Modelling of reacting flows and industry applications: some examples

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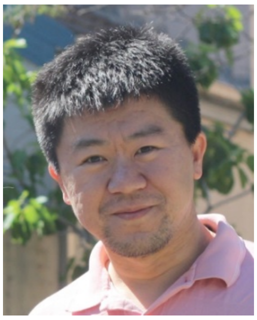
Abstract

Process design and control plays a significant role in modern industries. Most processes and reactors are very complex, as they usually involve not only multiphase flows but also heat and mass transfers related to chemical reactions and their interactions. The operation must be optimized in order to be competitive and sustainable, particularly under the more and more demanding economic and environmental conditions. This will need continuous innovative research and development. Computer simulation and modelling, supported by experiments, has emerged as an indispensable adjunct to the traditional modes of investigation for design, control and optimization of processes, reactors, and devices. In this presentation, A/Prof. Shen will report his core research on process modelling and design of reacting flows and the applications to a range of complex processes and reactors in conventional and emerging industries. Several examples of industry applications will be used for demonstration, including process metallurgy, coal preparation and utilization. The modelling works are indeed helpful to understand fundamentals and optimize & develop new, cleaner and more efficient technologies with measurable industrial outcomes.

Biography



Dr Yansong Shen is an Associate Professor in School of Chemical Engineering at University of New South Wales (tenured). He obtained his BEng and MEng degrees in Northeastern University (China) and PhD degree in UNSW. His research interests include process modelling and simulation and its applications in resource and energy sectors. He published over 100 peer-reviewed papers in top-tier multidisciplinary journals, secures 7 ARC and 5 ACARP/ARENA grants to date, in total over AUD 4M, established industry engagements in Australia and overseas, and won several honours/fellowships e.g. ARC APDI Fellowship and ATSE Emerging Future Leaders in Low Emissions Coal Technology Fellowship. His group designed and scaled-up several new technologies of iron ore and coal utilization and reactor design which have been implemented and practiced with measurable benefits. He is selected as Chartered member IChemE, TMS, AIST, and invited/plenary speakers in several international conferences.

Modelling and Simulation of Packing and Flow of Ellipsoidal Particles

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Abstract

Particle shape is one of the most important properties of granular materials, and it affects the packing and flow structures that are critical to transport properties such as permeability related to pore connection and thermal conductivity related to particle connection. Particle shape can be regular or irregular. To be more quantitative, recent studies are focused on particles of well-defined shapes. In particular, ellipsoids has attracted a lot of attention in recent years as it can represent a large number of shapes, e.g. from platy to elongated. In this presentation, a brief review is given on studies of ellipsoidal particles done at SIMPAS in the past years (for example, as shown in Figure 1), including particle packing, granular flow such as hoppers/rotating drums, and gas/liquid fluidizations. Key findings are shown by illustrating how particle shape affects packing and flow behavior of ellipsoids. The results demonstrate that discrete element method for ellipsoids provides an effective approach for fundamental understanding of particle shape effect on granular packing and flow.

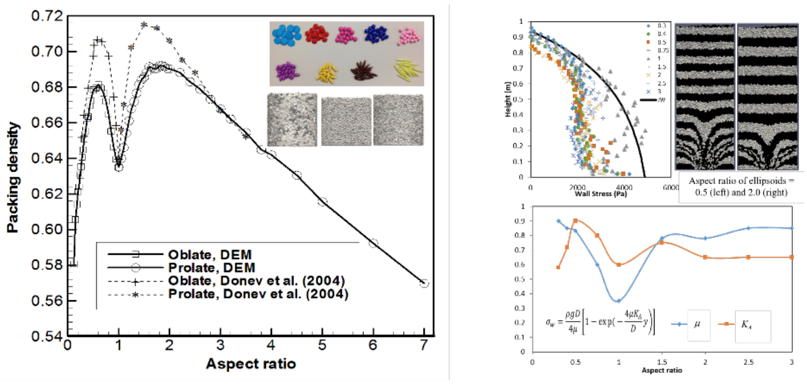

Figure 1: Relationship of packing density with aspect ratio (left) and stresses acting on side walls in a hopper.

