Analysis of a frictional–kinetic model for gas–particle flow

Anuj Srivastava, Sankaran Sundaresan*

Department of Chemical Engineering, The Engineering Quadrangle, Princeton University, Princeton, NJ 08544-5263, USA

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Abstract

A frictional–kinetic rheological model for dense assemblies of solids in a gas–particle mixture is described. This model treats the kinetic and frictional stresses additively. The former is modeled using the kinetic theory of granular materials. For the latter, we begin with the model described by Schaeffer [J. Differ. Equ. 66 (1987) 19] and modify it to account for strain rate fluctuations and slow relaxation of the assembly to the yield surface. Results of simulations of two model problems, namely, the gravity discharge of particles from a bin and the rise of a bubble in a fluidized bed, are presented. The simulations capture the height-independent rate of discharge of particles from the bin, the dilation of particle assembly near the exit orifice, the significant effect of the interstitial air on the discharge behavior of fine particles and the occurrence of pressure deficit above the orifice. However, the stagnant shoulder at the bottom corners of the bin is not captured; instead, one obtains a region of slow flow at the corners. The bubble rise example shows the significant effect of frictional stresses on the bubble shape. In both examples, a simplified version of the rheological model obtained by invoking a critical state hypothesis is found to be adequate.

Keywords: Bin discharge; Fluidized bed; Simulation; Frictional stress; Critical state

1. Introduction

Flows of dense assemblies of granular materials are encountered in a variety of industrial devices, such as bins, hoppers, rotary blenders, fluidized beds, circulating fluidized beds (CFBs), spouted beds, etc. [1]. In many of these applications, the interstitial fluid (say, gas) is essential for the operation of the device, while in others dealing with fine powders, the interstitial gas interferes sufficiently that, even when there is no forced gas flow, the system must be analyzed as a two-phase flow problem. Thus, there is a significant scientific and technological interest in understanding and modeling gas–particle flows involving dense assemblies of particles. In these systems, the particles interact with each other largely through enduring frictional contact between multiple neighbors and, to a lesser extent, through collisions. In many instances, the gravitational compaction of granular materials under their own weight is sufficient to ensure that frictional interaction is a significant, if not dominant, contributor to the particulate stress. As the particle volume fraction decreases, the collisional stress becomes more dominant. The development of a rheological model of the granular assembly in such flows (to be used with continuum models for such flows), its implementation in numerical codes for solving the continuum flow models, analysis of model flow problems to understand the consequences of the proposed closures and experimental validation are all practically important [2–7].

The volume fraction of solids in dense fluidized beds, hoppers and bin is high enough that particles make enduring contact with multiple neighbors. Particulate stresses in such dense phase flows are generated by frictional interactions between particles at points of sustained contact. Indeed, it is well known that frictional interactions play a very important role in many dense phase gas–solid flows. For example, it has been shown that frictional stresses play a critical role in maintaining stable operation of CFBs [8,9]. Constitutive models for frictional stresses under slow, quasi-static flow conditions are largely based on ideas which were originally developed in soil mechanics [10–13].

In fast-fluidized beds and risers, particle concentration is typically in the range of 1–30% by volume and particle–particle interactions occur largely through binary collisions. Constitutive models for the stresses in this system have been deduced in the literature by adapting the kinetic theory of dense gases [14,15]. This approach is often referred to in the literature as the kinetic theory of granular materials.
In many gas–particle flows of industrial significance, one can find regions in the flow domain where kinetic stresses dominate, other regions where frictional stresses dominate and finally, regions where contributions of both are comparable. Thus, it is of practical interest to synthesize rheological models that combine the frictional and kinetic contributions. However, given the disparate nature of theories of both contributions, it is still unclear as to how they should be combined.

In this article, we describe a frictional–kinetic closure for the particle phase stress, which treats the frictional and kinetic stresses in an additive manner [16,17]. The kinetic stresses are based on the kinetic theory of granular materials, which also takes into account the effect of the interstitial gas [18]. For frictional stress, we begin with a model for quasi-static flow proposed by Schaeffer [12] and modify it to account for strain rate fluctuations [19] and slow relaxation of the assembly to the yield surface. We then use the closure to analyze two model flow problems. The first example considers gravity discharge of particles from a 2-D bin, where we have simulated the dilation of particles in the vicinity of the exit orifice and also examined the effect of interstitial gas on the discharge characteristics. It will be seen that these simulations do capture the height-independent rate of discharge of the particles from the bin, the dilation of the granular assembly in the vicinity of the exit orifice and the pressure deficit above the orifice. These simulations, however, fail to capture the formation of stationary shoulders in the bottom corners of the bin. The second example is a detailed simulation of a rising gas bubble in a fluidized bed of Geldart B particles, where we see a significant effect of the frictional stress on the shape and size of the bubble. A simplified closure, which invokes a critical state hypothesis to evaluate the frictional stresses, is shown to be adequate in both examples.

