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A rate-dependent hydrodynamic-plastic model for crushable sand

Modèle hydrodynamique, plastique, et dépendant des taux de déformation appliqués, pour la modélisation des sables susceptibles de se fragmenter

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ABSTRACT: Granular materials can exhibit long-term rate-dependent relaxing response under fixed strain or stress conditions which has been attributed in the literature to be so-called ageing or creep phenomena, respectively. The grain-scale mechanisms that dictate this rate-dependent behaviour arise from the rearrangement of particles with or without crushing. Therefore, developing a formulation that can capture these grain-scale mechanisms in a continuum representation will be advantageous. This paper focuses on the constitutive modelling of granular materials within the concept of the hydrodynamic theory, which accounts for granular temperature as a specific state variable reflecting grain-scale dissipative mechanisms. Unlike previous hydrodynamic formulations, our formulation couples the hydrodynamic principles with mathematical ideas from the plasticity theory. Another novel feature of the current formulation is considering breakage as a state variable. We show that this formulation is capable of recovering: (1) rate-dependent friction coefficient and density; (2) rate-dependent breakage behaviour; (3) incrementally non-linear response; (4) granular material response during transient loading; and finally, (5) long-term ageing and creep phenomena.

RÉSUMÉ: Les matériaux granulaires peuvent présenter des dépendances, à déformation ou contrainte constante, qui, dans la littérature, ont été attribuées respectivement au vieillissement ou au fluage du matériau. À l'échelle des grains, les mécanismes à l'origine de ces dépendances dans les vitesses de déformation émergent des réarrangements des particules, avec ou sans fragmentation. En conséquence, il est nécessaire de développer une formulation capable de capturer ces mécanismes à l'échelle des grains dans une représentation continue. Cet article développe une loi de comportement pour les matériaux granulaire en se basant sur la théorie hydrodynamique, qui utilise la température granulaire comme une variable d'état rendant compte des mécanismes de dissipation à l'échelle des grains. Contrairement aux formulations précédentes, notre modèle couple les principes de l'hydrodynamique avec les concepts de théorie de la plasticité. De plus, un nouvel élément de notre formulation est de considérer le degré de fragmentation du matériau comme une variable d'état additionnelle, essentielle pour rendre compte du comportement du matériau granulaire. Nous montrons que cette formation permet d'expliquer: (1) les dépendances de la densité et du coefficient de friction avec les taux de déformation; (2) la dépendance du taux de fragmentation avec les taux de déformation; (3) les non-linéarités dans la réponse à un incrément de contrainte ou de deformation; (4) la réponse des matériaux granulaires en régime de chargement transitoire; et enfin, (5) les phénomènes de fluage et de vieillissement à long terme.

KEYWORDS: Sand, hydrodynamics, plasticity theory, breakage mechanics, creep.

1 INTRODUCTION

Granular materials exhibit rate-dependent macroscopic response, as shown in discrete element rheological studies by Da Cruz et al. (2005) and Jop et al. (2006), and experimental rate-transient shearing tests on sand by Nawir et al. (2003). These rate-dependent macroscopic phenomena originate from grain-scale interactions that cause dissipative mechanisms. Therefore, a constitutive model that is capable of capturing the rate-dependent macroscopic observations should consider a proper set of state variables to account for the grain-scale dissipative mechanisms. Granular temperature has been introduced in the literature as a variable that quantifies the extent of kinetic energy fluctuations of grains due to granular interactions. Following original ideas in Jiang & Liu (2009, 2015), Alaei et al. (2021) introduced their hydrodynamic based formulation for granular materials considering an energy form that depended on granular temperature. In order to introduce the explicit forms of the evolution equations for the state variables, Alaei et al. (2021) considered ideas from conventional plasticity, in particular bounding surface plasticity by Dafalias (1986). Therefore, their hydrodynamic-plastic formulation benefitted from the hydrodynamics theory to satisfy thermodynamic principles as well as conservation laws, and robust mathematical tools of plasticity theory to capture macroscopic observations.