Biography

Dr Zhou obtained his PhD in 2007 from UNSW, currently is a senior lecturer at Monash University and vice director of ARC Research Hub for Computational Particle Technology. His research expertise is in modelling and simulation of granular flow/dynamics and multiphase flow and heat transfer in various particulate systems in mineral, metallurgical and manufacturing industries. His significant contributions in the community of particle research include theoretical developments of CFD-DEM coupling approach, discrete approach for multiphase heat/mass transfer modelling, and non-spherical particles. Dr Zhou has successfully won many major ARC grants, and published more than 100 journal and conference papers with citations more than 3400 times, and h-index of 23 (SCOPUS data).

DEM-based models for flow, heat and mass transfer and chemical reactions in gas-solid flows

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Abstract

Intensive heat and mass transfer between continuum fluids and discrete particulate materials is quite common in many chemical processes. To understand and improve the operation of these processes, discrete particle models are very helpful when they are combined with flow, heat and mass transfer and chemical reaction models. However, due to the high computational cost with discrete particle models, it is not practical until now to study long transient processes. A transient discrete element method-based is developed recently through scaling and allows the study of the transient process at a particle scale. The scaled model can simulate the process faster (~two orders) and makes it practical to track long and transient process such as iron ore reduction from burden charge to the cohesive zone. This work will introduce the transient discrete element method and its applications. The results demonstrate that the scaled model can reasonably predict flow state, temperature distribution, and chemical reactions.

Brief Biography

Dr Qinfu Hou is an Australian Research Council (ARC) DECRA (Discovery Early Career Researcher Award) Fellow in the Department of Chemical Engineering of Monash University Australia. He was awarded a PhD in 2012 at UNSW Australia, ME and BE in 2003 and 2000 respectively at Northeastern University of China. Dr Hou has published 70+ articles in various prestigious journals and proceedings including Energy & Environmental Science (Impact Factor: 33.250). Dr Hou secured more than AUD$2M research funds from different sources including ARC. Dr Hou has also received various awards in the past, reflecting the recognition at different stages, and been invited to give plenary/keynote talks at different international conferences. Aiming to formulate safer, smarter, more sustainable and energy-efficient processes involving granular materials, his research mission centres in unravelling fantastic mechanics and thermochemical behaviours of granular (and multiphase) flows through rigorous cutting-edge multiscale modelling techniques, experiments and theoretical analysis. His main research areas include: (i) heat/mass transfer and chemical reactions in packed and fluidized beds, (ii) multiphase flows in water treatment, (iii) granular flow stability pertinent to segregation and mixing, and (iv) development of numerical techniques and virtual process models.

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Dense Medium Cyclones: from Fundamental Simulation to Process Optimisation

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Abstract

Dense Medium Cyclone (DMC) is a high-tonnage device that has been widely used in the Australian coal industry to upgrade run-of mine coal in the 0.5-50 mm size range. Its working principle is simple, however, the flow in a DMC is very complicated because of the presence of swirling turbulence, air core and segregation, and involves multi phases: gas, liquid, solid and medium particles of different sizes. It is known that a small improvement on the performance of DMC may greatly enhance industrial profitability. Therefore, it is very useful to develop an effective method to help optimize the design and operation of DMCs. Some efforts have been made to experimentally study the flow in a dense medium cyclone, but such an experimental method is technically difficult and expensive. Recently, based on the numerical experiments performed by Computational Fluid Dynamics (CFD) and its combination with Discrete Element Method (DEM), we have established a PC-based mathematical model that is promising to achieve this design and operational goal. It is found that this DMC model can indeed offer a convenient way for optimum design or operation of DMCs under different conditions.