2. Model equations

We treat the gas and solid phases as interpenetrating continua and model them through the volume-averaged equations of Anderson and Jackson [20].

\[
\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{u}) = 0 \tag{1}
\]

\[
\frac{\partial (1 - \rho_g)}{\partial t} + \nabla \cdot [(1 - \rho_g) \mathbf{u}] = 0 \tag{2}
\]

\[
\rho_g \left[ \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] = -\nabla \cdot \mathbf{\sigma}_g - \rho_g g + \mathbf{f} + \rho_g \gamma \mathbf{g} \tag{3}
\]

\[
\rho_s \left[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right] = -(1 - \rho_g) \nabla \cdot \mathbf{\sigma}_s - \mathbf{f} + (1 - \rho_g) \rho_s \mathbf{g} \tag{4}
\]

Here, \( \rho \) is the volume fraction of particles; \( \mathbf{v} \) and \( \mathbf{u} \) are the local average velocities of the particle and gas phases, respectively; \( \rho_s \) and \( \rho_g \) are the densities of the solids and the gas, respectively. \( \mathbf{\sigma}_s \) and \( \mathbf{\sigma}_g \) are the stress tensors associated with the two phases and are defined in a compressive sense; \( \mathbf{f} \) is the interaction force between the two phases per unit volume; \( \mathbf{g} \) is the specific gravity force.

A simple Newtonian closure is used for the effective gas phase stress \( \mathbf{\sigma}_g \) [21].

\[
\mathbf{\sigma}_g = \rho_g I - \mu_{g,\text{eff}} \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) I \right] \tag{5}
\]

Here, \( \rho_g \) is the gas pressure, \( \mu_{g,\text{eff}} \) is the effective gas phase viscosity and \( I \) is the unit tensor. More elaborate models, which account for the effect of gas turbulence, have been developed [22]. However, in the case of dense gas–particle flows under investigation where \( \rho, v \geq \rho_0 (1 - v) \), the deviatoric part of the gas phase stress plays a negligible role and hence, \( \sigma_{g,\text{eff}} = \rho_g \mathbf{f} \) is adequate [18].

In dense gas–solid systems, the dominant contributor to the interaction term \( \mathbf{f} \) is the drag force. In the simulations presented here, the drag correlation of Wen and Yu [23] is used.

\[
\mathbf{f} = \beta (\mathbf{u} - \mathbf{v}); \quad \beta = \frac{3}{4} C_D \rho_g \left( 1 - v \right) \left| \mathbf{u} - \mathbf{v} \right| \frac{d}{\left( 1 - v \right)^{2.65}} \tag{6}
\]

\[
C_D = \begin{cases} 
\frac{24}{Re_g} (1 + 0.15 Re_g^{0.87}) & Re_g < 1000; \quad Re_g = \frac{\rho_g (1 - v) d |\mathbf{u} - \mathbf{v}|}{\mu_g} \\
0.44 & Re_g \geq 1000
\end{cases} \tag{7}
\]

Here, \( \beta \) is the interphase drag coefficient, \( Re_g \) is the Reynolds number and \( d \) is the particle diameter.

Following Savage [16,19], it is assumed that the particulate stress tensor \( \mathbf{\sigma}_s \) is simply the sum of the kinetic stress tensor \( \mathbf{\sigma}_k^s \) and the frictional stress tensor \( \mathbf{\sigma}_f^s \) each contribution evaluated as if it acted alone:

\[
\mathbf{\sigma}_s = \mathbf{\sigma}_k^s + \mathbf{\sigma}_f^s \tag{8}
\]

The physical basis for such an assumption remains unproven, but it captures the two extreme limits of granular flow; the rapid shear flow regime where kinetic contributions dominate and the quasi-static flow regime where friction dominates. Frictional–kinetic theories based on this simple additive treatment have been used to examine a wide variety of flows such as flow down inclined chutes and vertical channels [19,24], plane shear between parallel plates [17,25] and flow through hoppers [26,27]. The additive theory has been shown to capture the qualitative features of such flows.

The kinetic stress tensor is now commonly modeled by the kinetic theory of granular materials [14,28]. Accord-
ingly, the averaged equations of motion are supplemented
by an equation representing the balance of pseudo-thermal
energy (PTE) of particle velocity fluctuations,
\[ \frac{3}{2} \rho_s v \left[ \frac{\partial T}{\partial t} + v \cdot \nabla T \right] = -\nabla \cdot q - \sigma_Y^s : \nabla \psi - J_{\text{coll}} - J_{\text{vis}} \]  
(9)

where \( T \) denotes the granular temperature. The first term on
the right-hand side of this equation represents the diffusive
transport of PTE, where \( q \) is the diffusive flux of PTE. The
second term represents the rate of production of PTE by shear,
with the implicit assumption that work done by the frictional
component of stress is translated directly into thermal internal energy and does not contribute to the
PTE of the particles [17]. The third term in the equation represents dissipation of PTE through inelastic collisions,
whereas the fourth term denotes the net dissipation of PTE through fluid–particle interactions.

Closure relations for \( \sigma_Y^s \) and \( q \) used in our study are presented in Table 1 (see Eqs. (1.1) and (1.3)). These expressions represent slight modifications of those proposed by Lun et al. [14] to account for the effects of interstitial gas on particle phase viscosity and thermal diffusivity [18,22,29]
(see Eq. (1.5)). Setting \( \mu^s \) and \( \lambda^s \) to \( \mu \) and \( \lambda \), respectively, will recover the model proposed by Lun et al. [14]. The rate of dissipation of PTE due to inelastic collisions \( J_{\text{coll}} \) is modeled following Lun et al. [14] (see Eq. (1.4)).

The net rate of dissipation of PTE by gas–particle interactions, \( J_{\text{vis}} \), consists of two terms as shown in Eq.
(1.8). The first term, \( 3\beta T \), denotes the dissipation of PTE due to
gas–particle slip and is modeled following Gidaspow [28]. The second term is the production of PTE by gas–
particle slip. The expression shown in Eq. (1.8) for this term, without the \( g_b \) term appearing there, was derived by Koch
[30] for dilute systems. Koch and Sangani [31] have developed a more elaborate closure for this term; the \( g_b \) term in Eq.
(1.8) accounts for bulk of the refinement in concentrated
suspensions.