Grain crushing is another essential process in sand material that can affect its macroscopic response (Hardin 1985; Lade et al. 1996; McDowell & Bolton 2000; Zhang 2012). To consider the consequences of grain crushing on the macroscopic response of granular media, one needs a corresponding thermodynamic state variable that can be exploited in a model in addition to the ones specified in Alaei et al. (2021). The concept of breakage B as a thermodynamic state variable that quantifies the variations of grain size distribution was introduced in the breakage mechanics theory by Einav (2007). Einav considered the experimental measurability of B based on the relative position from initial and ultimate grain size distributions. In this paper, we use the concepts introduced in the breakage mechanics theory and add B as a state variable within the hydrodynamic frame in addition to granular temperature. We will show that granular temperature effects can be important in the crushing regimes of granular media as it can guide the model to capture the long-term effects, e.g. creep breakage (Lade 2007).

2 HYDRODYNAMIC DERIVATION

The first law of thermodynamics, which describes the conservation of energy, can be expressed as

$$\partial_t U + \nabla_i E_i = \rho v_i G_i, \qquad (1)$$

where U is the conserved energy density in a moving reference frame, ρG_i is the gravitational force density and E_i is the energy flux. Alaei et al. (2021) considered the general structure of conserved energy for non-crushable dry sand in a single component continua to depend on entropy s, granular entropy s_g, density ρ, momentum g_i and elastic strain ε^e_{ij} as the state variables. Based on the theory of breakage mechanics by Einav (2007), here we consider an additional thermodynamic state variable B into the conserved energy density. In this case, the conserved energy U takes the following general form:

$$U = U(\rho, g_i, \varepsilon^e_{ij}, s, s_g, B). \tag{2}$$

The conjugates for the first five variables above can be written as

$$\mu_\rho \equiv \frac{\partial U}{\partial \rho}, \quad v_i \equiv \frac{\partial U}{\partial g_i}, \quad \sigma^e_{ij} \equiv \frac{\partial U}{\partial \varepsilon^e_{ij}}, \quad T \equiv \frac{\partial U}{\partial s}, \quad T_g \equiv \frac{\partial U}{\partial s_g}, \tag{3}$$

which are the chemical potential, velocity, elastic stress, thermal temperature and granular temperature, respectively. In addition, we consider the breakage energy (Einav 2007) that is conjugated to the state variable B:

$$E_B \equiv -\frac{\partial U}{\partial B}. \tag{4}$$

Following the hydrodynamics procedure, we define a stress measure:

$$\sigma_{ij} = \sigma^e_{ij} + \sigma^D_{ij} + p_T \delta_{ij}, \tag{5}$$

where σ_{ij} is the total stress that goes into the momentum equation, σ^D_{ij} is the viscous stress and p_T is the thermodynamic pressure defined as

$$p_T = -\frac{\partial(U/\rho)}{\partial(1/\rho)}\Big|_{\frac{s}{\rho}, \frac{s_g}{\rho}, v_i, \varepsilon^e_{ij}}. \tag{6}$$

The relation in equation (5) is consistent with the standard sign convention in soil mechanics of positive stresses under compression. The second law of thermodynamics (the balance of thermal entropy) can always be written as

$$\partial_t s + \nabla_i(s v_i - f_i) = \frac{R}{T} \geq 0, \tag{7}$$

where $s v_i$ and f_i are the convective and dissipative thermal entropy currents, respectively; and R is the thermal rate of dissipation (production rate of thermal entropy). Similarly, the evolution law for the granular entropy can be introduced as

$$\partial_t s_g + \nabla_i(s_g v_i - f^g_i) = \frac{R_g}{T_g}, \tag{8}$$

where $s_g v_i$ and f^g_i are the convective and dissipative granular entropy currents, respectively; and R_g is the granular rate of dissipation (production rate of granular entropy). Applying the hydrodynamic procedure (Alaei et al. 2021), one finds the following equation for the total rate of dissipation

$$R + R_g = f_i \nabla_i T + f^g_i \nabla_i T_g + \Phi_M \geq 0, \tag{9}$$

where the mechanical dissipation is expressed by

$$\Phi_M \equiv \sigma^D_{ij} \dot{\varepsilon}_{ij} + \sigma^e_{ij} \dot{\varepsilon}^p_{ij} + E_B \dot{B}. \tag{10}$$

In the above expression, the first two viscous and plastic contributions were defined in Alaei et al. (2021), and the third contribution from breakage dissipation was established by Einav (2007).

