BUILDING A NUMERICAL MODEL FOR BULK MATERIALS FROM STANDARD SHEAR TEST DATA

HERMANN FEISE AND ANDREAS DAISS

BASF AG, D-67056 Ludwigshafen, Germany
{hermann.feise, andreas.daiss}@basf-ag.de

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Abstract: While numerical methods have become an integral part of everyday work in process engineering for fluid processes, there is a curious lack of such methods in the field of solid handling. One of the reasons may be the inability of the most often used CFD codes to handle bulk solids. In this paper an attempt is made to show how the behaviour of bulk solids can be modelled using a CFD code without a specific constitutive model for bulk solids.

Another reason for not using numerical tools to handle bulk materials is the difficulty of generating the necessary material parameters. Those material models suitable for bulk solids that are available in commercial packages are mostly derived from soil mechanics. Their parameters are determined using a triaxial cell. This device is generally not available in the chemical industries and most often not suitable for bulk solids, due to the high stress levels applied in those tests. In the paper a method is presented which allows the use of standard shear test data, supplemented by data from a compression tests in a "lambda-meter", to determine the parameters of an extended Drucker-Prager model with a compressive yield cap. Model equations are given and parameters are determined for white polymer powder. With these parameters a simulation of silo discharge has been performed successfully using a CFD code.

To make CFD codes, which already have the much-needed multi-phase capability, capable of handling bulk solid flow, significant work remains to be done (*e.g.* shear stresses at rest and anisotropic stress tensors).

Keywords: constitutive model, FEM, silo flow material parameters stress

1. Introduction

While numerical methods have become an integral part of everyday work in process engineering for fluid processes, there is a curious lack of such methods in the field of solid handling. Noteworthy work in establishing numerical methods for solid handling applications has been done using mainly Finite Element Methods (FEM) and Granular Dynamics, also called Discrete Element Methods (DEM). Work on FEM is done at the University of Karlsruhe [1, 2], the Technical University of Braunschweig [3, 4], the University of Edinburgh [5], at the University of Guelph [6] and in Scandinavia [7]. Work using DEM to model bulk solids was done at the Universities of Birmingham [8], Surrey [9] and Stuttgart [10]. However, little of this has been translated into actual use of such methods in the chemical industry, for several reasons. The use of DEM is still restricted to fairly powerful computing equipment and comparably small numbers of particles. The invention of a useful "meta-structure", where one discrete element represents a cluster of actual particles has yet to be made and the description of particles other than spheres still entails even longer computing times. Finite Elements do not have the scale restrictions of DEM applications, however, the constitutive models found in FEM packages, such as ABAQUS or ANSYS, have been developed for soil mechanics applications. Their adaptation to bulk solid handling problems is not obvious and the required material parameters are not generally available for bulk solids. For process engineering applications we quite often need to model not only bulk solid flow but also the gas and/or liquid phase around the particles. This is a task usually unsuitable for FEM systems. The obvious choice for these applications would be a CFD package with multi-phase capabilities. However, these packages tend not to provide models suitable for bulk solids.

In this paper an attempt is made to show how the behaviour of bulk solids can be modelled using a CFD code without a specific constitutive model for bulk solids. It will also be shown how the necessary parameters can be derived from standard bulk solid tests.

2. Constitutive modelling

2.1. Flow function

The basis of constitutive modelling of bulk solid behaviour is the BINGHAM fluid model. This model is generally available in CFD codes and provides for static yield stress, which is necessary to describe bulk solids. The well-known flow equation of the Bingham-fluid is:

$$\tau = \tau_0 + \eta \cdot \dot{\gamma}. \tag{1}$$

For bulk solids, this simple equation has to be adapted to account for the tensorial quality of the stress state:

$$q = q_0 + \sqrt{3} \cdot \eta \cdot \|\dot{\gamma}\|. \tag{2}$$

Here, q is equivalent shear stress and $\|\dot{\gamma}\|$ is the second norm of the strain rate tensor. Viscosity, η, is not generally significant for bulk solids, which tend not to exhibit viscous behaviour, and it will not be considered here. In such cases, it can be used to dampen numerical fluctuations and speed up convergence.

