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Publisher's version / Version de l'éditeur:

Computational Technologies for Fluid/Thermal/Chemical Systems with Industrial Applications-ASME-PVP (Pressure Vessels and Piping Division), 397-1, pp. 137-148, 1999

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Proceedings of the 2nd ASME International Symposium for
Computational Technologies for Fluid/Thermal/Chemical Systems
with Industrial Applications, Boston, MA, August 1-5, 1999.
PVP-Vol. 397-1, pp. 137-148.
NRC no. 41995.

NUMERICAL STUDY OF TWO-PHASE GRANULAR FLOW FOR PROCESS EQUIPMENT

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ABSTRACT

This paper reports on a research program of modeling single and multi-phase granular flow. Both incompressible and compressible single-phase granular flow, as well as two-phase liquid/granular flow in a pressure vessel were considered. For the latter case, detailed results based on a viscous/Mohr-Coulomb closure were compared to existing formulations. Idealized test cases indicated that the numerical procedure is sound. Subsequent simulations of two-phase flow using realistic geometries and boundary conditions showed that the pressure distribution in the solid phase is fundamentally different for the Mohr-Coulomb system than for the conventional system. The effect of the angle of internal friction, geometry, and other parameters is discussed.

NOMENCLATURE

A	Area
A, B	Constants in equation of state
a_W, a_E, a_S, a_N, a_J	Coefficients in finite-volume equations
b	Forchheimer's constant
C	Source term coefficient
D	Diameter or width
d_0	Threshold rate of deformation
d_{ij}	Components of deformation rate tensor
d_I, d_{II}	Principle rates of deformation
g	Generation term
$\vec{g}$	Acceleration due to gravity
H	Height
k	Permeability
k'	Inter-phase slip coefficient
m	Exponent in equation of state

P	Solid phase pressure
p	Fluid pressure
r_f, r_s	Fluid, solid volume fraction
S	Source term in finite-volume equations
$\vec{u}$	Velocity vector
u, v	Velocity components
$\vec{u}_f, \vec{u}_s$	Fluid, solid phase velocity
V	Source term value
x, y	Displacement
Δ	Rate of deformation
η	Solid phase shear viscosity
κ	Kappa number
μ	Fluid viscosity
ρ, ρ_f, ρ_s	Density, fluid density, solid density
σ	Normal stress
$\bar{\sigma}$	Stress tensor
$\sigma_{11}, \sigma_{22}, \sigma_{xx}, \sigma_{yy}$	Normal components of stress tensor
σ_I, σ_{II}	Principle stresses
τ	Shear stress
τ_{12}, τ_{xy}	Shear component of stress tensor
τ_w	Wall shear stress
$\Phi_P, \Phi_W, \Phi_E, \Phi_S, \Phi_N$	Values of Φ in finite-volume equations
$\Phi_{iP}, \Phi_{iW}, \Phi_{iE}, \Phi_{iS}, \Phi_{iN}$	Values of Φ_i in finite-volume equations
ϕ	Angle of internal friction
ϕ_w	Angle of friction with wall
ψ	Angle of major principle stress
$\partial u / \partial n$	Wall velocity gradient

INTRODUCTION

The two-phase flow of granular materials within a viscous fluid is a subject with many important applications in the chemical and process industries, food and beverage, materials refining, energy, and other industry sectors. Figure 1 shows an example of an industrial reactor-vessel used to process wood chips into pulp. Solid wood chips and liquid material are introduced at the top, and removed at the bottom of a long pressure vessel. There are four main regions in the vessel: An impregnation zone, followed by (from top-to-bottom) heating, cooking, and washing zones. The unconsolidated porous matrix of solid particles is saturated with free liquid in the upper impregnation zone. The chips are then brought to the required cooking temperature in the heating zone. Chemical delignification of the wood fibers occurs in the cooking stage, while the chips are cooled and washed in the lower washing zone. Additional liquid, necessary to optimize the cooking process, is introduced at three locations in the apparatus; spent fluid being extracted at two sets of screens in the outer wall. Smooth flow of the granular material within the vessel, under the action of gravity and fluid drag, is critical to the successful operation of the apparatus, especially in the washing zone, where a counter-flow regime exists. Hanging of the chip column, or plugging of the extraction screens could lead to time-consuming and expensive downtime of the equipment.

In view of the elevated pressures and temperatures, caustic environment, and complex nature of the flow, performing even the simplest experiments is difficult or impossible. Under these circumstances, computational fluid dynamics can convey important information to the manufacturer and operator of the equipment. Although chemical kinetics, heat and mass transfer are present, these are considered beyond the scope of this paper, which is concerned only with the mechanics of the solid and liquid phases, knowledge of which is of paramount importance to the operator of the equipment.