3 TWO-STAGE IRREVERSIBILITY

Based on the original ideas from the development of the granular solid hydrodynamics theory by Jiang and Liu (2009, 2015), we employ the principle of two-stage irreversibility in granular media to account for energy decay through two separate granular and atomic scales. Adopting this concept, we consider that during a dissipative process in granular media the macroscopic energy can flow into thermal heat through two different ways; either directly or as a two-step process, whereby the energy first decays into the fluctuations of grains (granular heating), and only then into the fluctuations of atoms within the grains (thermal heating). In particular, the energy decays from the macroscopic scale to perturbing the grain scale degrees of freedom and the atomic ones (quantified by the granular and thermal rates of dissipation R_g and R, respectively), and from the grain scale into the atomic one, but never backwards ($R \geq 0$). Conventionally, the second law of thermodynamics also implies that the thermal rate of dissipation must be non-negative. The concept of two-stage irreversible energy decay implies that the total rate of dissipation must also be non-negative $R + R_g \geq 0$, as shown in figure 1.

Considering the principle of two-stage irreversibility and recalling the total rate of dissipation in equation (9), we propose the following relations for the thermal and granular rates of dissipation, respectively

$$R = f_i \nabla_i T + \eta T_g^2 \geq 0, \tag{11}$$

$$R_g = f^g_i \nabla_i T_g + \Phi_M - \eta T_g^2. \tag{12}$$

This choice of the above equations, along with the thermodynamic requirements on non-negativity of $f_i \nabla_i T$, $f^g_i \nabla_i T_g$ and η satisfies the non-negativity of the total dissipation rate, as well as the non-negativity of the thermal entropy production in equation (7).

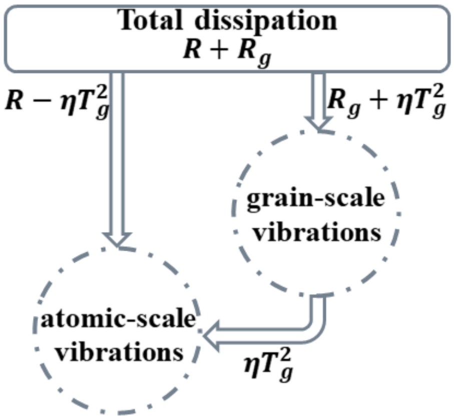

Figure 1. Principle of two-stage irreversibility (Jiang & Liu 2009, 2015). In granular media, macroscopic energy either dissipates directly to generate atomic vibrations (in the form of T), or in a two-stage process, first to generate granular vibrations (in the form of T_g) and only then decaying to form atomic vibrations (in the form of T).

4 CONSTITUTIVE CONSIDERATIONS

4.1 *Kinetic pressure*

Adopting the ideas in Alaei et al. (2021) on an explicit form of granular energy density, the hydrodynamic derivation leads to a pure kinetic expression for thermodynamic pressure in the case of dry granular materials:

$$p_T = T_g^2 \equiv p^k. \tag{13}$$

Similar to the procedure adopted in Alaei et al. (2021), we take the kinetic pressure p^k as an alternative state variable for T_g and devise its rate equation in the absence of non-local phenomena:

$$\dot{p^k} = \Phi_M - \eta p^k. \tag{14}$$

Now recalling equation (5), the total mean and deviatoric stresses can be correspondingly written

$$p = p^e + p^k, \tag{15}$$
$$q = q^e + q^D, \tag{16}$$

where p^e and q^e are elastic pressure and deviatoric stress while q^D is the deviatoric viscous stress.

4.2 *Inertial number and kinetic number*

Rheological $\mu(I)$ and $\phi(I)$ relationships (Jop et al. 2006 and Da Cruz et al. 2005, respectively) capture correspondingly the rate-dependent friction coefficient and solid fraction of granular media at critical state as functions of inertial number I. Inspired by this idea, we devise the explicit form of $\dot{p^k}$ equation, specifically the state function η. It could be shown that under monotonic shearing conditions ($\dot{\varepsilon_s} = \text{const} \neq 0$), critical state can be reached and maintained when the kinetic pressure rate vanishes $\left(\dot{p^k} = 0\right)$ and the mechanical dissipation reduces to $\Phi_M = \sqrt{2/3}|q|\dot{\varepsilon_s}$. We therefore find an expression for the state function η, such that a new kinetic number

$$I^k = \frac{p^k}{p}, \tag{17}$$

will be identical to inertial number $I = d\dot{\varepsilon_s}\sqrt{\rho_s/p}$ at critical state conditions:

$$\eta = \frac{M}{d}\sqrt{\frac{2p}{3\rho_s}}, \tag{18}$$

where M, d and ρ_s are the friction coefficient, grain size and solid density of grains.