The static part of equivalent shear stress is used to describe the pressure-dependent, velocity-independent flow of bulk materials. Here we use a formulation employing a Drucker-Prager yield surface with a cap. Such a model is suitable for cohesive, compressible bulk materials. The better known Mohr-Coulomb or Drucker-Prager models without a flow cap are restricted to absolutely free-flowing, incompressible materials. In the Drucker-Prager convention the yield locus (cone) reads thus:

$$q_0 = d + p \cdot \tan\varphi_\beta, \tag{3}$$

and the consolidation locus (cap) is as follows:

$$q_0 = R^{-1} \cdot \sqrt{R^2 \cdot [d + p_e \cdot \tan\varphi_\beta]^2 - (p - p_e)^2}. \tag{4}$$

All stresses are considered solid stresses only, not taking into account any pressures or pressure gradients in the gas phase (the effective stress concept). At a given bulk density, ρ_b, the yield locus is active if the acting hydrostatic component p of the stress tensor (pressure) is smaller than the respective value at steady-state flow, p_e. Beyond steady-state flow, the consolidation locus becomes active. Figure 1 shows the yield and consolidation loci in a q-p diagram.

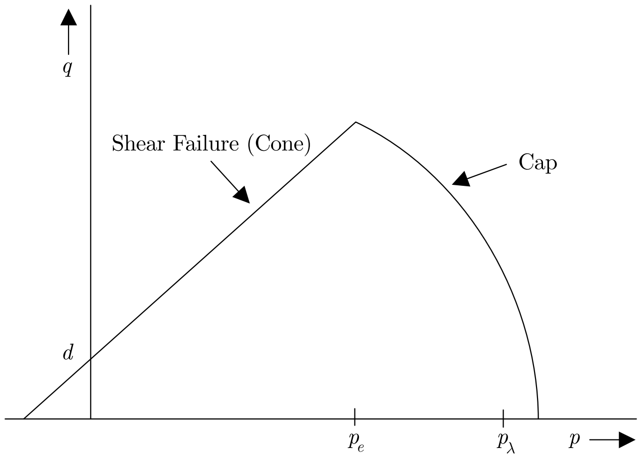

Figure 1. Drucker-Prager model with cap

At steady-state flow, there exists a unique correlation between p_e and ρ_b [11, 12]. Here, we assume a logarithmic dependence of porosity and stress at steady-state flow. This leads to the following equation:

$$\rho_b = \rho_{b_0} + \rho_s \cdot \Gamma \cdot \ln\left(\frac{p_e}{p_0}\right), \tag{5}$$

where p_0 is an arbitrary reference pressure and ρ_{b_0} – the bulk density at this pressure. Care has to be taken when using Equation (5), as both ρ_{b_0} and Γ depend on p_0.

2.2. Hardening functions

In cohesive, compressible bulk materials cohesion is a function of consolidation pressure. Equivalent cohesion, d, can be written as a function of bulk density, which in turn is a function of pressure at steady-state flow (see Equation (5)). For many materials a linear correlation between equivalent cohesion, d, and pressure at steady-state flow p_e may be assumed. This corresponds to a linear flow function in the sense of Jenike [13]. The resulting equation reads:

$$d = d_0 + m_d \cdot p_e, \tag{6}$$

where d_0 and m_d are material parameters and have to be determined from experiments.

The cap parameter R also depends on bulk density. Following the same arguments as above, it can be written as a logarithmic function of pressure at steady-state flow, p_e (see Equation (7)). The respective material parameters are R_0 and Γ_R:

$$R = R_0 + \Gamma_R \cdot \ln\left(\frac{p_e}{p_0}\right). \tag{7}$$

3. Material parameters

3.1. Powder characterisation for flow

Powder characterisation for flow is done using shear testers. The industrial standard is the Jenike Shear Cell, developed by Jenike in the 1960s [13]. Since this tester is rather cumbersome to use, new automated testers have been developed. Over the last ten years the Schulze ring shear tester [14] has been very successful; effectively, on the verge of becoming the new industry standard. Either of these devices – or other competing testers – measure one normal and one shear stress in the material only. To determine the entire stress state, much more complicated testers (*e.g.* true biaxial testers [15, 11]) have to be used. These devices are generally unsuitable for industrial use. A typical result of industrial shear tests is a set of yield loci as shown in Figure 2. Here, the shear stress at yield is given as a function of the normal stress applied. All measurements related to one yield locus have been made with the material first consolidated under steady-state flow, *i.e.* all such measurements have been made at the same bulk density. The stress at steady-state flow is represented by the larger of the two Mohr circles drawn for each yield locus. The major principal stress at steady-state flow σ_1 is considered the consolidation stress. The smaller Mohr circle defines the uniaxial compressive strength, f_c, of the material at the respective bulk density.