Previous solutions

Härkönen (1984, 1987) was among the first to attempt numerical modeling of such a system. He considered two-dimensional (2-D) steady-state flow within the axisymmetric reactor illustrated in Fig. 1. Fluid flow within the isotropic porous media was described by the Ergun-modified form of Darcy's law (Scheidegger, 1974, Ergun and Orning, 1949, Ergun, 1953). Terms due to confining and pore pressure, as well as Darcy friction and gravity were constructed in a force balance. Härkönen's numerical scheme involved the solution for a harmonic scalar potential function, satisfying overall continuity, followed by the iterative solution for the solid bed (inter-granular) pressure, volume fraction, phase velocities, and Darcian inter-phase slip coefficient. Härkönen's method was based on the notion that a solid pressure, P , distinct from the fluid pressure, p ; was present; however no shear forces were permitted within the granular material, other than at the wall, i.e. the bulk of the material was treated as an inviscid fluid.

Figure 1. Schematic of the reactor used in this study. From Härkönen (1984), with permission.

The Härkönen scheme has formed the basis for subsequent calculations: Michelsen (1995) and Michelsen and Foss (1994, 1996) considered transient one-dimensional (1-D) two-phase flow in an industrial digester. The solid material was treated as a Newtonian fluid with a kinematic viscosity of 10^{-3} (m^2/s). The chip and liquid heights were allowed to vary; however radial momentum was presumed insignificant in comparison to axial momentum. Saltin (1992) also considered a 1-D two-phase flow model. The Härkönen scheme suffers from a number of restrictions: (i) The method is based on a static balance, i.e. creeping flow, and inertial terms are excluded entirely. (ii) Because a scalar potential is employed, boundary layer effects (Brinkman, 1949) cannot be accounted for. (iii) The rheology of the chip column is idealized. (iv) The algorithm employed is highly specialized, i.e. non-standard.

Scope of the present study

The goals of this study are to: (a) Develop a model of 2-D single and two-phase granular flow with standard CFD methods and codes. (b) Validate the method against previous numerical work. (c) Introduce a more realistic rheology, which includes the frictional behavior of the solid phase. (d) Conduct parametric studies to ascertain the effects of the frictional properties of the solid phase on the flow.

Rheology of the solid phase

Flowing granular materials are known to behave differently from viscous fluids. The significant feature of that behavior is that the shear stresses, which arise during deformation, are proportional to the normal stresses. Such frictional properties give rise to one of the well-known observations concerning pressure distribution in bins. Janssen (1895), see also Brown and Richards (1970) considered the equilibrium of vertical forces on a section of the granular material to show that the

pressure on the walls of a bin increase linearly with depth, only near the top. The resulting vertical distribution of the pressure follows an exponential profile, tending to a constant maximum value that does not increase with further increase of depth.

The frictional properties of granular materials are commonly described by a Mohr-Coulomb criterion as follows

$$\tau = c + \sigma \sin \phi \quad (1)$$

where τ and σ are the shear and normal stress on the failure plane, c is the cohesion term, and ϕ is the angle of internal friction. Both ϕ and c are material properties (or constants). The angle, ϕ , is approximately equal to the angle of repose of the granular material.

The Mohr-Coulomb criterion for two-dimensional deformation can be graphically represented, as shown in Fig. 2. The vertical and horizontal axes represent the shear and normal stress, respectively. The stress states can be represented as circles. The yield envelope corresponds to a straight line, tangent to the stress circles. The case shown is for a cohesionless material, $c = 0$, with shear stresses vanishing at zero normal stress.

For 2-D Cartesian coordinates, x_1 and x_2 , the stress relations are

$$\sigma_{11} = -P(1 + \sin \phi \cos 2\psi) \quad (2)$$

$$\sigma_{22} = -P(1 - \sin \phi \cos 2\psi) \quad (3)$$

$$\tau_{12} = -P \sin \phi \sin 2\psi \quad (4)$$

where σ_{11} , σ_{22} , τ_{12} are the normal and shear stresses, ψ is the angle between the major principal stress σ_I and the x_1 axis, and the magnitude of the solid pressure, P , is the average of the major and minor principal stresses,

$$P = -\frac{\sigma_I + \sigma_{II}}{2} \quad (5)$$

At low rates of deformation, it is usually assumed that granular material can be modeled as a plastic continuum, and the Mohr-Coulomb criterion is used to represent the frictional behavior. Drucker and Prager (1952) developed the first adaptation of the theory of plasticity to the deformation of granular materials. The model was based on an associated flow rule, with a generalized Mohr-Coulomb criterion as the plastic potential. There have since been a large amount of related investigations. Most of the relevant results may be found in soil mechanics textbooks, e.g. Scott (1963). At high rates of deformation, flowing granular materials exhibit a behavior that is somewhat different. Particle-particle collisions give rise to stresses that depend on the magnitude of the rate of deformation; i.e. of a turbulent nature. Savage (1984) gives a thorough review of that behavior.

