Research Statement (Aibing Yu BEng MEng PhD DSc FTSE FIChemE)

Much of our environment, and the benefits that we derive from our surroundings, are strongly influenced by the interactions of the three primary phases of matter - solids, liquids, and gases. These interactions often occur at surfaces, with the individual phases being discrete in form. Particles and powders, which can be either wet or dry, and range in size from nanometers to centimeters, are one very important example of such a multiphase system. They have properties that are characteristic of each of the three primary phases. That is, they can withstand deformation like solids, flow like a liquid and exhibit compressibility like a gas. These features give rise to another state of matter - **particulate/granular matter** - that is poorly understood, posing a challenge to the scientific and engineering community for years.[1]

Therefore, understanding and modelling the physics of this matter has been a major research focus worldwide. However, progress in this area has been slow in the past. As pointed out by de Gennes, the Nobel Prize Laureate 1991, "granular matter, in 1998, is at the level of solid-state physics in 1930".[2] Particulate and multiphase processing rarely reach more than 60% of the design capacity because of inadequate understanding of the fundamentals.[3] Although widely used, many processes are actually operated as "black box" reactors. In fact, limited by the research techniques, previous work has mainly been targeted on a large scale and focusing on phenomenological descriptions, but rarely touching on the basic fundamentals. This is evidenced by the study of the dynamics of a particulate system which includes at least three aspects: velocity, structure and force. Previous studies have been limited to velocity because of the difficulty in obtaining information for the other two. In fact, the newly developed Positron Emission Particle Tracking (PEPT) and Nuclear Magnetic Resonance cannot provide any information about the interaction forces;[4] and scientists are still searching for a technique for measuring such forces even just on the external surfaces of a particle system.[5] Consequently, there have been problems in probing the underlying physics and solving practical problems reliably.

How to overcome this problem has become one of the most important research areas in particulate research. To date, probably the only technique that can overcome this problem is computer simulation, particularly based on **Discrete Particle Simulation (DPS)**. The concept involved is simple: it considers a finite number of discrete particles interacting by means of contact and non-contact forces, and every particle is described by Newton's equations of motion (when coupled with fluid flow, **Computational Fluid Dynamics (CFD)** should also be used to describe the flow of fluid(s)). Then, by tracing the motion of all the particles in a considered system, the

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[1] See, for example, Jaeger HM, Nagel SR, 1992, Physics of the granular state, Science, 255, 1523-1531; Jaeger HM, Nagel SR and Behringer RP, 1996, Granular solids, liquids, and gases, Reviews of Modern Physics, 68, 1259-1273.

[2] de Gennes PG, 1999, Granular matter: a tentative view, Reviews of Modern Physics, 71, s374-s382.

[3] Merrow EW, 1985, Linking R&D with problems experienced in solids processing, Chemical Engineering Progress, 81, 14-22; Ennis BJ, Green G, and Davies R, 1994, The legacy of neglect in the U.S., Chemical Engineering Progress, 90, 32-43.

[4] Parker D J, Broadbent CJ, Fowles P, Hawkesworth MR and McNeil PA, 1993, Positron emitting tracking - a technique for studying flow with in engineering equipment. Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors & Associated Equipment, 326, 583-592; Gladden LF, 2003, Magnetic resonance: Ongoing and future role in chemical engineering research, AIChE Journal, 49, 2-9.

[5] Majmudar TS, Behringer RP, 2005, Contact force measurements and stress-induced anisotropy in granular materials, Nature, 435, 1079-1082.

dynamics information - key for fundamental understanding - can be generated. Although it sounds simple and straightforward, the implementation of this approach requires comprehensive knowledge and skills from a broad range of disciplines including mathematics, physics, engineering and computational technology.

Such a multidisciplinary approach is indeed reflected in Prof Yu's research **"simulation and modelling of particulate systems"**. It aims to understand and model the physics governing particulate and multiphase processing, with its application oriented to mineral/metallurgical/material/chemical industries. Over years his research team at UNSW has developed a sustainable and systematic way to study particulate matter at various time and length scales including, for example, the determination of contact forces between particles at an atomic or sub-particle scale, dynamics of particles at a particle scale, and performance of an operational unit at a process equipment scale. The outcomes of his research include theories, computer models and simulation techniques, and knowledge at both microscopic and macroscopic levels; hence the implications are both extensive and generic. Such mutltiscale research is critical to advancing particle science and technology, as well as process technology. The resulting breakthroughs have led to extensive publications in this field, which also represent his research contributions in particle packing and flow. The major contributions are highlighted below:

