

INCLUSION OF A SOIL MECHANICS BASED SOLIDS RHEOLOGY MODEL INTO THE KINETIC THEORY OF GRANULAR FLOW

Simon VUN^{1,2}, Jamal NASER^{1,2}, Peter WITT³

¹Swinburne University of Technology, Hawthorn, Victoria 3122, AUSTRALIA

²CRC – Clean Power from Lignite, Mulgrave, Victoria 3170, AUSTRALIA

³CSIRO Minerals, Clayton, Victoria 3169, AUSTRALIA

ABSTRACT

The kinetic theory of granular flow has become a popular choice for closure of the gas-solid, Eulerian-Eulerian momentum equations for fluidised beds. However the theory is limited to short term particle collisions and as the solid volume fraction increases convergence problems arise. A solution to this problem has been to include a frictional stress tensor developed from soil mechanics into the kinetic theory of granular flow frictional stress tensor with expressions for the bulk viscosity and shear viscosity. In the present paper a constitutive model representing the granular flow includes a frictional model developed by Dartevelle (2004). The frictional model is a function of the normal stress, which is based on an empirical critical state pressure given by Johnson & Jackson (1987). A comparison was conducted between the frictional viscosity model of Srivastava & Sundaresan (2003) and a modified Dartevelle model. In addition, validation with experimental work shows the predictions of both models compare well to the bubble diameter and time-averaged porosity plots of Kuiper's (1990). Moreover the Dartevelle model shows higher gas dispersion through the bed which better resembles the experimental time averaged porosity plots.

NOMENCLATURE

d	Diameter
e	Coefficient of restitution
P,p	Pressure
u	Velocity

Greek Letters

ε	Volume fraction
ρ	Density

Subscript

g	Gas
s	Solids
f	Frictional
KT	Kinetic Theory of Granular Flow.

INTRODUCTION

Interest in advanced gasification technology from the Australian brown coal power industry has led to further research into gas-solid, fluidised beds. Experimental research into the hydrodynamics of a fluidised bed can be difficult and costly, especially for large industrial scale systems. However computational fluid dynamics (CFD) has the advantage of numerically predicting the hydrodynamics from first principles and providing

information on various quantitative and qualitative data. Correctly predicting the hydrodynamics of a bubbling fluidised bed is of particular importance as it affects operational characteristics such as particle mixing, heat transfer, elutriation rate and reaction rates.

Early two-phase modelling of bubbling gas-solid fluidised beds concentrated on the stability of the code and the physical feasibility of the numeric results such as Lyczkowski (1978), Gidaspow & Ettehadieh (1983) and Witt et al (1998). The majority of these models treated the gas and solids phases as interpenetrating continua using the constant viscosity model with experimental correlations for the pressure terms. Subsequent research (Bouillard et al (1989), Kuipers (1990)) compared the numerical predictions to experimental measurements of bubble properties and bed porosity thus providing validation for the two-phase flow equations.

Development of the kinetic theory of granular flow modified from the Chapman & Cowling's (1970) kinetic theory of gases, offered an analytical solution to the particle stress. The theory considers the effective particle stress to have contributions from both kinetic effects and short term collisional interactions. Originally adapted (Savage & Jeffery (1981), Savage (1983), Lun et al (1984)) for purely granular flows Ding & Gidaspow (1990) revised the equations to include an interstitial fluid providing closure relation for the solids stress and viscosity. However in the application of dense bubbling fluidised beds the kinetic theory assumption of instantaneous particle collisions gives way to prolonged contact and sliding between particles, which is dominated by frictional forces.

The addition of a frictional shear stress viscosity accounts for the long term particle interactions present at high solids concentrations. The majority of models implemented into two-phase flows were developed from soil mechanics (Johnson et al (1990), Boemer et al (1997), Laux (1998), van Wachem et al (2001), Srivastava & Sundaresan (2003), Patil et al (2005)) and found to improve the convergence and bed properties. However there are varying opinions on the frictional model and its implementation into kinetic theory.

The current work presents a three-dimensional frictional model developed by Dartevelle (2004) based on the yield function of Gray & Stiles (1988).

MODEL DESCRIPTION

The continuity and momentum equations used in this work assume an interpenetrating continua and form the basis of Eulerian two-fluid model. Various forms of the governing

equations have been discussed by Gidaspow (1994), Witt & Perry (1996) and Van Wachem et al (2001) and in the present study the Model A formulation, so named by Gidaspow (1994), was used where the pressure drop between phases was shared.