Figure 2. Mohr-Coulomb diagram for a cohesionless material. The circles represent possible stress states.

At present, there is no indication that treatment of the present problem requires the relatively complex models that correspond to the high rate of deformation regime. Consequently, we incorporate the frictional behavior of the solid phase by employing a plasticity approach representing the slow deformation regime. The impact on performance of using models for the high rate regime is left for future investigations. Such work may also consider the theory of Savage (1998) which incorporates particle fluctuations in a plasticity framework, and may be relevant to the present situation.

GOVERNING EQUATIONS

Two distinct classes of problem are considered in the present work. (i) The motion of incompressible bulk granular material. Interstitial fluid effects are assumed negligible. The objective is to verify that the present numerical scheme can deal with plastic rheology. (ii) The simultaneous motion of both granular and viscous fluid phases, and the coupling between them. This case is considered in order to examine actual flow conditions in the industrial pressure vessel.

Incompressible single-phase granular flow

The continuity and momentum equations of the bulk granular material may be written as follows:

$$\bar{\nabla} \cdot (\rho \bar{u}) = 0 \quad (6)$$

$$\bar{\nabla} \cdot (\rho \bar{u}; \bar{u}) = \rho \bar{g} + \bar{\nabla} \cdot \bar{\sigma} \quad (7)$$

where $\bar{u}$ is the velocity, ρ is an effective density, $\bar{g}$ is the acceleration due to gravity, and $\bar{\sigma}$ is the stress tensor. Tensile normal stresses are considered positive in Eqs (6) and (7).

The relationship between the stress and the rate of deformation may be expressed as¹

¹ Cartesian tensor notation is adopted for reasons of brevity. The vector forms in Cartesian and polar co-ordinates may easily be derived (Aris, 1962).

$$\sigma_{ij} = -P\delta_{ij} + 2\eta d_{ij} \quad (8)$$

where $d_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ are the components of the rate of deformation, P is the pressure, see Eq. (5), and η is a solid phase shear viscosity. Bulk viscosity is considered negligible in Eq. (8). The Mohr-Coulomb criterion and associated flow rule are introduced into the flow algorithm by giving the shear viscosity, η , the following value,

$$\eta = \frac{P \sin \phi}{\Delta} \quad (9)$$

The rate of deformation, Δ , is given by

$$\Delta = \max(|d_I - d_{II}|, d_0) \quad (10)$$

where d_I and d_{II} are principle values of the deformation gradient tensor, and d_0 is a threshold rate-of-deformation. The reader will note that for the present case, $|d_I - d_{II}| = \sqrt{g}$, where the generation term, g , is frequently used in fluid mechanics codes for calculations involving heat transfer and turbulence. For relatively large rates of deformation, $\Delta > d_0$, the rheology is plastic, with stresses independent of the magnitude of the rate of deformation components. At small rate of deformation values, $\Delta \leq d_0$, the shear viscosity is constant, and the deformation is viscous. Thus, the present model employs a viscous-plastic formulation to approximate rigid-plastic conditions. The threshold rate of deformation, d_0 , is assigned a very small value in order to maintain a predominantly plastic deformation. Equations (6) to (10), together with the appropriate boundary conditions are sufficient to determine the velocities and components of the stress tensor.

Compressible two-phase fluid/granular flow

For this type of analysis, we add the equations of motion of the fluid phase, terms describing the coupling between solid and fluid phases, and an equation-of-state for the solid phase (needed to model the bulk compressibility of the granular material).

The continuity and momentum equations for the fluid phase are

$$\bar{\nabla} \cdot (r_f \rho_f \bar{u}_f) = 0 \quad (11)$$

$$\bar{\nabla} \cdot (r_f \rho_f \bar{u}_f \bar{u}_f) = r_f \rho_f \bar{g} - r_f \bar{\nabla} p + \bar{\nabla} \cdot (\bar{\nabla} r_f \mu_f \bar{u}_f) + k'(\bar{u}_f - \bar{u}_s) \quad (12)$$

where r_f is the fluid volume fraction, $0 \leq r_f \leq 1$, ρ_f and $\bar{u}_f$ are liquid velocity and density, respectively, μ is the fluid viscosity, and p is a fluid or pore pressure. The inter-phase slip coefficient, k' , is given by,

$$k' = r_f \frac{\mu}{k} + \rho_f r_f^2 b |\bar{u}_f - \bar{u}_s| \quad (13)$$

where k is permeability, and b is Forchheimer's constant (Scheidegger, 1974). For the solid phase, i.e., the bulk granular material,

$$\bar{\nabla} \cdot (r_s \rho_s \bar{u}_s) = 0 \quad (14)$$

$$\bar{\nabla} \cdot (r_s \rho_s \bar{u}_s \bar{u}_s) = r_s \rho_s \bar{g} - r_s \bar{\nabla} p + \bar{\nabla} \cdot (\bar{\nabla} r_s \bar{\sigma}) + k'(\bar{u}_s - \bar{u}_f) \quad (15)$$