2.1. Frictional stress model

At high particle volume fractions, individual particles
interact with multiple neighbors through sustained contact.
Under such conditions, the normal reaction forces and the
associated tangential frictional forces at these sliding contacts are dominant. The frictional model used here is largely
based on the critical state theory of soil mechanics [10,11]. It is assumed that the granular material is noncohesive and follows a rigid–plastic rheological model of the type proposed by Schaeffer [12] and Tardos [13] which is given by

\[ \sigma_Y^f = p_I I + A(p_I, v) \frac{S}{\sqrt{S} : S} \]  
(10)

where

\[
P_I = \frac{\sigma_{xx}^f + \sigma_{yy}^f + \sigma_{zz}^f}{3}
\]

\[
S = \frac{1}{2} \left\{ \nabla \psi + (\nabla \psi)^T \right\} - \frac{1}{3} (\nabla \cdot \psi) I
\]

and \( A \) is a function to be specified. According to Eq. (10), the frictional stresses manifest an order-zero dependence on
the rate of strain. Such a behavior is well known in the
 quasi-static regime of flow [10,11]. The following properties
of Eq. (10) can be proven readily:

(i) the principal axes of stress and rate of deformation are coaxial, and
(ii) the granular material is isotropic and its deformation satisfies an extended von Mises yield condition

\[ F(\sigma_1,\sigma_2,\sigma_3,v) = (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 - 3A^2 = 0 \]  

(11)

Here \( \sigma_i \), \( i = 1,3 \) denote the principal stresses. The yield function \( F \) can equivalently be expressed in terms of the stress components \( \sigma_{ij} \) referred to an \( (x, y, z) \) coordinate system by

\[ F = \sigma_{xx}^2 + \sigma_{yy}^2 + \sigma_{zz}^2 + 2\sigma_{xy}^2 + 2\sigma_{xz}^2 + 2\sigma_{yz}^2 - 3p_t^2 - A^2 = 0 \]  

(12)

Additionally, if the postulate is made that the material obeys an associated flow rule, the following compatibility condition can be deduced [13,32]

\[ \nabla \cdot \mathbf{v} = -\sqrt{S : S} \frac{\partial A}{\partial p_t} \]  

(13)

A variety of models for \( A(p_t,v) \) have been described in the soil and granular mechanics literature [13,26]. In our illustrative examples, we have considered a form discussed by Prakash and Rao [26]

\[ A = -\sqrt{2}p_t\sin\phi \left\{ n - (n - 1) \left( \frac{p_t}{p_c} \right)^{\frac{1}{n}} \right\} \]  

(14)

where \( \phi \) is the angle of internal friction, \( p_c = p_c(v) \) is the critical state pressure and \( n \) is an exponent that determines the shape of the yield surface. Combining Eqs. (10), (13) and (14), we get

\[ \frac{\sigma_s^f}{p_c(v)} = \frac{p_t}{p_c} - \sqrt{2}\frac{p_t}{p_c} \sin\phi \left\{ n - (n - 1) \left( \frac{p_t}{p_c} \right)^{\frac{1}{n}} \right\} \times \frac{S}{\sqrt{S : S}} \]  

(15)

and

\[ \frac{p_t}{p_c(v)} = \left\{ 1 - \frac{\nabla \cdot \mathbf{v}}{n\sqrt{2}\sin\phi \sqrt{S : S}} \right\}^{\frac{1}{n}} \]  

(16)

If the assembly dilates as it deforms, \( \nabla \cdot \mathbf{v} > 0 \) and \( p_t < p_c(v) \). Similarly, if the assembly compacts as it deforms, \( \nabla \cdot \mathbf{v} < 0 \) and \( p_t > p_c(v) \). At the critical state, where the granular assembly deforms without any volume change, \( \nabla \cdot \mathbf{v} = 0 \), Eq. (16) reduces to \( p_t = p_c(v) \), and Eq. (15) becomes

\[ \frac{\sigma_s^f}{p_c(v)} = 1 - \sqrt{2}\sin\phi \frac{S}{\sqrt{S : S}} \]  

(17)

This expression, which is valid only at the critical state, is sometimes used as a simpler representation of the stresses in the granular assembly even when \( \nabla \cdot \mathbf{v} \neq 0 \).

Returning to Eqs. (15) and (16), the dilation and compaction branches of the yield surface are usually modeled separately (see, for example, Prakash and Rao [26]). In our work, we retain the same functional form for \( A(p_t,v) \) in both branches, but choose different values of \( n \) for \( p_t(v) \) in dilation and compaction as discussed below (Fig. 1).

Setting \( n = \sqrt{3}/2\sin\phi \) in the dilation branch ensures that the granular assembly is not required to sustain tensile stress anywhere on the yield surface. On the compaction side, \( n \) can assume any value greater than unity; however, it appears from literature data that \( n \) is only marginally larger than unity [27,33]. The value of \( n \) is thus set to 1.03, which is the value determined by Jyotsna [33] for Leighton–Buzzard sand. Fig. 2 shows the master curve for the family of yield loci represented by Eqs. (15) and (16) in 2-D principal stress space for \( \phi = 28.5^\circ \) and \( n = 1.03 \).