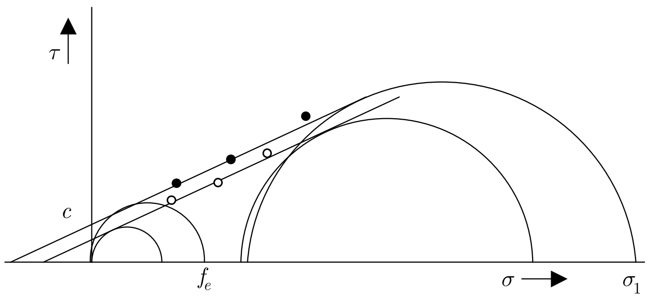

Figure 2. Yield loci from shear tests

The yield locus is approximated by a straight line corresponding to the linear yield surface (cone) of the Drucker-Prager model. Its inclination is given as φ_i and the intercept with the τ axis – as c. The following relation exists between uniaxial strength, f_c, and the cohesion, c:

$$c = \frac{1-\sin\varphi_i}{2\cdot\cos\varphi_i}\cdot f_c. \tag{8}$$

3.2. Powder characterisation for compaction

The consolidation locus cannot be determined from shear tests alone. While the consolidation procedure at steady-state flow gives some information about the consolidation locus, a dedicated compaction experiment is necessary. This can best be done in a compaction cell equipped to measure radial and axial stresses as well as axial strains ("soft oedometer", "lambda-meter") [16]. Figure 3 shows such a cell.

Meaurements with a compaction cell provide information about the consolidation process. In the compaction test, increasing normal loads (usually vertical) lead to increasing densities and increasing horizontal stresses. Therefore, the tests move

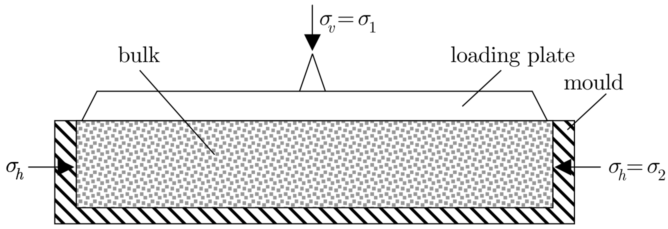

Figure 3. Lambda-meter [16]

through a number of consolidation loci, since all points of a specific consolidation locus belong to one specific density.

In a typical compaction test the horizontal stress increases linearly with the vertical stress, ignoring an initial transient period. The ratio of horizontal to vertical stress can therefore be considered as a constant:

$$\lambda = \frac{\sigma_h}{\sigma_v}. \tag{9}$$

Kwade *et al.* [16] have mentioned that wall friction effects may lead to errors in determining proper horizontal and vertical stresses in the measurement plane. Therefore, they have proposed to correct the decrease of vertical stress with depth with the Janssen equation [17]. In this paper only corrected values of λ are used.

The increase of density with vertical stress in a compaction test follows the same logarithmic dependency as in steady-state flow (see Equation (5)). Feise [11] and Nowak [18] have shown that the logarithmic constant is applicable in both tests. However, steady-state flow always leads to higher densities at the same stress level. Therefore the density-stress function for compaction reads as follows:

$$\rho_b = \rho_{b\lambda} + \rho_s \cdot \Gamma \cdot \ln\left(\frac{p_\lambda}{p_0}\right). \tag{10}$$

4. Determining Drucker-Prager parameters from shear tests

Bound by the restricted capabilities of the ring shear tester, an evaluation of shear test measurements has to assume that the third principal stress has no influence on the yield locus. This restriction does not apply to the Drucker-Prager model. To be able to calculate the Drucker-Prager parameters from shear test data, we assume that the data has been obtained from plane strain deformation [19]. This gives the following for the cone angle β:

$$\tan\varphi_\beta = \sqrt{3} \cdot \frac{\sin\varphi_i}{\sqrt{1 + \frac{1}{3}\sin^2\varphi_i}}. \tag{11}$$

For the equivalent cohesion we find:

$$d = \sqrt{3} \cdot \frac{\cos\varphi_i}{\sqrt{1 + \frac{1}{3}\sin^2\varphi_i}} \cdot c. \tag{12}$$

The cap parameter R follows from:

$$R^2 = \frac{(p_\lambda - p_e)^2}{(d + p_e \tan\varphi_\beta)^2 - q_\lambda^2}. \tag{13}$$

To determine p_e from standard shear test data, we have to make an assumption on the value of the third principal stress during steady-state flow. Following Nowak [18], we assume that the ratio of the three principal stresses during steady-state flow is a constant. For lack of better information, it is taken that $\sigma_3 = 0.65 \cdot (\sigma_1 + \sigma_2)/2$.