(a) Particle packing and transport properties

- The packing of spherical particles: identified the packing mechanisms and developed mathematical models, corresponding to these mechanisms, to predict the relationship between porosity or packing density and particle size distribution, which has been widely used for property and/or process control in practice;
- The packing of non-spherical particles: established the similarity between spherical and non-spherical particle packings, and on this basis developed an effective method to evaluate the packing characteristics of non-spherical particles and formulated a mathematical model, by transforming that developed for spherical particles, to describe the packing of non-spherical particle mixtures as a function of size and shape distributions;
- The packing of cohesive fine/wet particles: identified the governing mechanisms in terms of microscopic cohesive (van der Waals and capillary) forces, proposed a model framework for modelling this complicated packing system, on this basis formulated mathematical models, the only ones in the literature, to estimate the porosity of mixtures of fine or wet particles;
- Computer simulation: developed a simulation technique, in connection with the DPS development for granular dynamics, to simulate the packing dynamics of particles, which can explicitly consider the interparticle forces including van der Waals cohesion and/or capillary force and related dynamic variables, offering an effective way to generate reliable structural results under different conditions; and
- Structural analysis and modelling: developed an effective method for analysing the randomness and connectivity of particle packing, and applied various simulation techniques to study structural properties of particle packing in

relation to process/products control, and liquid and glassy structures; and developed a new method for evaluation of transport properties in porous media such as permeability (related to pore connectivity) and effective thermal conductivity (related to particle connectivity) at pore or particle scale, opening up a new direction to understand and analyse the transport mechanisms in porous media.

(b) Particle and multi-phase flow

- Discrete particle simulation (DPS): developed novel techniques, including the determination of interparticle forces/torques, for DPS simulation to study important operations such as granulation, mixing and stockpiling to conduct effectively particle scale research; quantified the flow and force structures under various flow/operation conditions, which are critical to understanding the mechanisms governing particle flow but not possibly to be obtained experimentally;
- Particle-fluid flow simulation: developed and validated a comprehensive theory to combine the continuum-based (Computational Fluid Dynamics) model for fluid phase and the discrete-based (Discrete Particle Simulation) model for solid phase; the DPS-CFD modeling technique is now widely accepted as a most effective way to study the fundamentals governing the particle-fluid or multiphase flow at the individual particle level.
- Local average theory: proposed an averaging technique to link microscopic variables at particle scale to macroscopic variables for continuum modelling, and applied this novel technique to analyse particle flow and, after extension, to particle-fluid flow under different conditions;
- Particle flow: developed a new computational mathematical (continuum-based) model to describe the solids flow under complicated conditions (e.g. coupled gas-solid flow in a blast furnace and hopper flow involving different flow regimes), and proposed a method to determine the transition between moving and non-moving particles, ie the profile of stagnant zone; the work in this direction continues with the new developments above; and
- Multiphase flow: identified the mechanisms governing the powder entrapment in a multi-phase flow packed bed (counter-current gas/powder (upward) and liquid (downward) flow) and proposed an effective experimental technique to quantify the interactions between powder and other phases, developed mathematical models to describe gas-liquid, gas-powder, and gas-liquid-powder-solid flows; and continued developing new theories for multiphase flow modelling.

(c) Process modelling and optimisation

- Bulk density prediction and control of coal in coke making: formulated a predictive model to calculate bulk density of coal as a function of particle size distribution, moisture content and oil addition, and proposing a cost-effective method for the control of bulk density of coal and its distribution in a coke oven;
- Porosity and permeability prediction and control: proposed comprehensive models to predict porosity and permeability as a function of particle characteristics such as particle size and shape distributions under different

conditions, which are useful for property and/or process control in powder processing and advanced materials (ceramic/composite) manufacturing;

- Modelling of multi-phase flow in a blast furnace: developed and validated computer models (e.g. models for gas-powder, gas-liquid, gas-solid two-phase flows) to describe the so-called four-fluid flow or gas-powder-liquid flow in moving particles under blast furnace conditions, leading to the development of better control/design strategy for blast furnace practice; and
- Simulation of mineral processes: Applied the newly developed modelling techniques to simulate various processes in mineral industries, including powder flow and mixing, stockpiling, sedimentation, filtration, grinding and granulation, fluidization, pneumatic conveying, and (gas-, hydro- and dense medium) cyclones, to understand the fundamentals and formulate strategies for process design, control and optimization.

In addition, research has been expanded to newly emerging areas including, for example, the development of sensors for combustible gases, synthesis and application of nanoparticles, molecular modelling of organoclays/nanocomposites, the crystal formation of aluminium in rapid cooling, and theories for particle-structure-property relations. Such research effort is very much in connection with his work on particles, and the focus has been to understand why and how atoms and particles behave differently because of the different forces in time and length scales.