It only remains to discuss the critical state pressure \( p_c(v) \), which is used to collapse the nest of yield surfaces to a single surface. \( p_c(v) \) is the mean stress at the critical state corresponding to that value of \( v \). In general, \( p_c \) increases monotonically with \( v \) and is expected to become very large (\( \sim \) diverge) as \( v \) approaches random close packing \( v_{\text{max}} \). Various expressions have been proposed for the functional dependence of \( p_c \) on \( v \) in the literature [9,10,12,13,17,19,26]. In our test simulations, we have used the form considered by Johnson and Jackson [17],

\[ p_c(v) = \begin{cases} F \left( \frac{v - v_{\text{min}}}{v_{\text{max}} - v_{\text{min}}} \right) & v > v_{\text{min}} \\ 0 & v \leq v_{\text{min}} \end{cases} \]  

(18)

where \( F, r \) and \( s \) are constants. This model asserts that frictional interactions do not occur at values of \( v < v_{\text{min}} \).

![Fig. 1. Yield loci in 2-D principal stress (\( \sigma_1, \sigma_2 \)) space for different values of the solids volume fraction \( v \). C1 and C2 denote critical states at volume fractions \( \nu_1 \) and \( \nu_2 \), respectively. The segments OC1 and OC2 represent dilation branches; C1V1 and C2V2 represent compaction branches. The dotted lines represent the critical state loci.](image-url)
2.2. Modification of frictional–kinetic model

Savage [19] argued that even in purely quasi-static flow there exist fluctuations in the strain rate associated with the formation of shear layers and that these fluctuations will lower the shear stress in the assembly. These shear layers are typically tens of particle diameters in thickness. The length scales, therefore, associated with the microscale, i.e. particle diameter \( d \), and the macroscale, i.e. thickness of a shear layer, are not very different. Using this reasoning, Savage suggested a simple estimate for the root mean square strain rate fluctuation, \( \varepsilon \), as

\[
\varepsilon = \frac{\psi}{d} T^{1/2}
\]

(19)

where \( \psi \) is a constant of order unity. In the present manuscript, we consider an ad hoc modification of Eqs. (15) and (16), which recognizes the effect of strain rate fluctuations in an approximate manner, and write

\[
\frac{\sigma_s}{p_c} = \frac{p_c}{p_e} I - \sqrt{2} \frac{p_c}{p_e} \sin \phi \left\{ n - (n - 1) \left( \frac{p_t}{p_c} \right)^{\frac{1}{1-n}} \right\} \times \frac{S}{\sqrt{S : S + T/d^2}}
\]

(20)

with

\[
\frac{p_t}{p_c} = \left\{ 1 - \frac{\nabla \cdot \mathbf{v}}{n \sqrt{2 \sin \phi \sqrt{S : S + T/d^2}}} \right\}^{\frac{1}{1-n}}
\]

(21)

With such a formulation, numerical singularity is avoided in regions where \( S : S \) is zero as long as the granular temperature \( T \) is nonzero. If, however, the physical system does contain regions where both \( S : S \) and \( T \) are zero, the present model will fail. Thus, in a bin discharge problem, the stagnant shoulders at the bottom corners of the bin, which are indeed physically real features, cannot be captured by this rheological model unless we bring in additional considerations. This, however, is beyond the scope of this paper and we will simply investigate the consequence of the above closure—one can anticipate that in the bin discharge problem the stagnant shoulder will be replaced by a region of slow flow when we simplify the above rheological model everywhere. Eq. (17), which invokes the critical state hypothesis, is also modified in an analogous manner.

\[
\frac{\sigma_s}{p_c} = I - \sqrt{2 \sin \phi} \frac{S}{\sqrt{S : S + T/d^2}}
\]

(22)

2.3. Test simulations—grid-scale flutter

The frictional–kinetic model described in the preceding sections was implemented within the framework of the finite-volume based MFIX code [34]. This code uses a staggered grid arrangement and the SIMPLER algorithm of Patankar [35] to solve the volume-averaged equations of motion.

A number of test simulations involving discharge of granular material from a two-dimensional rectangular bin were run to examine the robustness of the code. In all the test cases, persistent grid-scale flutter in the solids volume fraction profile and velocity field was observed after some time steps [32]. This flutter did not arise if the critical state hypothesis was invoked (i.e. \( p_t = p_c \)). The origin of this flutter was traced to Eq. (21), which requires the frictional pressure to respond to the rate of deformation instantaneously. As discussed in a greater detail elsewhere [32], a simple and physically reasonable approach to remedy this problem, without compromising on the essential features of the frictional model, is to let the granular material relax to the state dictated by the compatibility condition. This can be represented as

\[
\frac{\partial (p_t/p_c)}{\partial t} + \nabla \cdot (p_t/p_c) = \frac{(p_t/p_c)^* - (p_t/p_c)}{\tau}
\]

(23)

where

\[
(p_t/p_c)^* = \left\{ 1 - \frac{\nabla \cdot \mathbf{v}}{n \sqrt{2 \sin \phi \sqrt{S : S + T/d^2}}} \right\}^{\frac{1}{1-n}}
\]

(24)

and \( \tau \) being the relaxation time. This relaxation time can be viewed as a physically meaningful quantity if one argues that particles do not respond instantaneously to deformation. On
the other hand, it can simply be viewed as a small numerical damping introduced to eliminate grid-scale flutter from simulations as well. With this relaxation model implemented in MFIX, all test simulations ran robustly and did not manifest any grid-scale flutter.