Governing Equations

$$\frac{\partial(\varepsilon_g \rho_g)}{\partial t} + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g) = 0 \quad (1)$$

$$\frac{\partial(\varepsilon_s \rho_s)}{\partial t} + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s) = 0 \quad (2)$$

$$\begin{aligned} \frac{\partial(\varepsilon_g \rho_g \mathbf{u}_g)}{\partial t} + \nabla \cdot [\varepsilon_g \rho_g \mathbf{u}_g \otimes \mathbf{u}_g - \varepsilon_g \mu_g \{\nabla \mathbf{u}_g + (\nabla \mathbf{u}_g)^T\}] \\ = -\varepsilon_g \nabla p + \beta(\mathbf{u}_g - \mathbf{u}_s) + \varepsilon_g \rho_g \mathbf{g} \end{aligned} \quad (3)$$

$$\begin{aligned} \frac{\partial(\varepsilon_s \rho_s \mathbf{u}_s)}{\partial t} + \nabla \cdot [\varepsilon_s \rho_s \mathbf{u}_s \otimes \mathbf{u}_s - \varepsilon_s \mu_s \{\nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T\}] \\ = -\varepsilon_s \nabla p + \beta(\mathbf{u}_g - \mathbf{u}_s) + \varepsilon_s \rho_s \mathbf{g} - \nabla \sigma_s \end{aligned} \quad (4)$$

Where

$$\sigma_s = P_s - \left(\zeta_s - \frac{2}{3} \mu_s \right) \nabla \cdot \mathbf{u} \mathbf{I}$$

Constitutive Equations

The inter-phase momentum transfer describes the drag forces between the particle and the surrounding fluid. For high particle concentrations ($\varepsilon_g < 0.8$) the inter-phase momentum coefficient Gidaspow (1994) provided an equation (eqn (5)) based on an empirical pressure drop developed by Ergun (1952). In the regions of dilute flow ($\varepsilon_g > 0.8$) the Ergun equation inter-phase momentum coefficient becomes inadequate and instead the Wen & Yu (1966) expression (eqn (6)) is used.

$$\beta = 150 \frac{(1 - \varepsilon_g)^2 \mu_g}{\varepsilon_g d_p^2} + 1.75 \frac{\rho_g |\mathbf{u}_g - \mathbf{u}_s| (1 - \varepsilon_g)}{d_p} \quad (5)$$

$$\beta = \frac{3}{4} C_d \frac{\varepsilon_g \rho_g |\mathbf{u}_g - \mathbf{u}_s| (1 - \varepsilon_g)}{d_p} \varepsilon_g^{-2.65} \quad (6)$$

$$C_d = \begin{cases} \frac{24(1 + 0.15 \text{Re}^{0.687})}{\text{Re}} & \text{Re} \leq 1000 \\ 0.44 & \text{Re} > 1000 \end{cases} \quad (7)$$

$$\text{Re} = \frac{\rho_g |\mathbf{u}_g - \mathbf{u}_s| \varepsilon_g d_p}{\mu_g} \quad (8)$$

The kinetic theory of granular flow (referred to as kinetic theory from here on) was adapted by Jenkins & Savage (1983), Lun et al (1984), and Ding and Gidaspow (1990) from the kinetic theory of dense gases (Chapman & Cowling 1970) and both are based on mono-sized particles with the same densities. Kinetic theory assumes the local

solids-phase consists of a random fluctuating velocity represented by the quantity $1/3 \langle C^2 \rangle$. This quantity named the ‘granular temperature’ (denoted here by Θ) is analogous to the thermal temperature found in the kinetic theory of gases. This is an important quantity as it is a measure of the local average fluctuating energy of the solid-phase and is obtained from the fluctuating energy equation (eqn 9).

$$\frac{3}{2} \left[\frac{\partial(\varepsilon_s \rho_s \theta)}{\partial t} + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s \theta) \right] = -\nabla p_s : \nabla \mathbf{u}_s - \nabla \cdot \mathbf{q} - \gamma_s \quad (9)$$

