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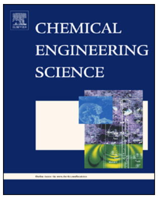

Modification of kinetic theory of granular flow for frictional spheres, Part I: Two-fluid model derivation and numerical implementation

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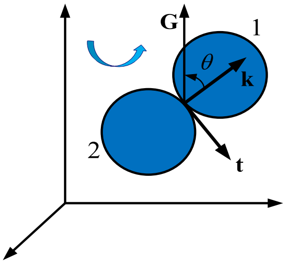
HIGHLIGHTS

- A kinetic theory of granular flow is derived for 3D frictional spheres in dense systems.
- The Chapman–Enskog approach of successive approximations is used.
- A balance equation for the rotational granular temperature is derived.
- The stress tensor contains anti-symmetric components associated with a rotational viscosity.

GRAPHICAL ABSTRACT



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ABSTRACT

We derive a kinetic theory of granular flow (KTGF) for frictional spheres in dense systems, including rotation, sliding and sticking collisions. We use the Chapman–Enskog solution procedure of successive approximations, where the single-particle velocity distribution is assumed to be nearly Maxwellian both translationally and rotationally, as assumed by McCoy et al. (1966). An expression for the first-order particle velocity distribution function is derived, which includes the effects of particle rotation and friction. Using a simple moment method, balance equations for mass, momentum and energy are derived with closure equations for viscosities, and thermal conductivities and collisional energy dissipation rates of angular and translational kinetic energy. Because the internal angular momentum changes are coupled to the flow field, the stress tensor contains anti-symmetric components which are associated with a rotational viscosity. In the resulting closure equations, the rheological properties of the particles are explicitly described in terms of the friction coefficient. The model has been incorporated into our in-house two-fluid model (TFM) code for the modeling of dense gas–solid fluidized beds. For verification, a comparison of the present model in the limit of zero friction with the original (frictionless) KTGF model is carried out. Simulation results of both models agree well. In the next part, simulation results obtained with the new model will be compared with experimental data and discrete particle model (DPM) simulations.

1. Introduction

Gas–solid fluidized beds find a widespread application in processes involving combustion, separation, classification, and catalytic cracking (Davidson et al., 1985; Kunii and Levenspiel, 1991). Understanding the dynamics of fluidized beds is a key issue in improving efficiency, reliability and scale-up. Owning to enormous increase in computer power and algorithm development, fundamental modeling of multiphase reactors has become an effective tool.

For larger scale applications, the Euler–Euler approach (Kuipers et al., 1992; Gidaspow, 1994; Lu and Gidaspow, 2003; Lu et al.,

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Nomenclature

$\mathbf{c}$	translational particle velocity, m/s
$\mathbf{v}$	mean particle translational velocity, m/s
$\mathbf{C}$	translational fluctuating particle velocity, m/s
$\mathbf{c}'$	translational particle velocity after collision, m/s
$\mathbf{G}$	relative particle velocity at contact point, m/s
$\mathbf{J}$	impulse force, kg m/s
$\mathbf{k}$	unit normal vector at contact point
$\mathbf{j}$	unit tangential vector at contact point
$\mathbf{F}$	external body force (acceleration) acting on the particle, m/s^2
$\mathbf{T}$	external torque (angular acceleration) acting on the particle, rad/s^2
$\mathbf{g}$	gravitational acceleration, m/s^2
$\mathbf{r}$	position of the particle, m
$f^{(0)}$	single particle distribution function, first approximation (Maxwellian)
$f^{(1)}$	single particle distribution function, second approximation
$f^{(2)}$	pair particle distribution function
I	moment of inertia, kg m^2
m	mass of the particle, kg
n	particle number density, m^{-3}
U_{mf}	minimum fluidization velocity, m/s
e	normal restitution coefficient