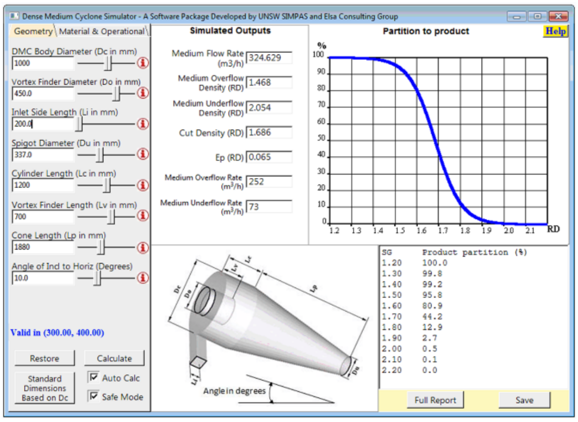

Figure 1. DMC simulator interface.

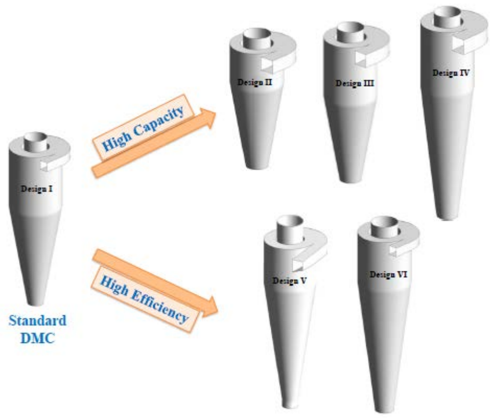

Figure 2. Optimization of DMC designs.

Biography

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Qualification:

PhD School of Material Science and Engineering
2010-2014 University of New South Wales, Australia
Supervisor: Professor Aibing Yu
MEng School of Material Science and Engineering
2009-2010 University of New South Wales, Australia

Supervisor: Professor Aibing Yu
BEng School of Materials Science and Engineering
2003-2007 Tongji University, P.R. China

Career:

10/14 -present Research Fellow, Department of Chemical Engineering, Monash University, Australia
04/14 –06/16 Research Associate, School of Materials Science and Engineering, University of New South Wales, Australia

Awards/Prizes/Distinctions:

2010-13 Australia Postgraduate Award Industry (APAI)
2010-13 UNSW International Research Scholarship (Tuition Fee Remission)
2011.9 5 minutes Postgraduate Presentation Competition - Winner for Round 6 (School of Materials Science & Engineering, UNSW)
2013 Membership (Material Engineer), Engineer Australia (EA)
2014 Contestant, Third prize of Start-up Competition (Suzhou, China)

Professional Experience:

My current research is devoted to the numerical simulation of multiphase flows in both fundamental and applied levels. These research activities directly impact in a wide range of application fields in the coal sectors but also indirectly in other fields, like the chemical engineering sectors. I have focused in the use of ANSYS Fluent CFD tools (combined with DEM) both for academic as well as for industrial consultancy purpose. I have been involved in a variety of national and international research projects and industrial consultancies.

Research Interests

- Particle/Powder Technology
- Multiphase System
- Process Modelling, Simulation and Optimisation
- Physical Separation
- PM2.5 Collection and Clean Coal Technology

Industry Experience/Research Projects

- **Project Member:** CFD study of Dense Medium Cyclone, *Australian Coal Association Research Program (ACARP) Projects C16043 and C29035, Australia* (2009-2011)
- **Project Consultant:** Optimize cyclones using CFD, *Minco Tech Australia* (2010-2013)
- **Project Member:** CFD study of Natural Medium Cyclone, *RecyCoal UK Ltd*, (2011-2013)
- **Project Consultant:** CFD study of mineral equipment service, *Shandong Borun Process Industrial Technology Corp., Ltd, China* (2012-2014)
- **Project Member:** Mesoscopic averaging theory of granular systems: Formulation and application, 91534206, *NSFC, China* (2016-2019)
- **Project Member:** ARC Research Hub for Computational Particle Technology, IH140100035, *ARC* (2015-2020)
- **Project Leader:** Particle-scale Modelling and Simulation of Coal Gasification Reaction, 2016YFB0600101-04, *MOST, China* (2016-2021)
- **Project Member:** Numerical Investigation of Separation Mechanism of High Concentration Hydrocodone and its Application, BK20171402**,** *Department of Science and Technology of Jiangsu, China* (2017-2020)
- **Project Manager:** Investigation of Inhalation Drug Delivery System and its Application, JITRI, China (2018-2020)