By assuming that the generation and dissipation of granular temperature is in equilibrium, equation (9) was simplified (Syamlal et al 1993, Boemer 1997) to give an algebraic form for the granular temperature and is used here. One of the main purposes of kinetic theory is to provide solutions for the solid phase stress terms and hence viscosity from first principles. Contributions to the solids stress tensor arise from kinetic and collisional forces that occur due to particle-particle interactions. Using the definition of granular temperature Ding & Gidaspow (1990) and Gidaspow (1994) derived equations (10-12) for solids stress, solids viscosity and solids bulk viscosity.

$$P_s^{KT} = \varepsilon_s \rho_s \theta_s + 2(1+e)\varepsilon_s^2 g_0 \rho_s \theta_s \quad (10)$$

$$\begin{aligned} \mu_s^{KT} = \frac{2}{(1+e)g_0} \left[\frac{5\sqrt{\pi}}{96} \rho_s d_s \sqrt{\theta} \right] \left[1 + \frac{4}{5}(1+e)g_0 \varepsilon_s \right] \\ + \frac{4}{5} \varepsilon_s^2 \rho_s d_s g_0 (1+e) \sqrt{\frac{\theta}{\pi}} \end{aligned} \quad (11)$$

$$\varepsilon_s^{KT} = \frac{4}{3} \varepsilon_s^2 \rho_s d_s g_0 (1+e) \sqrt{\frac{\theta}{\pi}} \quad (12)$$

The radial distribution function appears in the solids-phase kinetic theory equations and acts to prevent non-physical interaction between particles (Chapman & Cowling 1970). The function behaves as a resistance to the onset of particle compaction by tending to infinity as the particles reach maximum solids packing. There have been various forms of the radial distribution function reviewed by Boemer (1994), Van Wachem (2001) and Goldschmidt et al (2002). In the present study the Ding & Gidaspow (1990) model eqn (13) is used in the region below the maximum packing and above this limit a Taylor series expansion eqn(14) was used (Van Wachem et al 1998).

$$g_0 = \frac{3}{5} \left[1 - \left(\frac{\varepsilon_s}{\varepsilon_{s_{\max}}} \right)^{\frac{1}{3}} \right]^{-1} \quad (13)$$

$$\begin{aligned} g_0 = 1.08 \times 10^3 + 1.08 \times 10^6 (\varepsilon_s - \varepsilon_{s_{\min}}) + 1.08 \times 10^9 (\varepsilon_s - \varepsilon_{s_{\min}})^2 \\ + 1.08 \times 10^{12} (\varepsilon_s - \varepsilon_{s_{\min}})^3 \end{aligned} \quad (14)$$

Frictional Stress at High Solids Concentration

At high solids concentration ($\varepsilon > 0.5$) the interaction between adjacent particles and the dissipation of energy is predominantly of a frictional nature. In this limit there are

multiple particles sliding over each other and as a result collisions predicted by the kinetic theory of granular flow can no longer be simply considered as binary and of a short duration. This divides granular flows into at least two regimes: rapid granular flow predicted by kinetic theory and slow or quasi-static granular flow predicted by a frictional flow model. However in numerous gas-solid systems such as bubbling fluidised beds these two granular regimes simultaneously co-exist and thus a constitutive model that is able to predict both is required.

A combined kinetic theory and frictional flow theory was first implemented by the addition of the two stress tensors (eqn (15)) (Johnson & Jackson (1987)). The frictional shear stress originated from the simple two-dimensional, Coulomb yield condition and was a function of the normal stress.

$$\sigma_s = \sigma_{KineticTheory} + \sigma_{Friction} \quad (15)$$

A similar approach by Boemer et al(1997) implemented a two dimensional frictional model originally developed by Schaffer (1987). The frictional flow model consisted of a solids viscosity that was a function of the internal angle of friction, solids strain rates and the kinetic theory solids pressure. Results indicated improvement in predicted porosity profiles due to the high frictional shear viscosities in the bed. Subsequent research (van Wachem et al 2001) replaced the kinetic theory solids pressure in favour of an experimentally observed, algebraic representation of the normal stress as the bulk density increases (Johnson et al 1990) (eqn (16)).

$$P_{sf} = Fr \frac{(\epsilon_s - \epsilon_{s,min})^r}{(\epsilon_{s,max} - \epsilon_s)^s} \quad (16)$$

Laux (1998) compared viscosities terms from that used by Boemer et al (1997) based on the extended von Mises yield condition and a model developed based on the Drucker-Pager yield condition. The numerical simulations of flow in an hour glass suggested that although a frictional flow model was required to account for the frictional dominated flow, the choice of model wasn't crucial when predicting the angle of repose. Nevertheless whether this result can be said for frictional models in fluidised beds remains to be demonstrated.