Greek

ρ	density, kg/m^3
Θ	granular temperature, m^2/s^2
β_0	tangential restitution coefficient
σ	particle diameter, m
γ	energy dissipation rate, J/(m^3 s)
β_A	inter-phase momentum transfer coefficient, kg/(m^3 s)
$\boldsymbol{\tau}$	stress tensor (Pa)
ε	volume fraction
$\boldsymbol{\omega}$	rotational velocity, rad/s
κ	thermal conductivity, kg/(m s)
χ_c	collisional source of particle properties
θ_c	collisional flux of particle properties
$\boldsymbol{\Omega}$	rotational fluctuating particle velocity, rad/s
μ_t	translational shear viscosity, kg/(m s)

Subscript

1	particle 1
2	particle 2
s	solid phase
r	rotational contribution
i	coordinate direction i
j	coordinate direction j
k	coordinate direction k
n	normal direction
w	wall

2003) is considered to be the most effective. The so-called two-fluid model (TFM) has emerged as a very promising tool as a result of its compromise between computational cost and amount of detail provided. In TFM, both the gas phase and the solid phase are treated as fully interpenetrating continua and are described by separate governing balance equations of mass and momentum. The challenge of the model is to establish an accurate hydrodynamic and rheological description of the solid phase. State-of-the-art closures have been obtained from the kinetic theory of granular flow, initiated by Jenkins and Savage (1983), Lun et al. (1984), Jenkins and Richman (1985), Lun and Savage (1987), Ding and Gidaspow (1990), Lun (1991), and Nieuwland (1995). This theory is based on the classical kinetic theory of dense gases (Chapman and Cowling, 1970).

The original KTGF models of Jenkins and Savage (1983), Lun et al. (1984), Jenkins and Richman (1985) and Gidaspow (1994) are derived for frictionless and nearly elastic particles with translational motion only. Various extension have been proposed. For example, Sun et al. (2009) presented a KTGF with anisotropic second-order velocity moments for inelastic and frictionless particles. An extra model for the third-order velocity moment was used to close the equations for the second-order velocity moments. With this they predicted that in a fluidized bed the simulated second-order moment in the vertical direction is 1.1–2.5 (or even 4 for small particles) times larger than the second moment in the lateral direction. It was found that the relatively large anisotropy values always occurred at sufficiently dilute conditions. Similarly, Chen et al. (2012) found obvious anisotropy in the second moments in dilute riser flow. In dense gas–solid fluidized beds the anisotropy in the second velocity moments is much weaker however. In the present work we focus on applications in dense gas–solid fluidized beds. We will therefore assume that the second moments can be described by an isotropic granular temperature combined with relatively small deviations which are controlled, as we will show in this paper, by gradients in the average velocity field.

As mentioned above, most KTGF models focus on frictionless particles. In reality, however, granular materials are frictional. The roughness of the granular materials has been shown to have a significant effect on stresses at least in the quasi-static regime (Sun and Sundaresan, 2011). After a binary collision between rough particles, the particles can rotate due to surface friction. Thus, translational kinetic energy may exchange with rotational kinetic energy. Attempts to quantify the friction effect have been somewhat limited.

Lun and Savage (1987) developed a kinetic theory for a system of inelastic, rough spherical particles to study the effects of particle surface friction and rotational inertia. Two collisional parameters were used. One was the normal restitution coefficient and the other was the roughness coefficient to characterize the effects of surface friction. In their theory only dense systems, where the major stress contribution arises from particle collisions, was considered. However, at low solids concentrations the kinetic stress contribution becomes dominant. Lun (1991) extended the kinetic theory to be appropriate for both dilute and dense granular flows including kinetic as well as collisional contributions for stresses and energy fluxes. Translational and rotational granular temperatures were involved to characterize the kinetic fluctuation energies. An extra energy balance equation for the rotational granular temperature was derived. Goldshtein and Shapiro (1995) developed a kinetic theory for rough inelastic spheres combining the translational and rotational granular temperatures into a total granular temperature. Their theory has been improved by Wang et al. (2012a, 2012b) to develop kinetic theory for granular flow of rough spheres. Chou and Richman (1998) derived a theory for homogeneous shear flows of identical, smooth and highly inelastic spheres in which the solids volume fraction, mean velocity and each component of the full second moment of fluctuation

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