Numerical and Experimental Investigation of Aerosolisation and Deposition Process in the Inhalers and Realistic Respiratory Tract

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Abstract

The inhaled drugs are generated as aerosol in dry powder inhalers (DPIs) and then transported into respiratory tract. The deposition in the target sites mainly depends on a number of factors related to anatomical structure variation, particle characteristics and inhalation conditions (inhaled angle and breathing pattern e.g.). This project aims to numerically and experimentally investigate the inhalation parameters affecting fine particle deposition in the US pharmacopeia throat (USP), idealized mouth-throat (IMT) and realistic mouth-throat (RMT) models with a commercial inhaler (Handihaler®). The results indicate that the deposition fraction and spatial distribution are highly sensitive to the geometrical variation and respiratory conditions such as the inhalation airflow rate, particle size and inhalation angle. Moreover, the effect of geometrical variation on the particle deposition pattern is more dominant. In the RMT model, inhalation angle creates quite obvious effect on the aerosol delivery in mouth, and optimal inhalation can be achieved by controlling the aerosol entering the model with the flow streamlines parallel to the tongue. This study could be used to develop an in vitro method which aims to better predict in vivo lung deposition mechanisms of pharmaceutical aerosol.

Keywords: computational fluid dynamics, aerosolisation, dry powder inhalers, mouth-throat geometry, deposition efficiency.

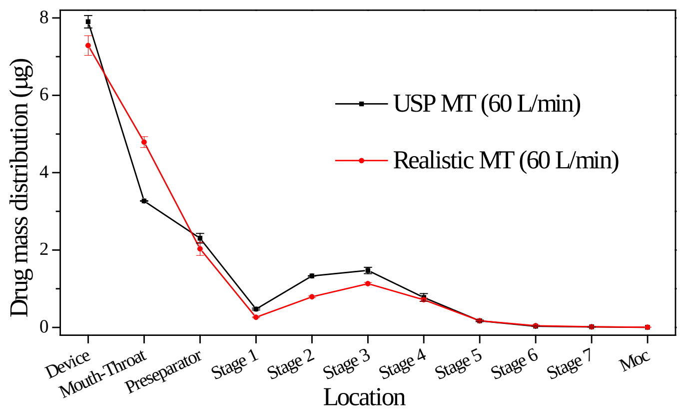

Figure 1 Drug mass distributions per discharge of HandiHaler® at 60 L/min

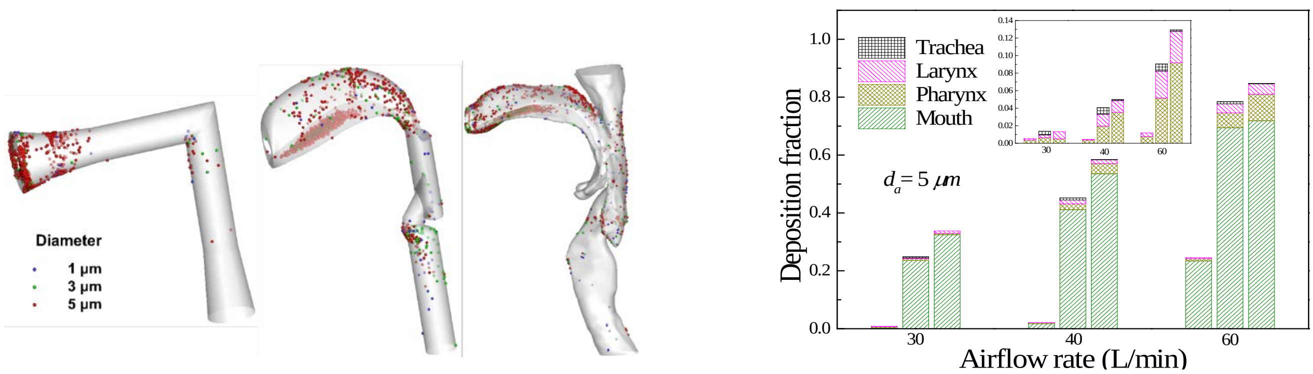

Figure 2 Spatial deposition distribution of fine particles in three MT models with airflow rate 60 L/min