3. Simulations

3.1. Discharge from a two-dimensional bin

Simulations of particle discharge from a 2-D rectangular bin, 8 cm wide, 100 cm high and open at the top, were performed. The width of the central orifice at the bottom varied between 1.4 cm and 2 cm. A schematic of the simulation domain is shown in Fig. 3a. A 5-cm high region below the bin was included in the domain so that a boundary condition was not required right at the exit of the bin. Symmetry of the solution about the vertical centerline of the bin was assumed.

The grid resolutions are 1 and 2 mm in the horizontal and vertical directions, respectively. Such a fine mesh was required to effectively resolve variations in the velocities and solids volume fractions near the orifice region. Initially, the bin was filled with particles at a solids volume fraction of 0.60. The initial granular temperature was taken to be non-zero everywhere (1 cm²/s²). As noted earlier, our simulations require that $SS + T/d^2$ is not zero at any location. Table 2 lists the values of the model parameters used in the simulations, most of which were taken from Johnson and Jackson [17]. The flow behavior of particles of two different sizes were investigated—100 μm (Geldart A) and 1 mm (Geldart B) particles.

![Fig. 3. Schematic diagrams showing the geometries used in the test simulations. (a) Bin discharge; (b) Bubble rise in a fluidized bed.](image)

| Table 2: Values of model parameters used in simulations |
|---------------------------------|------------------|
| $\rho_g$ gas density            | $1.3 \times 10^{-3}$ g/cm³ |
| $\eta_g$ gas viscosity          | $1.8 \times 10^{-4}$ g/cm.s |
| $\rho_s$ solids density         | 2.9 g/cm³           |
| $d$ particle diameter           | 1 mm, 100 μm (bin discharge), 400 μm (rising bubble) |
| $\tau$ relaxation time for solids| $10^{-3}, 10^{-2}, 10^{-1}$ s |
| $\phi$ angle of internal friction| 28.5°               |
| $\delta$ angle of wall friction | 12.3°               |
| $\phi'$ specularity coefficient | 0.25                |
| $e_p$ particle–particle coefficient of restitution | 0.91               |
| $e_w$ coefficient of restitution at wall | 0.91               |
| $n$ parameter for shape of yield surface | $\sqrt{3}/2\sin\phi$ (dilation branch), 1.03 (compression branch) |
| $F$ Constant in equation for $p(c)$ | 0.5 dynes/cm²      |
| $r$ exponent in equation for $p(c)$ | 2                   |
| $s$ exponent in equation for $p(c)$ | 5                   |
| $\nu_{\min}$ threshold volume fraction | 0.5                 |
| $\nu_{\max}$ maximum solids packing | 0.65               |

Fig. 3. Schematic diagrams showing the geometries used in the test simulations. (a) Bin discharge; (b) Bubble rise in a fluidized bed.
The momentum and PTE boundary conditions for the particulate phase at the walls of the bin were taken from Johnson and Jackson [17]. These can be written as

\[
\mathbf{n} \cdot (\sigma_s^b + \sigma_s^p) \cdot \frac{\mathbf{v}_{sl}}{|\mathbf{v}_{sl}|} + (\mathbf{n} \cdot \sigma_s^p \cdot \mathbf{n}) \tan \delta
\]

\[+ \frac{\pi \sqrt{3}}{6v_{max}} \phi \rho_s v_{gs} T^{1/2} \mathbf{y}_{sl} = 0 \]  \hspace{1cm} (25)

\[\frac{\mathbf{n} \cdot \mathbf{q}}{\rho_g v_{gs}} = \frac{\pi \sqrt{3}}{6v_{max}} \phi \rho_s v_{gs} T^{1/2} |\mathbf{v}_{sl}|^2 - \frac{\pi \sqrt{3}}{4v_{max}} (1 - e_s^2) \rho_s v_{gs} T^{3/2} \]  \hspace{1cm} (26)

where \(\mathbf{n}\) is the unit normal from the boundary into the particle assembly, \(\delta\) is the angle of wall friction for the material, \(\phi\) is the specularity coefficient, \(e_s\) is the coefficient of restitution at the wall and \(\mathbf{v}_{sl}\) is \(\mathbf{v} - \mathbf{v}_{wall}\), the slip velocity of the particle assembly at the wall. The gas was allowed to slip freely at the wall.

At the open boundaries of the integration domain, the gas pressure was set to be atmospheric. For all other dependent variables, the usual continuation condition (i.e. zero gradient in the direction normal to the boundary) was applied.

### 3.2. Rising bubble in fluidized bed

Simulations involving the rise of a single bubble in a fluidized bed were done for two reasons: (a) to contrast the flow patterns obtained with and without the frictional stresses, and (b) to examine the consequences of assuming that the granular material is in a critical state everywhere (for the purpose of computing the stresses), i.e. \(\nabla \cdot \mathbf{v} = 0\) and \(p_t = p_c\). This assumption leads to considerable simplification of the frictional model.

The simulation domain was a two-dimensional fluidized bed, 14 cm in width and 70 cm in height. The grid resolution was 3 mm in both the horizontal and vertical directions. Symmetry of the solution about the vertical centerline was assumed. Initially, the fluidized bed was filled with particles at a solids volume fraction of 0.58 up to a height of 40 cm. A schematic of the simulation domain is shown in Fig. 3b. The temporal variation of the discharge rate of 1 mm particles from the bin with an orifice width of 1.4 cm is shown in Fig. 4. In these simulations, the gas phase was turned off and only the particle phase equations were solved. The three different curves in this figure correspond to three different values of the relaxation time constant \(\tau\). At early times, there was a rapid increase in the discharge rate, which was then followed by a plateau region where the discharge rate did not vary appreciably with time. We will loosely refer to this plateau as the steady discharge region. It is worth noting that the discharge rate in this plateau did not change much even when \(\tau\) was varied over two orders of magnitude. In all the results presented below, \(\tau\) was set to \(10^{-3}\) s.