where $r_s = 1 - r_f$ is the solid volume fraction and ρ_s and $\bar{u}_s$ refer to the solid phase. The components of the solid phase stress tensor $\bar{\sigma}$ are given in Eq. (8). For compressible flow, the solid (granular) pressure, P , is related to the volume fraction according to the equation-of-state, or compressibility equation;

$$r_s = A + B P^m \quad (16)$$

for $P \geq 0$. The fluid pressure, p , is solved-for but the solid pressure, P , is obtained algebraically, by inversion of Eq. (16) as,

$$P = \frac{10^4}{0.831 - 0.139 \ln \kappa} (r_s - 0.356)^{1.695} \quad (17)$$

from Härkönen (1987), with a constant value of $\kappa = 195$ (Michelsen, 1996), and $r_s > 0.356$. The reader will note that while the fluid pressure, p , acts on both fluid and solid, the solid pressure, P , has no effect upon the fluid. Thus, p is sometimes referred to as a 'shared' pressure.

NUMERICAL SCHEME

Both incompressible single-phase granular flow, and compressible two-phase fluid/granular flow were considered in this study. For the former case a finite-volume method based on the well-known SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm of Patankar and Spalding (1972) may readily be employed. The domain is divided into a number of finite-cells, and it is postulated that the governing partial differential equations may be approximated by linear algebraic equations having the form

$$a_W(\Phi_W - \Phi_P) + a_E(\Phi_E - \Phi_P) + a_S(\Phi_S - \Phi_P) + a_N(\Phi_N - \Phi_P) + S = 0 \quad (18)$$

where Φ_P is the value of some intrinsic property Φ at cell P , and Φ_W , Φ_E , Φ_S , Φ_N refer to values at the west, east, south, north neighbors of P , and $S = C(V - \Phi_P)$ is a linearized source-term. A so-called staggered scheme (Harlow and Welch, 1965) is employed for velocities, $\Phi = u, v$. The momentum equations are

solved assuming a guessed pressure field. If the pressure field is incorrect, the velocity field will not satisfy continuity, and pressure and velocity correction factors are computed until satisfactory convergence is achieved. For multi-phase flow, the system of equations having the form,

$$\begin{aligned} a_w(\Phi_{iW} - \Phi_{iP}) + a_E(\Phi_{iE} - \Phi_{iP}) + a_S(\Phi_{iS} - \Phi_{iP}) + \\ a_N(\Phi_{iN} - \Phi_{iP}) + a_J(\Phi_{jP} - \Phi_{iP}) + S = 0 \end{aligned} \quad (19)$$

$i = 1, 2, j = 2, 1$, may be solved using the IPSA (Inter-Phase Slip Algorithm) of Spalding (1980, 1981). The main features of this algorithm are: (i) The notion of a 'shared' pressure, p , between the fluid and the solid, with an associated 'extra' pressure, P , in the solid due to inter-granular stresses (Markatos and Kirkcaldy, 1983). (ii) The use of a partial elimination algorithm to mitigate the cross coupling in the inter-phase term in Eq. (19). (iii) The sum-to-unity requirement for volume fractions, r_f, r_s . Phase-continuity equations are used to solve for volume fractions, while overall continuity is used to correct the pressure, p , and velocity fields in the phase momentum equations in a fashion analogous to the SIMPLE algorithm.

The commercially available research-oriented code, PHOENICS, was modified to perform all the calculations described in this paper. This was achieved by modifying parts of the source code, supplied by the vendor, in order to compute (a) η according to Eq. (9) (all cases) (b) k' according to Eq. (13) (two-phase cases) and P according to Eq. (17) (compressible cases), at the end of each 'sweep' or iterative cycle. In addition source terms were introduced, as described below.

Boundary and initial conditions

Treatment of a granular flow at a wall is as follows. The shear stress on the wall is assumed to be,

$$\tau_w = \frac{P \sin \phi_w}{\Delta} \frac{\partial u}{\partial n} \quad (20)$$

where $\partial u / \partial n$ is the velocity gradient at the wall, ϕ_w is the angle of friction between the granular material and the wall, $0 \leq \phi_w \leq \phi$, and the rate of deformation, Δ , is computed with Eq. (10). By changing ϕ_w , the wall shear stress may thus be varied from no slip to pure slip.

For the liquid phase, the fluid regime is dominated by gravity and Darcy (inter-phase) friction, in the inertial regime, so wall effects were not considered in this study. Other boundary prescriptions are straightforward; both fixed mass and momentum sources, and fixed pressure-type boundary conditions were imposed at inlets and exits, as appropriate. For two-phase flow, solid and liquid were presumed to enter with no initial inter-phase slip.