A more recent frictional model by Srivastava & Sundaresan (2003) developed a three-dimensional frictional viscosity (eqn (17)) that unlike most other frictional models implemented in fluidised beds, accounted for compressibility of the solids phase. Furthermore the model includes an ad hoc expression for the particle strain rate fluctuations theorized by Savage (1998), which is a function of the particle diameter and the granular temperature. The frictional model (eqn (17)) was applied to a bubbling fluidised bed showing major differences in the bed porosity as compared to simulations without a frictional model.

$$\mu_{fs} = \frac{P_{fs} \sqrt{2} \sin \phi}{2\epsilon_s \sqrt{(\mathbf{S}:\mathbf{S}) + \frac{\Theta}{d^2}}} \quad (17)$$

A variation of the frictional flow model was introduced into a set of rheological equations proposed by Dartevelle (2004) for the application in geophysical granular flows.

The extended von Mises yield condition was modified by Gray & Stiles (1988) to provide a three dimensional yield condition that demonstrates key phenomena of quasi-static granular flow such as dilatancy, consolidation and critical state. Resembling the frictional viscosity of Srivastava & Sundaresan (2003), Dartevelle's viscosity (eqn (18)) is a function of the normal stress, internal friction angle and the magnitude of the rate of deformation. In addition to account for the particle strain rates Savage's expression was similarly added. Furthermore unlike the previous frictional flow models a bulk viscosity was formulated (eqn 19).

$$\mu_{fs} = \frac{P_{fs} \sin^2 \phi}{2\epsilon_s \sqrt{4\sin^2 \phi (\mathbf{S}:\mathbf{S}) + (\nabla \cdot \mathbf{u}_s)^2 + \left(\frac{\Theta}{d^2}\right)}} \quad (18)$$

$$\zeta_{fs} = \frac{P_{fs}}{\sqrt{4\sin^2 \phi (\mathbf{S}:\mathbf{S}) + (\nabla \cdot \mathbf{u}_s)^2 + \left(\frac{\Theta}{d^2}\right)}} \quad (19)$$

NUMERICAL SIMULATIONS

The frictional flow models were introduced into the kinetic theory of granular flow code of ANSYS CFX4.4 and compared against data from Kuipers (1990). The simulations carried out in this study were conducted in two-dimensional geometries using the Van Leer discretisation scheme. The transient simulations used a time step of 0.0002 seconds and were run for 2 seconds of real time. The conditions simulating the experiments of Kuipers (1990) are presented in Table 1.

The frictional theory was implemented in conjunction with the kinetic theory by addition of the stress tensors at a particle concentration higher than the minimum solids volume fraction ($\epsilon_{s,min}$).

The fluidised beds were initially fluidised at the specified bed height. A central jet injected air into the bed while a uniform velocity entered from the base. The boundary condition on the two side walls was set to free slip for the solids phase and no slip for the gas phase. The outlet at the top of the geometry was set to a fixed pressure boundary condition with Neumann conditions applied to the velocities.

The experiments by Kuipers (1990) consisted of a 0.57m x 1.0m pseudo two dimensional fluidised bed with a central jet of 0.015m width. The grid spacing for the numerical simulations is given in Table 1.

RESULTS / DISCUSSION

The purpose of the numerical simulations was to determine if selection of the frictional viscosity model greatly affected the behaviour of the bed. The frictional viscosity models of Dartevelle (2004) will be compared with the model of Srivastava and Sundaresan (2003).

	Property	Value
ρ_g (kg/m ³)	Gas density	1.2
μ_s (Pa.s)	Gas viscosity	1.85E-05
d_s (μ m)	Particle diameter	500
ρ_s (kg/m ³)	Solids density	2660
e	Coefficient of restitution	0.95
ϵ_{max}	Max. solids vol. fraction	0.65
$\epsilon_{s,min}$	Minimum solid volume fraction for transition to frictional model.	0.5
H_{bed} (m)	Bed Height	0.5
U_{mf} (m/s)	Min. fluidisation vel.	0.25
U_{jet} (m/s)	Jet velocity	10.0
Δx (m)	Horizontal mesh spacing	7.5E-03
Δy (m)	Vertical mesh spacing	0.01
Fr (N/m ²)	Frictional normal stress multiplier (eqn 16)	0.05
r	Frictional Constant (eqn 16)	2
s	Frictional Constant (eqn 16)	5
ϕ	Internal angle of friction.	28.5

Table 1: Physical Properties applied to numerical simulations following the experimental work of Kuipers (1990).