During the period of steady discharge, the depth of material in the bin varied considerably. For example, at time \(t=1.5\) s, the depth was 85 cm while at time \(t=4.5\) s it was 53.9 cm. The discharge rate was, therefore, roughly independent of the height of the material in the bin. Experimentally, it has long been known that the flow rate of Geldart type B granular material from bins and hoppers is independent of the surcharge level [36].

Simulations including the gas phase equations yielded essentially the same discharge rate, showing that the gas had a negligible effect on the discharge behavior of the 1-mm particles, which is entirely reasonable [36,37].

The particle phase velocity (at an instant of time in the plateau region) in the bottom region of the bin is shown in Fig. 4. The rate of discharge of 1-mm particles as a function of time. See Fig. 3a for a schematic of the geometry of the bin. The results corresponding to three different relaxation times are shown. The gas phase equations were not considered in these simulations. In calculating the discharge rate, the thickness of the bin was taken to be 1 cm.
Fig. 5. The corresponding solids volume fraction distribution is superimposed. The width of the orifice in this case was 1.4 cm. The region far above the orifice was characterized by a nearly uniform particle concentration where the material was effectively in (nearly) plug flow. As particles approached the orifice region, the flow converged towards the orifice, as one would expect. At the orifice, there was a substantial decrease in the particle concentration accompanied by a simultaneous increase in the velocities as the particles were discharged. There was further dilation and increase in the downward velocity as particles accelerated down after discharge.

It is clear from Fig. 5 that there was some flow even in the corners of the bin, regions which should truly be stagnant. The frictional model was thus unable to predict the formation of the experimentally observed stagnant zones on either side of the orifice. This was due to the addition of the term \( T/d^2 \) in the denominator; the conduction of PTE from regions of high shear near the orifice to the corners ensured that granular temperatures in the latter regions were nonzero.

Fig. 6 shows solids volume fraction profiles at three elevations below the plane of the orifice for the preceding simulation. The vertical lines indicate the positions of the edges of the orifice. Just below the orifice, the profile displayed a marked convexity. At lower depths the profiles manifested greater lateral spreading as the material dilated after being discharged, with the particle concentration being maximum on the centerline. Very similar experimental profiles were observed by Fickie et al. [38] for discharge of 1-mm particles from a wedge-shaped hopper.

The variation in the solids volume fraction along the vertical centerline (during the steady discharge rate period) as a function of height above the plane of the orifice is shown in Fig. 7 (as solid line). From a value of 0.60 high in the bin, \( \dot{m} \) fell rapidly on approaching the orifice, reaching a value of 0.52 at the plane of exit. Below the orifice, particle concentration decreased rapidly as the stream of particles accelerated under gravity. Experimental investigations such as those of Bransby et al. [39] and Fickie et al. [38] do reveal considerable changes in the particle concentration from point to point within the hopper. Discrete element simulations of discharge from a hopper also show the same trend [40].

The bin discharge simulation described in Figs. 4–7 was repeated invoking the critical state hypothesis for the frictional stresses (i.e. postulate that \( p_f = p_c \)). It was found that the results were virtually indistinguishable. This is illustrated in Fig. 7, where the broken line corresponding to the critical state hypothesis overlaps very nearly the solid line obtained with the more detailed stress model. The variation of the ratio \( p_f/p_c \) along the centerline, obtained with the detailed stress model, is shown in Fig. 8. Only a small region near the orifice is shown in this figure. It is clear that this ratio was very close to unity well above the orifice; as the granular assembly approached the orifice, it dilated and the ratio decreased. Note that this ratio dropped by only \( \sim 10\% \).
even though there was appreciable dilation. This was because of the large rate of strain (and hence $S$) near the orifice. Thus, even in the presence of appreciable dilation near the orifice, critical state hypothesis is reasonable for the purpose of estimating the stresses in the present problem. This is in line with the finding of Tardos [13] who analytically showed that flow in a wedge plane hopper takes place under conditions very close to the critical state.

Many of the early attempts to predict the mass flow rate of Geldart type B particles discharging from a bin under the action of gravity were based on dimensional analysis or semi-empirical correlations. All these studies have tended to rely heavily on the concept of a “free-fall surface” in the neighborhood of the orifice. Above the free-fall arch, particles are in contact with one another and the granular material is usually treated as a noncohesive incompressible Coulomb powder. Below the arch, particles are no longer in contact with one another and accelerate freely under gravity.

