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A two dimensional combined discrete and finite element scheme for simulating the flow and compaction of systems comprising irregular particulates

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Abstract

The paper describes the development and application of a combined discrete finite element scheme to simulate the flow and compaction of irregular randomly packed particles to form a tabletted product. The techniques which have been adopted to achieve computational efficiency are described. These include contact detection, particle level deformation analysis and the presentation of results via a homogenisation strategy.

The computing scheme in question is validated against published data and is shown to be capable of simulating the expected trends associated with the effects of particle shape, size and friction on the flow rate. The flow simulations also exhibit noticeable differences when compared with a geometric packing model. Over the relevant compaction regime, for which elastic behaviour is applicable, the present scheme also compares well with published work that uses a distinct element simulation approach and with experimental data. The advantage of the current scheme is the flexibility that it offers to capture a mixture of material properties and particle shape and that no restrictions are necessary on the contact models since these are integral in the calculation procedures.

Keywords: Discrete element; Finite element; Contact detection; Viscoelasticity; Homogenisation

1. Introduction

A very large range of products are manufactured using particulate processing.[1] These include tablets, for example, pharmaceutical, food and domestic products together with a diverse range of engineering components. In pharmaceutical applications the tablets are generally simple in shape, but the powder mixture may be complex in nature. Whereas for engineering components, the shapes are becoming increasingly complex, but the powder itself is comparatively simple. In all instances, processing involves powder flow. The starting point is flow from a silo or hopper and the finishing point is die filling. This is subsequently followed by compaction. There is a growing industrial awareness that a detailed understanding of these stages in the processing cycle is becoming increasingly important in order to guide process improvement and optimize the end product. The current paper reports on the development of a combined discrete and finite element scheme for simulating the flow and compaction in powder systems which may well include both regular and irregular particle geometries. A review of the most pertinent published works is given which is followed by a brief description of the

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[1] In this work, particulate will be used to describe both powder and granulate systems.

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combined discrete and finite element scheme. The computational algorithm will then be illustrated via a number of case studies which will include both flow and compaction processes.

2. Review of relevant literature

2.1. Powder flow

Numerical techniques have been developed to simulate powder flows over a range of length scales. For example, previous work has included applications, such as drag line bucket filling [1], silo filling [2] and hopper flows [3]. Extensive studies have focused on silo filling since these are well documented and often form a good case study [2]. Other more complex examples include the die filling stage in powder forming. This is an extremely difficult problem due to the particle size range, complex cavity geometry and the need to account for the flow of both particulate and air phases [4]. Exhausting air from the die is particularly important for the filling process when fine particles are involved as the air is known to impede the flow into the die. The ultimate aim of this type of simulation is to determine the initial fill density which is known to have a marked impact on the green density of the compact, especially for multilevel component shapes.

Simulation of particulate type flows have been carried out principally using discrete element techniques and references [5,6] provide a full overview of previous studies. Early work focused on two dimensional simulations, but with the development in computing speed there are a number of instances where three dimensional analyses have been undertaken. These rely on a parallel code structure to achieve realistic simulation times for more complex geometries [5].

Despite this progress, a number of developments are still required to enhance discrete element simulation for particulate flow problems. For example, many previous studies have focused on spheres (or cylinders in two dimensions), monosize distributions and single materials, as opposed to mixtures. Many analyses have been concerned with predicting the kinematic behaviour accounting for various contact mechanisms. However, the majority of simulations do not calculate the stresses that occur within each particle. Computing the stress state within the particulate is relevant when mechanical damage of the particulate is to be avoided. Stresses arising from contact may also be important in conveying applications where collision during flow along a conveyor could lead to product damage. The complexity arises when there is a requirement to calculate the stress state within each particle and this will need to respond to the loads that are applied at the contacts between the particles themselves and also between the particles and rigid surfaces. An example implementation is set out in [7] in which discrete simulations are coupled with a finite element deformation analysis of discrete bodies. This was aimed at masonry structures comprising large blocks having restricted movement, unless collapse occurs. Examples of application at the particulate scale are also set out in [8] in which particle yielding effects are also included. The experience gained from these simulations highlights the computational demands, for example, even two dimensional simulations comprising typically hundreds of particles requires several hours of computing time on scalar PC platforms.

2.2. Powder compaction

Simulation of the compaction stage is important for a number of reasons. In engineering products, it is necessary to establish the density uniformity that is required to ensure that sintering shrinkage is controlled, or to establish the likelihood of crack formation within the compact. In a tabletted product, the density uniformity is important to ensure control of the dissolution rate, whereas a knowledge of the stress levels within the particles is important to prevent their failure. The stress intensity may be controlled by the addition of particulates with a lower modulus of elasticity, thus designing the mixture response to the compaction process. Also, where the deformation is significant, the contact area between particles will provide an indication of the tablet strength [9].

Compaction modelling provides a method whereby the stress and density state within the tablet may be predicted whilst also accounting for the rheological characterisation, particle size, size distribution and mixture proportions. These materials exhibit nonlinear characteristics due to large scale deformation and in some cases a rate dependent behaviour is also observed. Also the interaction between each particle and between the particles and the tooling may also exhibit nonlinear laws.

Despite these complexities, compaction simulation has been tackled using two different schemes. The first has been applied extensively to compaction simulation for engineering components where a continuum-based finite element model, derived from geomechanics applications was utilised [10,11]. Recently, this approach has also been extended to pharmaceutical systems [12]. An alternative approach is to use the discrete element method, first developed by Cundall and Strack [13]. In common with continuum simulations, this development was also motivated by geotechnical research. The early discrete element method treated each particle as a rigid body with no deformation being allowed. Later models have incorporated contact laws that range from Hertzian through to plastic behaviour and these are often derived from studying interactions between regular particles [14]. Some studies [15] have also attempted to integrate the discrete and continuum schemes by modeling material behaviour at the particulate scale and to combine this with continuum simulations in order