4.3 *Rate- and breakage- dependent limits of solid fraction*

Adopting the idea of minimum and maximum limits of solid fraction discussed in Alaei et al. (2021), we consider the attainable solid fraction values to be confined by its rate-dependent limits:

$$\phi^k_{min}(I^k) = \phi_{min}(1 - I^k), \tag{19}$$
$$\phi^k_{max}(I^k) = \phi_{max} - (\phi_{max} - \phi_{min})I^k, \tag{20}$$

where ϕ_{min} and ϕ_{max} are the minimum and maximum solid fractions at rest. Breakage affects both the minimum and maximum limits of the solid fraction (Rubin & Einav 2011; Tengattini et al. 2016). Rubin & Einav (2011) introduced expressions for experimentally measurable minimum and maximum limits of porosity n. Considering their expressions and recalling the direct relationship between solid fraction and porosity $\phi = 1 - n$, we define the following experimentally measurable limits of solid fraction which depend on breakage

$$\phi_{min} = \phi_{min}(B) \equiv 1 - (1 - \phi_l)(1 - B)^l, \tag{21}$$
$$\phi_{max} = \phi_{max}(B) \equiv 1 - (1 - \phi_u)(1 - B)^u, \tag{22}$$

where ϕ_l and ϕ_u are the lower and upper limits of solid fraction at zero breakage, while the coefficients l and u are model constants.

4.4 *Rate-dependent friction coefficient*

Based on the empirical rheological relationship by Jop et al. (2006) capturing a rate-dependent ratio of total deviatoric and mean stresses at critical state conditions, and definition of kinetic number at section 4.2 we define

$$M(I^k) = \frac{q}{p} \equiv M_0 + bI^k, \tag{23}$$

where M_0 is the static friction coefficient and b is a model constant, previously defined by Jop et al. (2006).

4.5 *An extension to effective stress principle*

The total pressure in the current work, for the case of dry granular materials, is composed of the elastic and kinetic pressures. Since the elastic pressure is actually sustained by the skeleton of grains, we take a physical assumption that it is equivalent to effective pressure (Einav & Liu 2018). The effective stress principle (Terzaghi 1936) denotes that the shear resistance of a soil is related to the effective pressure applied to its skeleton. Therefore, shear resistance in the current work should be a function of p^e.

Total shear stress (equivalently the deviatoric stress) in the current work is composed of the elastic and viscous contributions. The original effective stress principle does not distinguish between the total and effective shear stresses, since rheological stress contributions are normally neglected in the case of geotechnical quasi-static regimes. However, rheological stresses can be important under elevated loading rates as well as transient loading conditions (Nawir et al. 2003). Here, following Alaei et al. (2021) we introduce an extended effective stress principle that relates the elastic (effective) stress ratio to the state of the material:

$$\frac{q^e}{p^e} \equiv M^e(\text{state}). \tag{24}$$

Our preliminary studies on the effective stress ratio in discrete element simulations reveal that the state function M^e follows a $M(I^k)$ type of relationship. Note that the above elastic shear resistance concept is in addition to the idea of rate dependent total shear resistance in equation (23). The concept of an extended effective stress principle was validated in Alaei et al. (2021) against discrete element simulation results by Macaulay & Rognon (2020).

Combining equations (23) and (24) will lead to an expression for the viscous stress as a function of the state of the material and the shearing rate it is subjected to, without introducing any new model constants (see Alaei et al. 2021).

5 RATES OF BREAKAGE AND PLASTIC STRAIN

In this section, we present a formalism to introduce incrementally non-linear (unlike elasto-plasticity) equations for the breakage and the plastic strain rates, using the bounding surface plasticity type of formulation in Alaei et al. (2021). We devise the expressions for the rate of B and $\dot{\varepsilon^p_{ij}}$:

$$\dot{B} = \lambda_B A_B, \quad \lambda_B \equiv \sqrt{\xi}\langle\lambda_A\rangle, \tag{25}$$
$$\dot{\varepsilon^p_{ij}} = \lambda_p A_{ij}, \quad \lambda_p \equiv \sqrt{\xi}|\lambda_A|, \tag{26}$$

where the choice of λ_B and λ_p are resolved to guarantee that the state of the material is maintained inside a bounding surface, while the plasticity multiplier λ_A is calculated to maintain the state on the auxiliary loading surface (see Alaei et al. 2021). In the above equations, $0 \le \xi \le 1$ is a current-to-bounding mapping ratio that determines how far the loading surface is from the bounding one (0 value indicates the farthest distance from bounding surface, while 1 value indicates that loading and bounding surfaces are identical). The Macaulay brackets function is considered with $\langle x \rangle = x$ if $x \ge 0$, and $\langle x \rangle = 0$ otherwise. This will satisfy the experimental observation that upon an isotropic unloading $\dot{\varepsilon_v} < 0$ and $\dot{\varepsilon_s} = 0$, negligible breakage growth is expected.