Since the discharge rate of granular materials from a bin is dependent on conditions near the orifice, it has been argued that the free-fall surface scales with the orifice diameter or width ($D_o$). Ignoring the possible effects of particle diameter $d$, dimensional analysis suggests that particle velocity $v$ at the orifice then scales as $(gD_o)^{1/2}$. Scaling for the discharge rate $W$ of material from a hopper or bin should therefore be

$$W = \begin{cases} \rho g^{1/2} D_o^{3/2} & 3 - D \text{ bin or hopper flow} \\ \rho g^{1/2} D_o^{3/2} H & 2 - D \text{ channel} \end{cases}$$

where $\rho$ is a density characteristic of the flowing material and $H$ is the thickness of the hopper/bin. Indeed, semi-empirical correlations found in the literature are of the form shown above. The well-known Beverloo correlation [41] for discharge from two-dimensional hoppers and bins can be written (when the orifice diameter is much larger than that of the particles) in simplified form as

$$W = C\rho_i g^{1/2} D_o^{3/2} H$$

(28)

where $\rho_i$ is the initial density achieved during the filling process and $C$ is an empirical constant in the range $0.55 < C < 0.65$. The variation of the discharge rate with orifice width for our system is shown Fig. 9 where the discharge rate is seen to scale as $D_o^{1.4}$. This compares well with the expected value of 1.5 for the exponent. However, the steady discharge rates obtained in our simulations yield $C \approx 1.6$, which is significantly larger than the typical experimental value. It is possible that this discrepancy is due to the fact that simulation failed to capture the stagnant shoulder; however, it should be noted that theoretical analyses tend to overestimate the discharge rate of particles from a small-angled hopper as well.

Tardos [13] studied the discharge of compressible powder from a wedge-shaped hopper, using an equation of the form $p_c m^{1/n} = \text{constant}$ for the critical state pressure. He found that as $n$ was varied from 0 to 0.25, corresponding to the granular flow becoming increasingly compressible, the coefficient $C$ reduced from 2.0 to 0.90.

As mentioned above, most theoretical analyses of bin or hopper discharge postulate the existence of a free-fall arch at the exit orifice, where the normal stress is assumed to vanish. Kaza and Jackson [42] have argued that this sce-
nario with the density of the material remaining constant up to the free-fall surface, below which it accelerates, is inconsistent with the laws of motion. The results of our simulations support this argument. For example, there is no evidence of a discontinuous change in the slope of $v$ in Fig. 7, as one would expect at a free-fall surface of the type described previously. Furthermore, the decrease in the bulk density of the granular material starts well within the regime where frictional interactions are dominant and makes the zero normal stress boundary condition questionable.

The decrease in the particle concentration $n$ also has implications for semi-empirical correlations. Such correlations require a density $\rho$ for dimensional consistency as shown in Eq. (28), but there is significant controversy as to the appropriate value to use. Beverloo et al. [41] used the initial density achieved during the filling process, $\rho_i$, in their correlation. Kotechanova [43] argued that the bulk density in the vicinity of the orifice region should be used although how this value is to be evaluated is unclear according to Nedderman [44].

4.2. Bin discharge—100 $\mu$m particles

The temporal variation in the discharge rates of 100 $\mu$m particles in the presence and absence of air is shown in Fig. 10. In the absence of air, the discharge rate manifests the plateau region as is expected. It is noteworthy that the steady state discharge rate is almost the same as that for the 1-mm particles. Indeed, the frictional model is independent of the diameter of the particle in the regions where the $S.S$ term dominates over the $T/d^2$ term, as is the case for the orifice region in bin discharge.

The discharge rate is significantly lower in the presence of air than that in the absence of air. It is well known that the discharge rate decreases as the particle size decreases [45] primarily because the motion of the particles is significantly impeded by drag exerted by the air and that the Beverloo correlation cannot be used to predict discharge rates of particles less than 400 $\mu$m in size [44].
Nedderman [44] has shown that for a hopper, in the absence of voidage changes, the gas and solids flow through with the same velocities and there is no drag on the particles. Thus, the influence of drag on the discharge of fine particles must be due to relative velocities between the two phases induced by changes in the particle concentration. The variation of the time-averaged solids volume fraction along the centerline (in the plateau region where the discharge rate is nearly constant) is shown in Fig. 11. Indeed, the presence of air changes the $v$-profile near the orifice region appreciably. It is noteworthy that the magnitude of the change in $v$ in the presence of air is much smaller than that in the absence of air. There is some experimental evidence to support this observation. The experiments of Fickie et al. [38] for 1-mm particles, which are insensitive to fluid drag, reveal considerable changes in particle concentration along the centerline of the hopper. The experiments of Spink and Nedderman [45] for the discharge of 110-$\mu$m sand particles from a hopper, show a relatively small but rapid change in the particle concentration immediately above the orifice.

During discharge of a fine material through a hopper or a bin, a subatmospheric pressure is known to develop just above the orifice [45], when both the top and the bottom of the bin are exposed to atmospheric pressure. This was indeed observed in our simulations. The time-averaged pressure profile along the centerline is shown in Fig. 12. Just above the orifice region the air pressure was lower than the ambient pressure just below the orifice. The magnitude of this pressure deficit is comparable to the values recorded experimentally [45,46].

Fig. 11. The variation of solids volume fraction with height along the centerline. See Fig. 3a for a schematic of the geometry of the bin. The horizontal line indicates the location of the exit orifice. Discharge of 100-$\mu$m particles from the bin. The results represent a time-average of data in the steady discharge rate plateau. The solid curve was obtained from a simulation which ignored the interstitial air. The broken line was obtained in a simulation which included the effect of the interstitial air.

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Fig. 12. The variation of gas pressure (scaled with atmospheric pressure) with height along the centerline. See Fig. 3a for a schematic of the geometry of the bin. The horizontal line indicates the location of the exit orifice. Discharge of 100-$\mu$m particles from the bin. The results represent a time-average of data in the steady discharge rate plateau.
4.3. Rising bubble in fluidized bed

Instantaneous snapshots of the solids volume fraction profile of a bubble (circular cap) in a fluidized bed at time $t=0.5$ s are shown in Fig. 13a–c. Panel (a) was obtained with the full frictional model. The relaxation time constant $\tau$ was $10^{-3}$ s for this case. Panel (b) was obtained from a simulation where the critical state hypothesis was used to determine the frictional stresses. Finally, panel (c) represents the situation where frictional stresses were turned off and only the kinetic stresses were considered.

