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Continuum numerical simulation of multiphase granular suspension flow in the context of applications for the mechanical processing industry

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ABSTRACT

Simulation of industrial-scale, highly dynamic processes of suspensions, for example suspension flow in vertical rotating disk mills, inherit the challenge of a spatially and in-time resolved dynamic multi-phase coupling between for example the bulk material suspension and the granular beads — all in a highly dynamic setting of moving geometries. The basis of the simulation software GRAIN is the physical model for single-phase continuum granular flow of (Latz and Schmidt, 2010). It has been validated intensively and has proven its applicability to industrial processes in various cases. We describe herein the extension of that model to multiphase suspension flow, where the single continuum granular phase is coupled to the fluid phase by modeling a suspension viscosity with the goal of simulating TiO_2-suspension flow in bead mills. The beads are treated as a granular material within GRAIN and are fully coupled with the suspension flow simulation to the CoRheoS FLUID module. For vertical mills the interface between the wet suspension in the mill and the dry top region is also dynamically calculated. The simulation result in the dynamic calculation of local quantities like density distribution of suspension and beads, velocity fields, pressure distribution, shear forces for all phase and energy dissipation. Virtual performance tests are done by varying throughput rates and rotational speeds. Regarding local stresses and energy dissipation rates the grinding efficiency can be characterized.

1. Introduction

As much as CFD, and in general simulation tools, have become industry standard process and product design tools the simulation based design of products and processes involving complex rheologies has only recently started to developed towards CFD-like standards. This is especially true for processes involving granular material. Partly this is an intrinsic effect caused by the sheer complexity of the underlying physical models. Contrary to usual CFD setups, many of the physical constitutive relations for complex rheologies are nonlinear and in some cases not known for a certain material.

Hence, the simulation of such processes requires a simulation infrastructure, providing means to obtain material-and process-dependent closure relations, rather than a pure software solution. Fraunhofer ITWM in collaboration with industry and during the course of many funded research projects has developed CoRheoS, a framework for complex rheology solvers.

GRAIN is a part of the CoRheoS simulation infrastructure for the design of products and processes which involve granular media. This infrastructure consists of the software itself, based on the CoRheoS software platform as well as the characterization of actual processes and the industrially handled materials. Application areas of GRAIN include the simulation of single phase bulk handling processes, milling devices, and detailed study of the flow behavior inside silos. GRAIN can be fully dynamically coupled to CoRheoS FLUID models to simulate multiphase flows including granular material like suspension flow in ball mills, mixing of suspension as well as pneumatic transport, fluidized beds or air handling processes in silos or mixers.

We describe in this text both the physical modeling as well as, to a certain degree, the details of the numerical implementations which form the core of GRAIN. We show basic validation of this model and the numerics and finally show the applicability of our approach to industrial bead mill simulations.

2. Complex fluid dynamic modeling and numerics

The challenges concerning software for numerical simulation of industrial processes involving fluids with complex rheology especially granular media differ significantly from those in standard CFD simulation. The latter has been carried out for decades and is a well-known and established working procedure in the industry. However, for complex processes involving multi-phase flow with coupling effects and non-Newtonian fluids, standard methods cannot be directly applied. Important efforts are required to find a physical model which simultaneously describe all the relevant phenomena of the process and involve physical parameters which are easily measurable during a robust calibration procedure. Additionally, some efficient and stable numerical

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methods must be developed and implemented into a CFD or CAE-like infrastructure which allows the flexible input of functional material parameter dependencies as well as pre- and post-processing procedures.

In the following, we will present the multi-physics framework which has been developed to model suspension flow in granular beads. We will first detail the granular solver and the fluid model before detailing how the coupling between them is treated.

2.1. Single phase granular and bulk flow in GRAIN

To describe the granular phase, we employ a hydrodynamic model which has been recently developed to describe both dilute and dense granular regimes (Latz and Schmidt, 2010). This model combines the properties of the granular gas kinetic theory, a well verified theory on dilute granular systems (Brilliantov and Pöschel, 2004) and critical state plasticity, a framework widely employed for soil mechanics applications (Schoeld and Wroth, 1968). On a spatial scale which is large in comparison to the size of the grains, the balance equations for mass density ρ and momentum ρv_i are given on a Cartesian coordinate system by

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho v_i)}{\partial x_i}=0,$$
$$\frac{\partial(\rho v_i)}{\partial t}+\frac{\partial\left(\rho v_i v_j\right)}{\partial x_j}=\rho g_i-\frac{\partial P}{\partial x_i}+\frac{\partial \widetilde{\sigma}_{ij}}{\partial x_j}+\beta(u_i-v_i),$$

where $\widetilde{\sigma}_{ij}$ is the dissipative stress tensor, g_i is the gravitational acceleration. The coupling of fluid and granular phases occurs through the friction term $\beta(v_i - u_i)$ (for details see Section 2.2). The Cauchy stress tensor is given by the sum of a pressure and the dissipative term

$$\sigma_{ij}=-P\delta_{ij}+2\eta\kappa_{ij}+\zeta\kappa_{ll}\delta_{ij},$$

where η is the shear viscosity, ζ the bulk viscosity and $\kappa_{ij}=\frac{1}{2}\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right)$ the strain rate. Like in the granular kinetic theory, the granular temperature T is defined as the spatial average of the fluctuating part of the velocity and obeys the following balance equation (Latz and Schmidt, 2010).

$$\frac{\partial(\rho T)}{\partial t}+\frac{\partial(\rho v_i T)}{\partial x_j}=\frac{2}{3}\left(\sigma_{ij}\kappa_{ij}+\frac{\partial}{\partial x_i}\left(\lambda\frac{\partial T}{\partial x_i}\right)\right)-\rho\varepsilon T,$$

where λ is the heat conductivity and ε is the rate of dissipation. This equation has a similar form as the classical heat transfer equation, except the last term which accounts for the dissipation due to the inelastic collisions.