Cases considered

The following four cases were examined:

- (1) Incompressible single-phase granular flow in a vertical channel.
- (2) Compressible granular/air flow through a hole in a square bin.
- (3) Two-phase viscous/viscous flow in the axisymmetric apparatus shown in Figs. 1 and 3.
- (4) Two-phase viscous/Mohr-Coulomb liquid/solid flow in the apparatus shown in Figs. 1 and 3.

Cases (1) and (2) were considered in order to demonstrate the accuracy of the model, and to help clarify the results for cases (3) and (4) which involved a problem with practical industrial applications. In case (1) both frictional and frictionless granular flow are considered and compared. The effect of the angle of internal friction, and of the channel width, D , on the solid flow regime is analyzed. In case (2) the stress distribution for a compressible granular flow in a short channel or bin is considered in detail. Cases (3) and (4) are both concerned with the apparatus of Fig. 1. Figure 3 shows further details of the equipment. The cross section of the 14.75 m vessel increases from the top to bottom, as shown. Solid and liquid material are introduced at the top of the pressure vessel. There are four main regions in the reactor: impregnation, heating, cooking and washing zones. Liquid is injected from three locations, and extracted through two sets of screens. The solids exit through the main outlet assisted by a mechanical scraper. An axisymmetric grid was constructed. The mesh was concentrated in the vicinity of the liquid inlet regions, and around the main outlet. Boundary conditions and property values are indicated in Fig. 3 and Table 1. These correspond to values given in Härkönen (1984, 1987).

For case (3), the inter-granular friction in the solid phase is presumed to be viscous, consistent with Michelsen (1996) with a shear viscosity, η , corresponding to a constant kinematic viscosity of $10^{-3} \text{ m}^2/\text{s}$. For case (4), the solid-phase rheology is extended to include friction using a Mohr-Coulomb plastic yield criterion. Comparison with case (3) reveals substantial differences. The effect of the angle of internal friction, ϕ , on the solid flow is discussed.

RESULTS AND DISCUSSION

Incompressible single-phase granular flow

Figures 4 to 7 show the results for gravity-driven single-phase incompressible granular flow in a straight vertical channel, Eqs. (6) to (10). The channel is open at both top and bottom. No-slip boundary conditions are imposed at the walls. The mass flow rate at the outlet is fixed corresponding to a bulk velocity of 1 mm/s and $\rho = 1132.4 \text{ kg/m}^3$, while the pressure, P , is fixed to zero, at the top of the channel.

Figure 3. Detailed schematic of the reactor vessel used in this study.

Figure 4. Velocity vectors for frictional granular flow, $D/H = 2:12$, $\phi = 20^\circ$.

Table 1. Boundary conditions and properties for solid and fluid phases for the problem of Fig. 3

Parameter	Value
Main inlet solid volume fraction, r_s	0.42
Main inlet solid pressure, P	5 000 (Pa)
Main inlet solid velocity, v_s	2.4×10^{-3} (m/s)
Main inlet fluid velocity, v_f	2.4×10^{-3} (m/s)
Main outlet fluid pressure, p	0 (Pa)
Solid density, ρ_s	1132.4 (kg/m ³)
Fluid density, ρ_f	1 000 (kg/m ³)
Fluid permeability, k	$\frac{\mu}{4.6 \times 10^3} \frac{r_f^2}{r_s^2}$ (m ²)
Forchheimer's constant, b	$\frac{3.9 \times 10^6}{\rho_f} \frac{r_s}{r_f^2}$ (1/m)

Figure 5. Fully developed velocity profiles for frictionless and frictional granular flow in a channel.

Figure 6. Effect of aspect ratio on pressure, P (Pa), for incompressible single-phase flow, $\phi = \phi_w = 30^\circ$.

Figure 7. Pressure, P (Pa), as a function of depth, $D/H = 2:12$. Various angles of internal friction, ϕ ($^\circ$).

Figure 4 shows velocity vectors in the channel. The flow is predominantly in the vertical direction. Note the formation of shear layers near the channel walls, as observed in the experimental work of Savage (1984), who also noted that the plug-like velocity profile in the central region of the vertical channel. Figure 5 is a detail of the fully-developed v -velocity profile. Results for both frictional, $\phi = 20^\circ$, and frictionless $\phi = 0^\circ$, granular material are shown. For the frictionless case, a flat profile is observed across the entire cross-section of the channel, corresponding to a slip boundary condition velocity at the wall: Since $\eta_w = \eta = 0$ in Eqs. (9) and (20), there is no shear force between the granular particles and the wall (or each other), and therefore no mechanism for the production of friction and hence shear.

