostatic pressure of the liquid phase and η its viscosity.

In case of a solid-fluid mixture, where solid particles are suspended into the fluid phase, the viscosity is assumed to be a function of the void ratio:

$$\eta = \eta(e)\,. \tag{16}$$

According to the formulation proposed by Marveggio (2018), the liquid viscosity expression retrieves, at low values of concentration, the one ofKrieger and Dougherty (1959) and Einstein (1905), whereas, when dense mixtures are considered, the viscosity tends to the one proposed by Carman (1937).

Steady state conditions

Under saturated steady conditions, the following balance of fluctuating energy is assumed:

$$\mathbf{s_c} : \dot{\mathbf{e}} = \Gamma_c + \Gamma_{SL} \,. \tag{17}$$

Equation 17 may be easily interpreted as the extension to saturated conditions of the relation expressed by Equation12, valid under dry conditions. In particular, in Equation17, the term Γ_{SL}, representing a coupling contribution between the solid and liquid phase, stands for the energy dissipated at the interface between the two phases.
Γ_{SL}, assumed to be related to the Stoke's force acting on a sphere moving in a Newtonian fluid, is a function of the void ratio and of the granular temperature (Marveggio, 2018):

$$\Gamma_{SL} = \Gamma_{SL}(e,T) \tag{18}$$

With respect to the dry case, in the steady-saturated extension of the constitutive model, one macro mechanical parameter has been introduced, which is the ambient viscosity of the liquid phase η.

Comparison with DEM results

The previously described model has been validated under steady simple shear conditions. In particular, in Figure 2, model predictions (lines) are compared with the DEM numerical simulations (markers) of Ness and Sun (2015), where the presence of the liquid phase has been accounted by adding some long range lubrication forces in the contact laws between particles. The DEM simulations have been performed imposing the same deviatoric strain rate $\dot{J}_e = \sqrt{\dot{\mathbf{e}} : \dot{\mathbf{e}}}$ =9.29e-41/s an ddifferent values of the void ratio *e*. The details of the DEM numerical simulations can be found inNess and Sun (2015).

In Figure 2a, the stress ratio is plotted against the inertial number both for DEM results and model prediction, whereas in Figure 2b, the results are reported in the voidratio-inertial number plane.

The qualitative and quantitative agreement between DEM numerical results and model predictions is satisfactory both for both low and high values of inertial number.

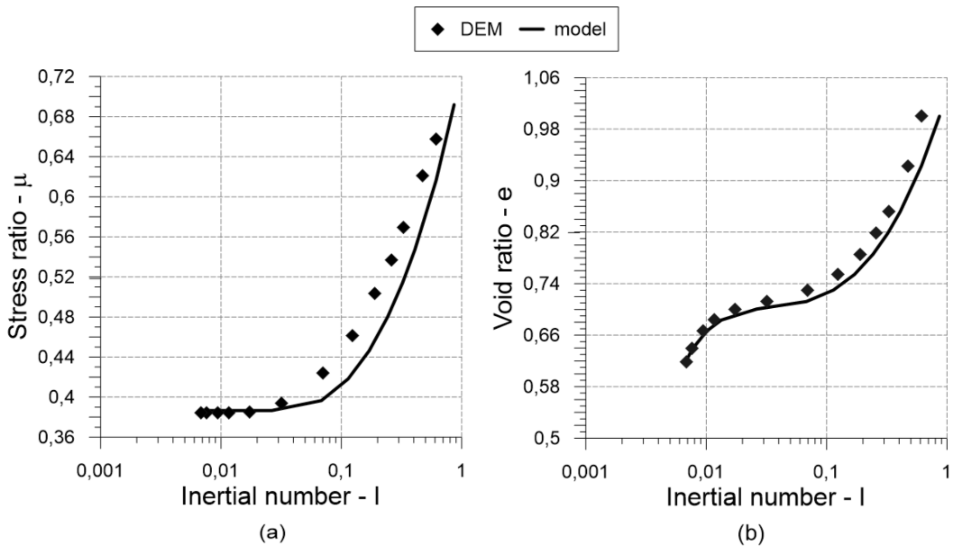

Figure 2 Comparison between DEM simulation results and theoretical model for saturated suspensions at steady state: (a) stress ratio versus inertial number, (b) void ratio versus inertial number

CONCLUSIONS

In this paper, a new constitutive approach capable of capturing the transition from solid-to-fluid like conditions, in dry or saturated granular materials, has been presented.
The stress tensor is computed by adding in parallel a liquid contribution and a granular contribution. The liquid

contribution, calculated by considering the liquid phase as an incompressible Newtonian fluid with viscosity depending on the void ratio, is nil in dry granular flows. The granular contribution is in turn calculated as the sum of a quasi-static and a collisional stress. The former one is evaluated according to elasto-plastic theories incorporating the critical state concept and dominates under quasi static conditions (i.e. for sufficiently small inertial number values). The latter one is calculated by employing the kinetic theory of granular gases and dominates in the collisional regime.

In dry granular flows, the energy can be dissipated by means of either force chains or grain inelastic collisions. When saturated granular mixtures are considered, a third dissipation mechanism is introduced, reproducing the energy dissipated at the interface between the solid and the liquid phases.

The void ratio and the granular temperature represent the unique state variables of the model.

Model predictions have been compared with DEM numerical results of the literature. The model is capable of capturing the dependence of the numerical response on inertial number, imposed deviatoric strain rate, imposed pressure, imposed void ratio and loading path both under dry and saturated steady conditions.

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