It is clear that neglecting the frictional stresses altogether changed the dynamics of the bed considerably. When only collisional stresses were present, as depicted in Fig. 13c, the spherical cap was more elongated along the vertical axis and rose faster than when frictional stresses were present. As the cap rose, it produced nonuniformities in its wake. These nonuniformities then grew as can be seen in the bottom portion of Fig. 13c.

Comparing Fig. 13a and b, it can be seen that the shapes of the circular caps in both panels are very similar. Thus, the assumption that the granular material is at a critical state everywhere appears to be quite adequate for dense fluidized beds as well as gravity discharge from bins. This has important implications in the modeling of frictional stresses. The critical state assumption leads to considerable simplification of the frictional stress model described here. In addition to the equations becoming much simpler, the critical state assumption obviates the need of solving Eqs. (23) and (24) for the relaxation of $p_f/p_c$. This speeds up the computations and also makes it more robust.

5. Summary

A frictional–kinetic constitutive model for particle phase stresses is described. This model assumes that the frictional and kinetic stresses are additive [16,17]. For the frictional stresses, we began with a model based on an extended von Mises yield criterion and an associated flow rule [12,13], modified it in a simple, but ad hoc, manner to account for strain rate fluctuations [19] and also allowed the granular material to relax slowly to the yield surface. A simplified version of the model was obtained by invoking the critical state hypothesis [10]. The kinetic stresses have been modeled using the kinetic theory of granular materials with some modifications to account for the presence of the gas phase [18,28,31]. These models have been implemented within the framework of the finite-volume based MFIX code [34].

Simulations of discharge of granular material from a 2-D rectangular bin were performed for two different particle sizes. The discharge rate for 1-mm particles was found to plateau out with time and become approximately independent of the height of the material in the bin [36,41]. As expected, the gas phase did not affect the rate of discharge of these large particles. These simulations also revealed a significant variation in particle concentration near the orifice region, which is in line with experimental observations [38].

Fig. 13. Instantaneous grayscale plots of solid volume fraction field in a bubble rise simulation. (a) Full frictional–kinetic model; (b) Critical state hypothesis; (c) Kinetic stresses only. 400 $\mu$m particles in air. See Fig. 3b for a schematic of the geometry.
The discharge behavior of 100 μm particles was affected by the interstitial gas appreciably. The discharge rate in the presence of air was substantially lower than that in the absence of air. This well-known effect [45] is correctly captured by the simulations.

Although the frictional stress model described here is able to qualitatively predict many of the features of gravity discharge from a bin, it suffers from two main defects. First, it cannot predict the formation of stagnant shoulders at the corners of the bin. Second, it overestimates the discharge rate.

Simulations of a rising bubble in a fluidized bed revealed that the shape of the bubble changed appreciably when the frictional stresses were dropped, demonstrating the significant effect of the frictional stress on the bubble shape.

The critical state hypothesis was found to be fairly accurate for both problems. It simplifies the frictional stress model, renders the code more robust and increases the computational speed.

**Nomenclature**

- \( A \): function defined by Eq. (14)
- \( C_D \): drag coefficient (see Eq. (7))
- \( d \): particle diameter
- \( D_o \): orifice diameter or width
- \( e_p \): coefficient of restitution for particle–particle collisions
- \( e_w \): coefficient of restitution for particle–wall collisions
- \( f \): interaction force between the two phases per unit volume
- \( F \): yield function (see Eqs. (11) and (12))
- \( g \): specific gravity force
- \( g_o \): see Eq. (1.7)
- \( I \): unit tensor
- \( J_{coll} \): rate of dissipation pseudo-thermal energy by inelastic collisions per unit bed volume (see Eq. (1.4))
- \( J_{vis} \): net rate of dissipation pseudo-thermal energy by gas–particle interactions per unit bed volume (see Eq. (1.8))
- \( n \): see Eq. (14)
- \( n \): unit normal from the boundary into the particle assembly
- \( p_c \): critical state pressure
- \( p_f \): frictional pressure in the particle phase
- \( p_g \): gas pressure
- \( q \): diffusive flux of pseudo-thermal energy (see Eq. (1.3))
- \( Re_g \): Reynolds number (see Eq. (7))
- \( T \): granular temperature
- \( u \): local average velocity of the gas phase
- \( v \): local average velocity of the particle phase
- \( v_{sl} \): slip velocity of the particle assembly at the wall

**Greek symbols**

- \( \beta \): interphase drag coefficient
- \( \nu \): volume fraction of particles
- \( \nu_{min}, \nu_{max} \): see Eq. (18)
- \( \rho_s, \rho_g \): densities of the solids and the gas, respectively
- \( \sigma_{so}, \sigma_g \): stress tensors associated with the solid and gas phases, respectively
- \( \sigma^k, \sigma^l \): kinetic and frictional stress tensors, respectively
- \( \sigma_i, i = 1, 3 \): principal stresses
- \( \mu_{g,eff} \): effective gas phase viscosity
- \( \phi \): angle of internal friction
- \( \varepsilon \): magnitude of strain rate fluctuation
- \( \tau \): relaxation time
- \( \delta \): angle of wall friction for the material
- \( \phi' \): specularity coefficient

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**References**