Figures 6 and 7 show profiles of the pressure, as defined in Eq. (5), versus channel depth at the centerline of the channel. In Fig. 6, the aspect ratio D/H is varied, with $H = 12\text{m}$, and $\phi = 30^\circ$. It can be seen that the pressure, P , increases with increasing depth, y , near the top of the channel, then reaches a maximum which is proportional to the channel width, D . This class of pressure distribution is always observed for granular materials (Brown and Richards, 1970, Shamlou, 1988). It differs from that observed in fluids, where the hydrostatic pressure increases linearly with depth, and is independent of the channel's width.

In Fig. 7, the aspect ratio D/H is fixed at 0.167, and ϕ is varied in the range $0 \leq \phi \leq 45^\circ$ with $\phi_w = \phi$. The case $\phi = 0^\circ$ corresponds to a frictionless material, i.e. a perfect fluid. For this case, P increases linearly with y , reaching a maximum of 1.3×10^5 Pa at the bottom of the channel (corresponding to the hydrostatic fluid pressure, with $g = 9.81 \text{ m/s}^2$). As the value of ϕ increases, the resulting pressure distribution departs from that for a fluid and increases asymptotically to a constant maximum, which decreases with increasing friction, ϕ . The reader will note that the local pressure distortion at $y = 12\text{m}$, Figs. 6 and 7, is due to the prescription of a fixed mass flux (velocity) at the

exit. An alternative would be to specify the downstream pressure.

The pressure distributions shown in Figs. 6 and 7 are in good agreement with the equation of Janssen (1895). A quantitative comparison is not considered meaningful, owing to the numerous simplifying assumptions inherent in the derivation of Janssen's formula. The results, presented here, clearly illustrate the important role of shear (or friction) terms.

Compressible granular/air flow

Figures 8 to 12 show results for flow of a mixture of air and granular material from a small 2-D bin. The bin is open at the bottom with a centrally-located hole of size $0.2D$, through which the mixture flows. The only influence of the air is on the compressibility equation (equation of state), Eq. (17), i.e. the flow is in effect a compressible single-phase granular flow problem². The inlet flow rate is prescribed at $1 \times 10^{-3} \text{ m/s}$ with $r_s = 0.4$.

Figure 8 shows the solid phase velocity field. The gravity-driven flow converges toward the bottom hole. A shear layer at the walls is also apparent. The flow accelerates from the top to a maximum of $4.6 \times 10^{-2} \text{ m/s}$ at the outlet. Figure 9 shows the values of the angle, ψ , between the major principal stress and the horizontal axis, at a horizontal section mid-way up the bin. The resulting distribution of ψ is asymmetric, with $-45^\circ \leq \psi \leq 45^\circ$. This asymmetry is to be expected and can be explained as follows: The shear stress on the bulk granular material at each wall acts upwards. Consequently, according to the present co-ordinate system, the shear stress would be negative near the right wall, and positive near the left wall. Hence, the horizontal distribution of ψ should be asymmetric. The value of $\psi = 0^\circ$ at the centerline indicate that the major principal stress acts horizontally. This is sometimes referred to as a passive stress state (Scott, 1963). This is expected when a channel or bin is being emptied. In contrast, an active stress state corresponds to the major principal stress along the centerline acting vertically. It usually arises when a channel is being filled, with the outlet blocked.

The present calculations give values of $\psi = \pm 45^\circ$ at the side walls, i.e. the major principal stress acts at an angle of 45° to the vertical side walls. This is a consequence of the imposed no-slip boundary condition at the walls. The results indicates that slip planes are inclined to the side walls. It is interesting to note that according to the Mohr-Coulomb criterion, deformation (or failure) of the granular materials occurs along slip planes which form at angles of $\pm(45^\circ - \phi/2)$ to the major principal stress (see for example Scott, 1963). It follows that such slip planes do not coincide with the side walls.

² The problem was actually solved as two-phase flow; However inter-phase friction and fluid pressure, p , have negligible influence upon the solid flow, and were hence neglected.

Figure 8. Solid phase velocity vectors.

Figure 9. The angle, ψ (°), between major principal stress and the horizontal, at $y = H/2$.

Figure 10. Normal stress component, σ_{xx} (Pa).

Figure 11. Normal stress component, σ_{yy} (Pa).

Figure 12. Shear stress component, τ_{xy} (Pa).

Figures 10 and 11 show the normal stress components, σ_{xx} and σ_{yy} , respectively. Negative values indicate compression. For σ_{xx} , two main regions are apparent. (a) A center 'core' where the horizontal stresses, σ_{xx} , have large magnitudes, between 2.6×10^3 and 5×10^3 Pa. (b) Outer zone(s) near the wall(s), where the stresses have relatively small magnitudes, compared to center-line values and $|\sigma_{xx}|$ decreases in a near linear fashion from 2.6×10^3 at the top to 1.3×10^3 at the bottom. For σ_{yy} , three distinct zones may be identified. (a) A center 'core' of the bin where $|\sigma_{yy}|$ has the smallest values, between 2.3×10^4 and 9.2×10^2 Pa. (b) Lower outer regions near the bin corners, where $|\sigma_{yy}|$ has large values in the range 2.6×10^3 to 3.4×10^3 Pa. (c) Upper outer region(s) where $|\sigma_{yy}|$ is almost constant around 2.4×10^3 Pa. The stress distributions in Figs. 10 and 11 follow intuitively expected patterns. For example, the vertical normal stress, σ_{yy} , decreases near the exit. Also, the value of σ_{yy} is greater than that of σ_{xx} in the vicinity of the exit. This is expected when emptying granular material, corresponding to the passive state mentioned above.