A comprehensive CFD model for ironmaking blast furnace

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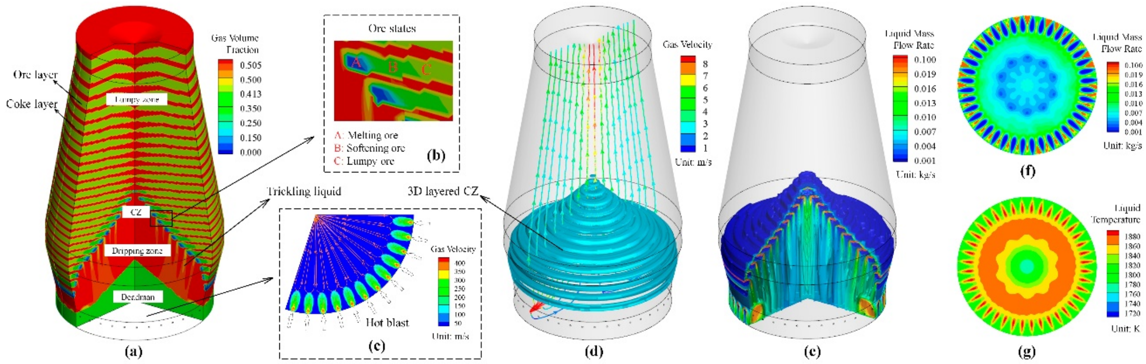
Abstract

Numerical simulation and modelling have been increasingly accepted as a viable method for understanding, designing and controlling ironmaking blast furnaces (BFs). This talk will discuss our recent efforts in developing a three-dimensional (3D) parallel BF process model using Computational Fluid Dynamics (CFD). The model explicitly describes layered burden and Cohesive Zone (CZ), gas and liquid re-distribution near raceways, trickling liquid flow in CZ and dripping zone, and stockline variation. Also, particle size reduction is modelled. The applicability of the model has been confirmed by the reasonable agreement between predicted and measured in-furnace states and global performance under experimental and industrial conditions.



Predicted 3D in-furnace states of the industrial BF: (a) layered burden structure, (b) three states of ore particles inside CZ, (c) gas velocity at tuyere-level, (d) 3D layered CZ and gas streamline inside an axial plane, (e) and (f) liquid mass flow rates, and (g) liquid temperature.

Brief Biography

Dr Shibo Kuang is currently a research fellow at ARC Hub for Computational Particle Technology, Monash University. His research interests centre around computational process engineering. A specific focus is on the development and application of numerical models at different time and length scales, with the support of physical experiments, for the fundamental and applied research on particle-fluid flow and granular dynamics. The research topics cover particle transportation, particle separation, and multi-phase reacting flows. In this field, he has authored/co-authored over 80 publications (including 60 journal papers collected in Web of Science, from which 48 ones are published in recent five years), with the H-index of 21 according to Google Scholar.

Fundamental study of chemically reacting liquid flow and its application to environmental and energy fields.

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I introduce our recent fundamental experimental study of chemically reacting liquid flow. These include fingering hydrodynamic instability phenomena with chemical reactions producing precipitate (Fig.1, [1,2]) or gel (Fig.2, [3]). In the cases involving precipitate, the coupling between precipitate particle dynamics and hydrodynamics should be important. Also, I introduce our recent trial of application of such fundamental studies to environmental and energy fields, especially to enhanced oil recovery. Finally, I introduce a recent interesting reacting flow phenomena in stirred tank reactor (Fig.3 [4]).