In the kinetic regime, the constitutive equations can be chosen as proposed by Bocquet et al. (2001), which was shown to provide good agreement with experimental measurements in a Couette geometry,

$$P_K=T\rho G(\rho),$$
$$\eta_K=\eta_0\sqrt{T}G(\rho),\quad \zeta_K=\zeta_0\sqrt{T}G(\rho),\quad \lambda_K=\lambda_0\sqrt{T}G(\rho),\quad \varepsilon_K=\varepsilon_0\sqrt{T}\rho^2G(\rho),$$

with $G(\rho)=\left(1-\frac{\rho}{\rho_{cp}}\right)^{-1}$, where ρ_{cp} is the random close packing, and η_0, ζ_0, λ_0, and ε_0 are material parameters.

In the dense flow regime, grains do not interact anymore through binary collision but mostly through long term contacts and the constitutive equation must be changed to describe the resulting macroscopic behavior. In a similar way as presented in Savage (1998), one can modify both the pressure and transport coefficients to capture the dense granular flow regime. The pressure can be assumed to be the sum of the kinetic one and a rate independent one P_Y which appears as a cross-over density ρ_{co}

$$P=P_K+P_Y \text{ with } \begin{cases} P_Y=0,\ \rho\le\rho_{co} \\ P_Y=T_o(\rho-\rho_{co})G(\rho),\ \rho>\rho_{co}\end{cases}$$

with T_o being a positive term which ensures that the pressure does not vanish at zero granular temperature. Viscosities, transport and dissipation coefficients are taken as

$$\eta=\eta_K\left(1+\frac{P_Y}{P_K}\right),\ \zeta=\zeta_K\left(1+\frac{P_Y}{P_K}\right)$$
$$\lambda=\lambda_K\left(1+\frac{P_Y}{P_K}\right),\ \varepsilon=\varepsilon_K\left(1+\frac{P_Y}{P_K}\right).$$

With these dependencies, both viscosities and transport coefficients increase for diminishing granular temperature, as it is generally observed in experiments (Pouliquen, 2008). Additionally, recent analytical works have shown that despite the relative simple choice of the constitutive equation, this model reproduces several key properties of granular systems like Bagnold scaling, frictional properties and the rate-independent plastic regime (Zemerli, 2013). It can be shown that in the dense limit of slow deformation, an elliptical yield surface is found as solution of the hydrodynamic equation and thus the material parameters are related to the size and the shape of the yield surface. Particularly, the internal friction angle ϕ in the critical state can be expressed as a function of the material parameters. It is given by:

$$\tan(\phi)=\sqrt{\frac{3\eta_0\varepsilon_0}{\rho}}.$$

This relation is very useful for the calibration of η_0 and ε_0 because it relates a directly measurable quantity to these parameters.

It is important to mention that the granular material is only and uniquely characterized by the macroscopic parameters ρ_{cp}, ρ_{co} η_0, ζ_0, λ_0, and ε_0. Therefore there is no assumption about microscopic particle behavior like particle shape, particle size distribution or restitution coefficient. ON the other hand, since the model is also correct in the dilute regime, it is possible (but not necessary) to use the kinetic theory for mono disperse granular balls to relate the transport coefficients η_0, ζ_0, λ_0, and ε_0 to the particle diameter and restitution coefficient for this specific case.

2.2. Flow solver-FLUID and coupling with GRAIN

The granular phase of GRAIN can be coupled with fluid phase, where the latter could be for example air, water or even non-Newtonian fluid. In this paper we will discuss the flow of the granular phase together with air-TiO_2 suspension modeled as two phase incompressible, immiscible fluid flow obeying the Navier–Stokes equations

$$\frac{\partial u_i}{\partial x_i}=0,$$
$$\rho_f\frac{\partial u_i}{\partial t}+\rho_f u_i\frac{\partial u_j}{\partial x_j}=\rho_f g_i-\frac{\partial P}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\eta_f\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)\right)+\beta(v_i-u_i),$$

where u_i is the fluid velocity, ρ_f fluid density and η_f fluid viscosity. The total density and viscosity of the fluid are given as the linear combination of the suspension and air densities and viscosities respectively

$$\rho_f=\alpha\rho_{TiO_2}+(1-\alpha)\rho_{air}$$
$$\eta_f=\alpha\eta_{TiO_2}+(1-\alpha)\eta_{air}$$

where α is the volume fraction of the TiO_2. Fluid equations are discretized with a finite volume scheme and solved with use of Chorin's projection type method (Niedziela et al., 2013). The coupling of fluid