Figure 12 shows the shear stress, τ_{xy} . This component is almost constant at the side walls. This behavior is in agreement with the results obtained in the above section for incompressible

granular material in a vertical channel, and is also in agreement with Janssen's formula as well as numerous observations of stresses in bins (Brown and Richards, 1970). The distribution of the shear stress displays asymmetry with respect to the centerline. This is expected, as mentioned in the discussion of the distribution of the angle ψ , shown in Fig. 9.

Two-phase viscous/viscous compressible solid/fluid flow

Figures 13 and 14(a) show the results for case (3), namely viscous/viscous solid/fluid flow in the apparatus of Fig. 3, generated using a grid of 72x164 cells. Figure 13 shows velocity vectors for both liquid and solid. It can be seen that for the solid, a plug-flow is apparent other than near the secondary inlets 1 and 2, where liquid injection entrains and disperses the solid particles as a result of inter-phase friction. Liquid velocities are axial in the impregnation and cooking zones, but radial in the heating and washing zones near the outlet screens, due to extraction. In the upper region, solid and liquid flow co-currently while in the lower washing zone a counter-current state is apparent at the wall, due to injection at inlet 3 (see Fig. 3). The reader will note that liquid and solid phases have relatively similar densities. These spatial velocity distributions are in good agreement with those of Härkönen (1984).

Figure 14(a) shows contours of solid pressure, P . The reader will note that a near linear pressure gradient is apparent in the central cooking zone, with somewhat larger gradients in the impregnation and washing zones. Though not readily apparent from Fig. 14(a), the pressure actually tends to zero in the vicinity of liquid injection sites 1 and 2, in addition to the main inlet. This indicates that there is no particle-to-particle contact here; i.e. the granular material is dispersed, since a state-of-tension cannot exist. In the impregnation zone, the compression increases slightly towards the bottom of the equipment, where a maximum of 3×10^4 Pa is observed. In the washing zone the pressure decreases near the side walls, due to liquid re-circulation between the injection inlet 3 and outlet 2. Liquid injection and extraction in the heating and washing zones disperses the solid in these regions, and a reduction in solid volume fraction, r_s , and pressure, P , results.

Figure 14(b) shows the distribution of solid pressure from Härkönen (1984). These are similar to the present results, Fig. 14(a). Inspection of Fig. 14(b) reveals that P increases from 5×10^3 Pa at the main inlet to 7×10^3 Pa at the main outlet, with the same pressure decrease in the vicinity of the lower liquid injection screens, as noted above. Some differences between Figs. 14(a) and 14(b) are observed near the main inlet and also the two lateral heating and washing zones. This may be due to the fact that inertial terms, considered here, were not included in the earlier work, or because the Härkönen formulation was for an inviscid fluid i.e. it did not contain a diffusion term within the bulk of the solid phase.

Liquid velocity Solid velocity
Figure 13. Velocity vectors, viscous/viscous compressible two-phase flow.

Two-phase Viscous/Mohr-Coulomb compressible solid/fluid flow

Finally, the results of case (4) are presented. This case corresponds to the full solution for two-phase flow, including the Mohr/Coulomb frictional behavior of the granular material. All other boundary conditions, transport properties etc. were identical to those given in case 3, above (as given in Table 1 and Fig. 3) other than the solid shear viscosity, η . The angle of internal friction, $\phi = 45^\circ$, used in the calculation of η is based on an industry-accepted average value, although this may vary substantially, in reality.

Fig. 14(c) shows the pressure, P , in the solid phase. It can be seen that P increases only very slightly from 5×10^3 Pa at the top, to 5.6×10^3 Pa at the bottom. For Mohr-Coulomb granular flow, the pressure is independent of height, which is in accordance with observed behavior of frictional granular materials, as discussed above. The minor increase in each of the four zones is due to the small increases in cross-section. It can also be seen that while P decreases near the liquid injection inlets 1 and 2 (Fig. 3), it does not approach zero, as in the previous case. This result suggests that frictional shear forces reduce dispersion of the solid particles by the pore fluid.

Figure 14. Solid pressure, P (Pa) contours (a) Viscous fluid formulation (b) From Härkönen (1984), with permission. (c) Mohr/Coulomb formulation.