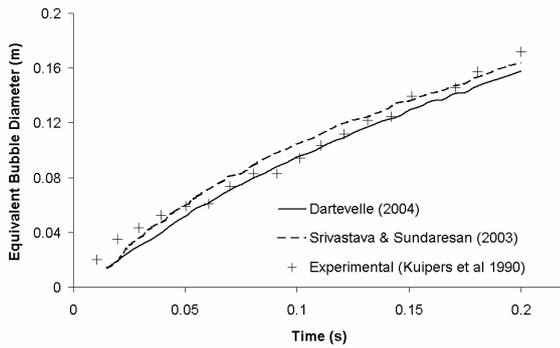


Figure 1: Comparison of equivalent bubble diameter.

The equivalent bubble diameter of Figure 1 was calculated following the work of Kuipers (1990) with a bubble boundary of 0.85 gas volume fraction. Growth of the bubble over the 0.2s period indicates both models compare well with the experimental data. Furthermore the Srivastava & Sundaresan model contains slightly more gas within the bubble than the Dartevelle model.

A comparison of frictional normal stress expressions by Patil et al (2005) suggested overestimation of the frictional normal stress causing an over prediction of gas leakage. As the frictional normal stress uses the same constants for both models it would stand to reason the difference in the results would come from the frictional viscosity. Thus the Dartevelle model predicts a higher frictional viscosity and consequently a higher gas leakage through the bubble.

The time averaged porosity profiles in Figure 2 were averaged over a 2 second period of real time. The figure shows predictions of both models below 0.4m are in good agreement with the experimental gas concentrations plotted at 0.375cm from the central axis. However higher in the bed the porosity reduces for both models which

would suggest the gas is being redistributed elsewhere. Furthermore both models experience a sharp gradient near the surface of the bed, which can also be seen at 9.375cm. The sharp gradient is more prominent in the Dartevelle model, beginning lower in the bed then rapidly increasing and overshooting the experimental measurements. This sharp rise in the gas porosity could be caused by the grid resolution having trouble predicting the rapid changes in volume fractions.

Additionally the predicted porosity profiles of both models at the horizontal position of 9.375cm under predict the porosity in the lower region of the bed. Given that the frictional stress models are added to the kinetic theory stress at or below 50% porosity, then the excess leakage of gas would be caused by the high frictional stresses. Similar graphs were found by Patil et al (2005) for the Srivastava and Sundaresan models.

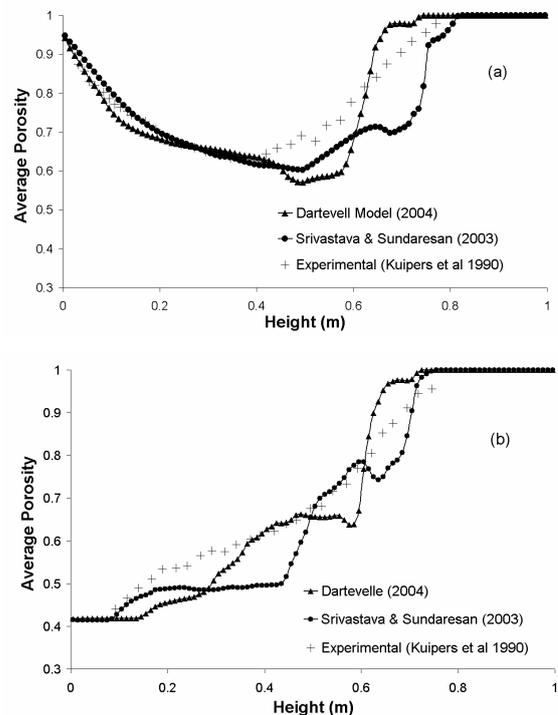


Figure 2: Average porosity profiles along the height of the bed at (a)x= 0.375cm and (b) x= 9.375cm from the central jet.