[1] Y. Nagatsu, S.-K. Bae, Y. Kato, and Y. Tada, Miscible viscous fingering with a chemical reaction involving precipitation, Phys. Rev. E, 77, 067302 (2008)
[2] Y. Nagatsu, Y. Ishii, Y. Tada, and A. De Wit, Hydrodynamic Fingering Instability Induced by a Precipitation ,Phys. Rev. Lett., 113, 024502 (2014)
[3] Y. Nagatsu, A. Hayashi, M. Ban, Y. Kato, and Y. Tada, Spiral pattern in a radial displacement involving a reaction producing gel, Phys. Rev. E, 78, 026307 (2008)
[4] T. Ueki, J. Iijima, S. Tagawa, Y. Nagatsu, Unpredictable Dynamics of Polymeric Reacting Flow by Comparison between Pre- and Post-Reaction Fluid Properties: Hydrodynamics Involving Molecular Diagnosis via ATR–FTIR Spectroscopy, J. Phys. Chem. B 123, 4587-4593 (2019)

Fig. 1 Fingering hydrodynamic instability phenomena with chemical reactions producing precipitate.

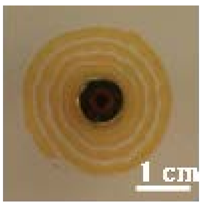

Fig. 2 Fingering hydrodynamic instability phenomena with chemical reactions producing gel.

Fig. 3 A recent interesting reacting flow phenomena in stirred tank reactor.

Modeling water movement in watersheds

Takashi Gomi
Tokyo University of Agriculture and Technology

Water resources management including mitigation of floods and droughts as well as related sediment disasters under changing environments is one of key factors for sustainable resource management. Safe and secure water supply is "essential" for promoting sustainable resource management and conservations. Much more comprehensive approaches for water resources management is required in various scales from regional to watersheds around the world. Detail information for understanding and modeling hydrological and geomorphic processes is necessary for not only progress of sciences but also developing for future prediction. Here we will present various field and modeling approaches for investigating complex processes of water in watersheds. This research team aims to develop a sustainable green infrastructure through appropriate forest and agricultural land management. Here, we focus on establishment of indicators of volume and quality of water and sediment dynamics in various scales.

Interfacial instabilities in porous media flows.

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Abstract:
Hydrodynamic instability plays a key role in determining both the feasibility and risks involved in the geological sequestration of CO2. Other porous media applications of interfacial instability are oil-recovery, chromatography separation, contaminant transport in aquifers etc. The displacement processes in the above processes encounter various hydrodynamic instabilities viz., Saffman-Taylor instability, Rayleigh-Taylor instability, to name a few. The viscosity contrast of underlying fluids in these systems results in an interfacial instability called viscous fingering (VF). Controlling such instabilities is of paramount interest and many theoretical, experimental and numerical studies have been focused on it. An overview of various control strategies ranging from an optimum flow rate to the use of reactive fluids will be presented using both linear stability analysis and robust direct numerical simulations of the model equations.

Let’s talk about modeling and simulation in your researches

Mikio Sakai

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Abstract

I believe that my group is world-leading in the modeling of granular and multiphase flows. My group concentrates on developments and applications of advanced multi-physics models in chemical engineering, nuclear engineering, environment & energy engineering, and food & pharmaceutical engineering. Our original approaches are related to the multi-physics simulations such as modeling of granular flows for dry and wet particles, modeling of gas-solid, solid-liquid and gas-solid-liquid multiphase flow in a complicated shape device and modeling of solid-liquid phase change. These models become helpful for a better understanding of complex phenomena and will give valuable information in your researches. I look forward to discussing our researches and our future joint projects.

Biography

Dr Mikio Sakai is currently Associate Professor in Resilience Engineering Research Center in The University of Tokyo. He earned his Ph.D. degree from The University of Tokyo in 2006. Then, he became Assistant Professor in 2007 and Associate Professor in 2008 in The University of Tokyo. He is Visiting Reader at Imperial College London since 2016. He extensively studies modeling of granular flows, multi-phase flows and the heat transfer, and besides the parallel computation techniques. He is a world-leading professor in computational granular dynamics, and hence has delivered lots of invited lectures in conferences. He holds important posts in powder technology community such as Director of Society of Powder Technology of Japan and Head of Simulation & Modeling Division in Association of Powder Process Industry and Engineering, JAPAN. At present, he is Associate Editor of Chemical Engineering Science and Editor of Granular Matter.