Figure 15. Solid phase pressure, P (Pa), for viscous and Mohr-Coulomb formulations.

Figure 16. Effect of angle of internal friction, ϕ (°), on the solid pressure, P (Pa).

Figure 15 is a comparison of solid pressure, P , midway across the reactor vessel, for case (3), viscous/viscous solid flow, and case (4), viscous/frictional Mohr-Coulomb solid. It is apparent that the two approaches generate fundamentally different profiles: For the viscous/viscous approach, the solid pressure increases from inlet to outlet (from 0 Pa to 1.8×10^4 Pa), in a relatively linear fashion, with depth, as expected for a Newtonian or perfect fluid. Local pressure extrema are associated with liquid injection. Conversely, for case (4) viscous/Mohr-Coulomb formulation, the pressure is relatively constant, around 5.3×10^3 Pa, along the length, but is sensitive to cross-sectional size.

The effect of the angle of internal friction, on the solid pressure distribution, midway across the vessel, is shown in Fig. 16, for $\phi = 10^\circ, 20^\circ, 40^\circ$. P is inversely proportional to ϕ , as demonstrated for case (1), above. For values of $\phi > 20^\circ$, the solid pressure in the impregnation zone is close to the inlet value of 5×10^3 Pa. For $\phi = 10^\circ$, gravitational forces predominate over shear forces, and the solid material is more closely-packed, leading to higher solid pressures.

Numerical considerations

The fluid pore pressure, p , was chosen to test for grid independence as a solved-for variable (unlike the solid pressure P , which is evaluated algebraically). Figure 17 shows profiles obtained using grids consisting of 18×41 (1x), 36×82 (2x) and 54×123 (3x) cells. The difference between inlet and outlet pressure is approximately 30% for the 18×41 and 36×82 grids, and 3% for the 36×82 and 54×123 grids. Results for a 72×164 (4x) grid are essentially identical to those for the 54×123 (3x) grid. This indicates that the present calculations achieve a satisfactory measure of grid independence. Comparisons suggested that there is only a small performance penalty associated with the use of the well-known IPSA algorithm, in the place of previously developed specialized numerical schemes to obtain a converged solution.

An assessment of the effects of numerical diffusion has yet to be conducted for the current problem. It is true that higher-order schemes than the 'hybrid' scheme (Patankar, 1980) adopted generate more accurate solutions e.g. for simple problems involving laminar single-phase flow. However, it is not readily apparent whether numerical considerations are the limiting factor in complex multi-phase flow. The governing equations, Eqs. (11) to (16), are based on assumptions introduced to close ensemble-averaged mass and momentum equations. The form of the (closed) inter-phase transport terms are presumed to be diffusive and/or convective in nature. The availability of 3-D multi-phase direct-numerical simulations (DNS) would be a useful tool in analyzing the combined effects of the precision of the discretization scheme and the accuracy of the closure assumptions.

Figure 17. Effect of grid size.

CONCLUSIONS

A multiphase flow model for chemical process equipment has been presented. The problem involves the simultaneous solution for two-phase flow of frictional bulk granular material and viscous-liquid. The two-phase flow is driven by gravity, and the imposed solid/fluid phase discharge at the inlets. Established single and two-phase Eulerian algorithms were modified to perform granular flow calculations, based on the solution of systems of coupled linear algebraic equations using a segregated flow solver.

The solid phase was modeled using two different approaches. In the first approach it was treated as a Newtonian fluid with constant shear viscosity, and an extra solid pressure, P (as in previous studies). The second approach extends the model to include Mohr-Coulomb viscous-plastic flow. This was achieved by introducing a shear viscosity such that the stress tensor is independent of the magnitude of the rate-of-deformation tensor. In fully-developed regions, where velocity gradients vanish, the viscosity coefficient is indeterminate, and the viscous-plastic threshold is reached. This, however, is a reasonable rheological behavioral assumption.

Idealized test cases showed that the present numerical scheme correctly handled the viscous-plastic regime. A solution of the full two-phase flow problem with realistic geometry and boundary conditions was then developed. The results show that the frictional properties of the solid phase play an important, previously neglected role. The pressure distribution down the vessel is quite different from that obtained by neglecting friction entirely, or by assuming a constant viscosity. The present model indicated a relatively constant pressure along the vessel walls; a result which is in agreement with numerous observations of granular materials in bins and hoppers, and contrary to the Newtonian model. The pressure distribution, and indeed the motion of the solid phase also appeared to be sensitive to the frictional properties of the granular material in the vicinity of fluid inlets, a situation with important ramifications to the equipment designer and operator.

ACKNOWLEDGMENTS

The authors acknowledge the assistance of the staff of Ahlstrom Machinery Inc., of Glens Falls NY, and in particular Mr. Aaron Leavitt. The advice and support of Dr. Donald Singleton and Mr. Ron Jerome at NRC, are gratefully acknowledged.

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