A contrast between frictional viscosity models can also be seen in the time averaged porosity plots of Figure 3. Both models show regions of very high solids concentration close to the wall with the gas concentration increasing closer to the central jet consistent with the experiment. Furthermore both models predict a similar expansion of the bed. The jetting region of the Srivastava & Sundaresan model follows a narrower central path, which as a consequence ejects particles higher into the splash region. In addition this causes a pronounced, upside-down parabolic shape of particle concentration in the central region of the Srivastava & Sundaresan model which was evident in the models reported by Patil et al (2005). In contrast the frictional viscosity of the Dartevelle model seems to allow the gas concentration to disperse and redistribute through the bed close to the central jet inlet.

Moreover it would seem from Figure 3 the inclusion of the bulk viscosity has an effect on the particle concentration at the surface region, which better resembles the experimental contours.

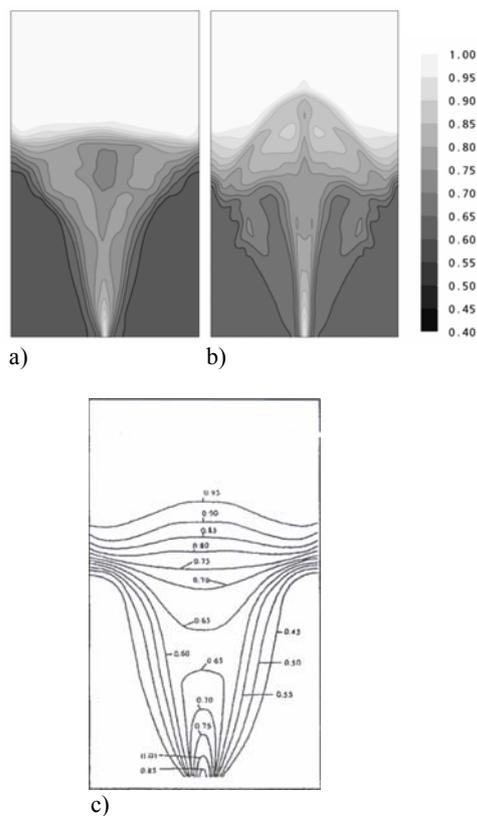


Figure 3: Time averaged (over 2 seconds) porosity contour plots of the a) Dartevelle model, b) Srivastava & Sundaresan model and c) experimental contours of Kuipers et al 1990.

A comparison in Figure 4 of the solids viscosities in the bed shows a considerable difference between the two models at 3.5 seconds. The Dartevelle model predicts very high viscosity near the wall and extends to the central jetting region. These high viscosity zones appear to be the cause of the narrow path of the central jet seen in Figure 3, slowing the radial dispersion of gas until higher in the bed. In contrast the Srivastava and Sundaresan model has smaller zones of high viscosity at the bottom corners of the bed but predicts lower viscosity in the bed, which allows the gas to disperse at greater radial distances close to the jet inlet. It is believed the bulk viscosity contribution is the cause of the higher viscosities and why the model shows better agreement to particle ejection above the bed surface in the Dartevelle model. However this will be studied further.

CONCLUSION

Various frictional models have been proposed in the literature and combined with the kinetic theory of granular flow to predict a comprehensive constitutive model of the granular flow in a bubbling fluidised bed. A new expression for the frictional stress tensor by Dartevelle (2004) that includes an explicit contribution for the bulk viscosity has been compared to the Srivastava and

Sundaresan (2003) frictional model. Both were found to have similar affects on the bubble diameter and average porosity with the Dartevelle model showing higher frictional stresses and redistribution of the gas. The Dartevelle model however was able to better predict the average particle concentration at the surface of the bed. Both models predict very high viscosities in the regions where frictional stresses are dominant, which has been attributed (Patil et al (2005)) to the normal pressure for frictional flow. An analytical expression for the normal pressure is required that could determine the stress in dilation, compression as well as at critical state.

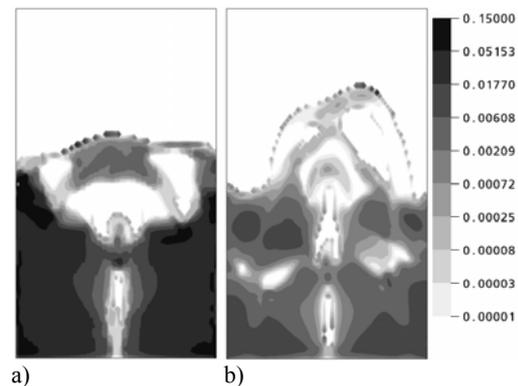


Figure 4: Comparison of average solids viscosities at 3.5 seconds; of the a) Dartevelle model and b) Srivastava and Sundaresan model.

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