The choices in equations (25) and (26) to correspondingly take $\langle \lambda_A \rangle$ and $|\lambda_A|$ is unlike the conventional bounding surface plasticity (Dafalias 1986) and employs an original idea in Einav (2012) to have freedom on the mathematical form of plasticity rules as long as the non-negativity of mechanical dissipation is satisfied. Advantages of adopting Einav's idea in a constitutive model were presented in Alaei et al. (2021), to capture material response upon shear unloading of samples with non-zero initial stress ratios and to satisfy a sub-symmetry of granular dissipation rate (R_g) upon time-reversal.

Note that although λ_A is set to maintain the state on a loading surface, in reality we take $\sqrt{\xi}\langle \lambda_A \rangle$ and $\sqrt{\xi}|\lambda_A|$ to determine the rates of B and ε_{ij}^p, respectively. Therefore, as long as $\xi \neq 1$ the state would not remain on a loading surface. However, as $\xi \to 1$ towards the bounding surface, we get $\lambda_p \to |\lambda_A|$ and $\lambda_B \to \langle \lambda_A \rangle$, thus the state is slowly being attracted to the bounding surface.

The simplified form of bounding surface (Mohr-Coulomb type) in Alaei et al. (2021) which does not yield on the isotropic compression line ($q = 0$) will result in pure elastic response under a pure isotropic compression ($\dot{\varepsilon_v} > 0$ and $\dot{\varepsilon_s} = 0$). In the current model however, a more realistic bounding surface yielding along the isotropic compression line is required (Figure 2). This yielding pressure, p_B, that represents the pressure at which the material starts to experience considerable breakage under pure isotropic loading conditions ($\dot{\varepsilon_v} > 0$ and $\dot{\varepsilon_s} = 0$) is defined by relating E_B and a critical breakage energy (Einav 2007).

Furthermore, the explicit form of the state functions A_B and A_{ij} should be defined to guarantee the non-negativity of the mechanical dissipation. To this goal, one can adopt the robust procedure in Tengattini et al. (2016) where they first proposed an explicit form of the mechanical dissipation and then derived the yield function and explicit form of flow rules from it, in their elasto-plastic type of model. Here, we derive the state functions A_B and A_{ij} from a bounding surface function (Figure 2) that could actually be taken to be identical to the breakage mechanics type of yield function in Tengattini et al. (2016).

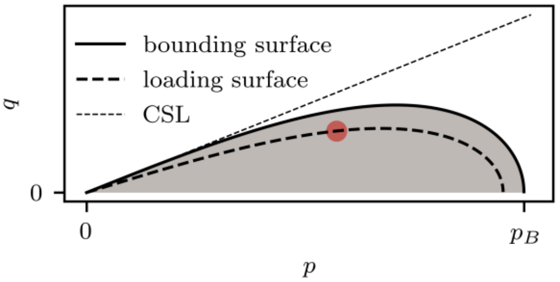

Figure 2. The bounding surface (thick line) and the loading surface (dashed line) passing through the stress state (marker), from which the value of ξ is determined. The thin dashed line represents the critical state line (CSL) and the grey area represents the attainable stress states inside the bounding surface.

Due to p^k −dependence of the friction coefficient, limits of solid fraction and total pressure, the plasticity multiplier λ_A will have free terms including p^k but without $\dot{\varepsilon}_{ij}$. As a result, under fixed strain or stress conditions following material loading, λ_A and consequently the breakage and plastic strain rates can be non-zero. This will help in capturing the long-term rate-dependent relaxing response related to ageing or creep phenomena (Lade 2007).