Equivalent shear stress in uniaxial compaction can easily be calculated from the horizontal stress ratio:

$$q_\lambda = 3p_\lambda \frac{1-\lambda}{1+2\lambda}. \tag{14}$$

5. Example: white polymer powder

5.1. Model material

Initial numerical test runs were done simulating a silo filled with white polymer powder. The powder was characterised using a Portishead ring shear cell for shear tests and a lambda-meter for compaction tests. Figure 4 shows equivalent cohesion, d, and the cap parameter, R, versus pressure at steady-state flow, p_e. As can be seen from the data, the approximation for d versus p_e holds very well. While the correlation for R versus p_e is not as good, it still gives a reasonable fit. One has to bear in mind, however, that R varies only marginally for this material.

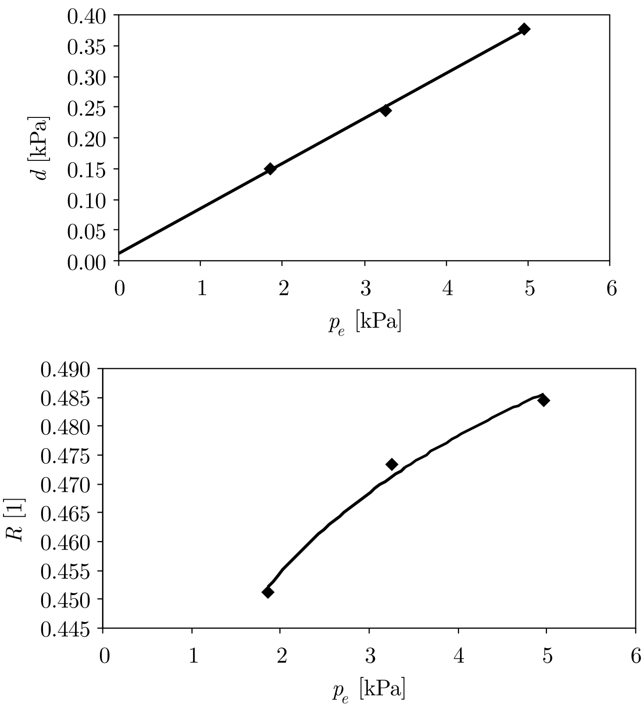

Figure 4. Test results

5.2. Numerical results

As an initial test for the material model described above, the predictions of the model for stresses in a silo have been checked. The silo used is an axial-symmetric silo with a shaft diameter of $D = 1$m and a total height of $h = 7$m. The hopper angle is $\Theta = 20^\circ$, which guarantees mass flow for this material, and the outlet diameter is $D_a = 300$mm. Figure 5 shows the results of the numerical calculation for the discharge state. The left-hand figure shows the vertical stress in the silo as colour coding. One can observe the typical increase of pressure with depth and a zone of very high pressure right at the transition. The typical mass-flow profile is captured in the hopper section. The wall stress is drawn versus height in the second diagram of Figure 5. The overall picture corresponds to the one for vertical pressure. However, while the typical switch stress is captured, we also see a drop in pressure right above the transition. This drop appears to be a typical feature of numerical simulations of mass-flow silos. It can be observed in the published results as early as in Häussler's work [1]. According to the numerical simulation the maximum vertical stress in the silo shaft is 3040kPa. This corresponds well with the result from the Janssen equation [17], giving $\sigma_{\max} = 3\,300$kPa.

