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Load-Dependent Contact Mechanics of Particulate Assemblies: Multi-Variant Particle Size, Shape and Surface Roughness in Advanced Materials and Process Applications

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Highlights not included as per agreement with Editor

ABSTRACT Many of the industrial manufacturing processes of particulate materials are presently modeled using Discrete Element Models, (DEM), and in some instances hybrid multi-phase models combining DEM with CFD and other hydrodynamic variants, see Chareyre^[1], Mehta^[2]. The early tribology work in 80's and 90's on load-dependent particle contact mechanics for use in computational algorithms relied on considerations of single-point contacts between smooth elastic and rigid-plastic spheres and curvilinear surface contacts between cylindrical shapes; see Johnson^[3]. Later developments included multiple-asperity surface contacts and elastic/plastic surface interactions as well as contact angle variations; see Tuzun et al^{[4][5][6]} that include many other references. In this paper, the established theoretical framework is reviewed first for calculating bulk assembly stresses and bulk shear patterns from single-particle contact mechanics highlighting the importance of the particle shape, size and surface roughness. Subsequently, illustrations are provided of the effects of relaxing the assumptions of mono-disperse particle size and shape on the bulk shear patterns observed during slow-shearing, packed assembly flows as seen in chutes and hoppers and in particle heaps respectively. Finally, an analogy is provided between the studies of the deformation response of material composites comprising of particles embedded within a matrix structure to sustained stress-loading and unloading cycles; see Hull and Clyne^[7] and those observed in flowing particle assemblies under compression and shear. Such an analogy can be particularly useful in predicting the flow behaviour of particles "tailor-made" for advanced functionality commonly encountered in applications as widely ranging as multi-phase catalytic reactors and separators, drug manufacture, renewable energy production and storage and in chemical and physical abatement of harmful environmental emissions.

Keywords: granular flows, composites, particulate chemical process modeling

MATERIAL AND PROCESS SIMULATION STRATEGIES

With the advancement of high-speed large-scale computer simulations of process flows, industrial applications being addressed demand simulations involving ever increasing complexity of particle shapes and sizes and in some cases with functional internal micro-structures to provide advanced functionality; see for example Cleary and Tuzun^[8], Biggs et al^[9].

In many simulation models, core algorithms firstly aim to define the physical interactions between adjacent particles in terms of the particle properties and those of the surrounding fluid. In gravity-driven packed-bed flows of coarse granular matter typically with particle sizes > 0.5 mm, the pressure losses due to hydrodynamic interactions between the particles and the carrier fluid are considered to be negligible where the viscous drag due to "skin friction" is inversely proportional to the square of the particle size as illustrated by the well-known Carman-Kozeny Equation;-

$$-\Delta P/L = C(\epsilon, S) \cdot \mu U / \epsilon d_p^2 \quad (1)$$

where $\Delta P/L$ denotes the pore pressure gradient over a characteristic length, L ; U/ϵ is the relative velocity between the solids and the percolating fluid of kinematic viscosity, μ . The function, $C(\epsilon, S)$ is related to the bed porosity (interstitial voidage), ϵ

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