6 MODEL EVALUATION

Considering the Karlsruhe sand material calibrated in Alaei et al. (2021), we conduct a two-stage test (Figure 3a) starting from an initial confining pressure $p_0 = 100$ kPa. During the first shearing stage we maintain a constant pressure $\dot{p} = 0$ and shear the model to produce $I = 0.5$ at critical state (CS), while in the second stage we maintain the total strain constant $\dot{\varepsilon}_{ij} = 0$. Figure 3a shows the evolution of the total deviatoric and mean stresses normalised by p_0 over time. During the shear stage of the test the kinetic pressure rises towards its CS value, causing the total stress ratio to reach its rate-dependent value which is greater than the static friction coefficient M_0 (see equation 23). During the second stage, q experiences an abrupt change due to the linear dependence of q^D on strain rate, a fact that has been observed experimentally (e.g., for sand by Lade 2007). Also during this stage, p^k gradually relaxes to zero causing a relaxation of the elastic strain since $\dot{\varepsilon}_{ij}^e = -\dot{\varepsilon}_{ij}^p$ where $\dot{\varepsilon}_{ij}^p \neq 0$. As discussed in the previous section, the multipliers λ_p and λ_B and consequently $\dot{\varepsilon}_{ij}^p$ and $\dot{B}$ may not vanish when $\dot{\varepsilon}_{ij} = 0$, since they are functions of p^k. The overall total stress relaxation response in the second stage is known as an 'ageing' response in soil mechanics.

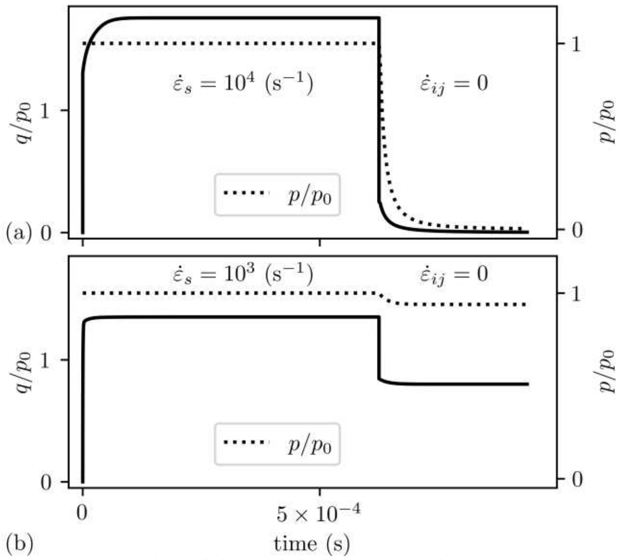

Figure 3. Relaxation of the total deviatoric q and mean p stresses in the current model implementations. Two simulated tests with the same initial total pressure $p_0 = 100$ kPa are initially subjected to the different shear rates to produce different inertial numbers $I = 0.5$ in (a) and $I = 0.005$ in (b), followed by a constant total strain stage. The stresses are normalised by the confining pressure p_0 during the initial shear stage.

We further examine this stress relaxation response by conducting another test with the same initial conditions, but with slower shearing during the shear stage, set to produce a smaller inertial number $I = 0.05$ at CS. As indicated by figure 3b, here again the model represents its rate-dependent features as the total stress ratio at CS reaches a value smaller than the one in figure

3a. At the second stage of this test, the stress relaxation effect is less pronounced where the deviatoric and mean stresses relax only slightly towards non-zero values, in contrast to the previous test (with higher I at CS). Similar rate-dependent stress relaxation response in granular materials has been observed in previous experimental studies (Lade 2007).

Breakage evolution in the above tests is not reported here as it showed negligible growth, due to relatively high crushing strength of the modelled Karlsruhe sand material compared to the applied stress magnitudes. Further evaluation of the model for relatively weaker materials, for example Carbonate sand, is required to reveal its capabilities in capturing the particle breakage effects (Hardin 1985; McDowell & Bolton 2000; Zhang 2012).

7 CONCLUSIONS

We have introduced a simple hydrodynamic-plastic framework for constructing a rate-dependent constitutive model for crushable granular media. An energy form depending on the most essential set of state variables for sand was considered to construct the general implicit form of the evolution equations for state variables. Then conventional plasticity was exploited to introduce their explicit forms. The model is set to recover well known rheological $\mu(I)$ and $\phi(I)$ type of relationships. Furthermore, the rates of breakage and plastic strain were defined in terms of the kinetic pressure (equivalently granular temperature) which also dictates rate dependent dissipative mechanisms. Our simulations reveal that inclusion of kinetic pressure in the stress measure, and expressions for friction coefficient and solid fraction limits will result in free p^k −dependent terms in the plasticity multiplier expression that helps in capturing the relaxation effects observed in the creep and ageing type of experiments.

8 ACKNOWLEDGEMENTS

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