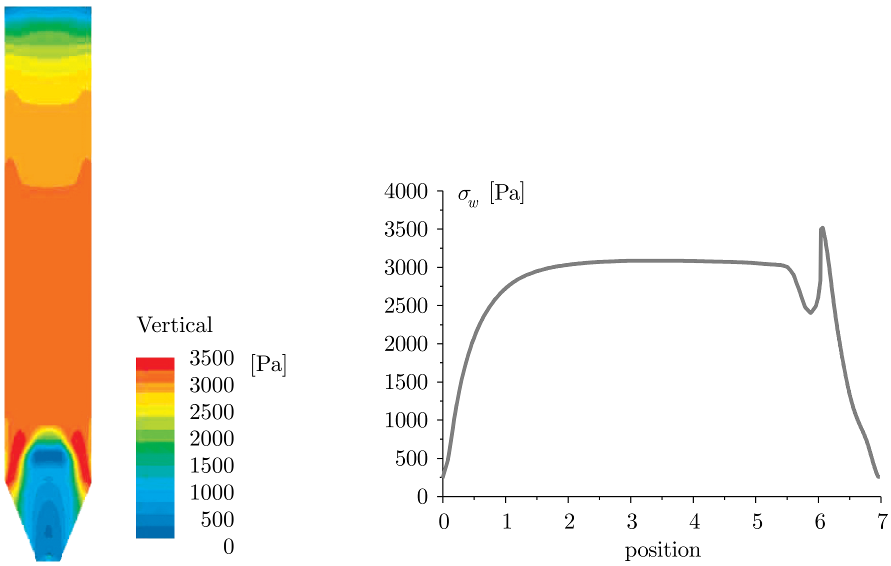

Figure 5. Numerical results

While the numerical simulation of silo discharge has worked reasonably well, we have been unable to simulate the filling state. This is due to the way the model is implemented into the software. The simulation of granular flows with finite volume CFD codes is a difficult task since the calculation of the flow field is based on the solution of the Navier-Stokes equations, which determine the stresses as functions of the local shear rate and viscosity, which is calculated from the Bingham viscosity model. This means that the stresses are not direct solution variables like in structure mechanics but are calculated from the flow-field solution. In the cylindrical part of a silo, significant shear rates occur only in the vicinity of the wall, where the apparent viscosity resulting from the Bingham model is rather small. In the core of the silo, however, the granular medium moves downward like a solid body. In this region, the shear rate is almost zero and viscosity goes to infinity. Thus, the program has to handle a very large viscosity gradient, which can lead to numerical instabilities. In order to practically reduce this problem, viscosity is limited to a maximum value.

This value has to be chosen so that the stability problem is reduced and that the chosen value has no significant influence on the solution.

It is impossible to calculate the stresses in a stationary granular bed with a finite-volume CFD code as no flow occurs there at all and, thus, the shear rate is zero everywhere. Since the calculation of stresses is based on viscosity and the shear rate, the stresses become indefinite (viscosity goes to infinity).

6. Conclusions

An attempt has been made to use well-established numerical methods (CFD) to model the behaviour of bulk solids. The material parameters have been estimated from standard shear test data. A suitable model has been formulated, based on the Drucker-Prager model of soil mechanics extended by a compressive yield cap to capture the capability of cohesive bulk solids to flow plastically during compaction. It has been possible to derive the necessary material parameters from standard shear test data plus some compaction data from a compaction test in a lambda-meter. Simple shear testing alone has not sufficed. The necessary equations have been given.

The numerical simulations of bulk solid behaviour using this approach have shown some promising results. It has been possible to get good qualitative and respectable quantitative coincidence of numerical and analytical calculations for the material chosen for silo discharge. It has been impossible, however, to simulate a stationary bulk solid. This is due to restrictions of the program used. This problem cannot be solved by the user alone but will require some changes in the code, *i.e.* co-operation from the software developers. The same holds for another important problem: finite volume CFD codes usually assume that normal stresses (pressure) are isotropic, which does not hold for granular flows. While it is possible to implement a Bingham viscosity model in a CFD code by user subroutines, it is quite difficult to incorporate the effect of anisotropic normal stresses by user programming alone.

To establish a similar level of numerical modelling for bulk solid flow in the chemical industry as there exists for fluid dynamics, a concerted action of the academia, software developers and users is needed to provide software and models suitable for use in the industry. Since in the chemical industry systems requiring numerical modelling are often concerned not only with bulk solids but also with the gas and/or liquid phase around it, there is a need for software which provides:

- constitutive models suitable for bulk solids in a multi-phase setup, and
- models using parameters that can be measured at reasonable expenditure of time and money (*e.g.* standard tests).

For CFD codes to allow the simulation of bulk solid flow, further work has to be done to provide for the capability of bulk solids to transmit shear stresses at rest (infinite viscosity) and the anisotropic characteristics of the stress tensor.

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