Hub Overview

The ARC Hub for Computational Particle Technology aims to develop and apply advanced computational particle technology to model and optimise complex particulate and multiphase processes in the mineral and metallurgical industries. This will be achieved through detailed analysis of the fundamentals governing the fluid flow, heat and mass transfer at different time and length scales, facilitated by various novel research techniques. Research outcomes including theories, computational models and simulation techniques, as well as well-trained young researchers, will generate a significant impact across a range of industries of vital importance to Australia’s economic and technological future.

It can significantly enhance the productivity and competitiveness of Australia’s important industries such as minerals, metallurgical, materials, chemical, energy, pharmaceutical and environment. Led by Prof. Aibing Yu in Monash University, the hub brings together key industry partners such as JITRI, Rio Tinto, Baosteel and Longking, and universities (Monash, UNSW, UQ, UWS, Macquarie University, and other four overseas universities) to drive its research program.

Overall research milestones has been progressing well. 10 students were graduated with their PhD degrees based on their works this year, which are relevant to the Hub’s research themes. Over 30 national and international scholars and technical staff visited the Hub this year and a number of workshops were organised between the Hub researchers and our industry partners. Four public lectures were given by researchers from the Hub during 2018 which gave a great social impact regarding how the scientific outcomes can make a change in our daily life.

We have had experts from Newcrest Mining visiting the research hub, discussion with the Hub director and researchers have provide more scientific insights and an effective approach to test new ideas and optimise operations in their current processes.

The Hub’s significant experience in modelling and simulation of the mineral processing, such as grinding, screening, hydro-cyclone, etc., could be a great help in their initiative.

We have also hosted a senior delegation from Longking on Oct 5th and had a constructive discussion with the researchers and students of the Hub. Longking is focused in flue gas clean-up, water treatment, soil remediation and material convey which are generally aligned with the research area of the Hub. Longking is one of the industry partners of the Hub with an annual output of over US$1.2 billion, and over 7000 employees, it is a leading environmental engineering company in China and has operations in both China and overseas.

In this issue, we are pleased to introduce our Chief Investigators from various Australian universities and our hub’s research programs & areas. Prestigious awards won by our hub’s postgraduate researchers, hub activities and high impact research outputs are also highlighted.

Please contact us or visit our website to learn more about our research and engagement activities.
INTRODUCING OUR CHIEF INVESTIGATORS

Prof Dongyuan Zhao  
Monash & Fudan University

Prof. Dongyuan Zhao got his Master degree from Chemistry Department at Jilin University (1987), and a Ph.D. degree from Jinlin University and Dalian Institute of Chemical Physics (1990). After postdoctoral research at the Weizmann Institute of Science (1993-94), University of Houston (1995-96), and University of California at Santa Barbara (1996-98), he joined the faculty of the Fudan University in Dec. 1998, where he is now Professor in the Department of Chemistry.


A/Prof Wenyi Yan  
Monash University

A/Prof Wenyi Yan received his Masters of Science Degree in Engineering from Beijing University of Aeronautics and Astronautics in 1992. He obtained his PhD degree from Tsinghua University, Beijing, China, in 1995. Dr Yan joined Monash University as a senior lecturer in 2007 and promoted to associate professor in 2014. Dr Yan has been awarded 11 research grants from Australian Research Council since 2006. Currently, he is supervising and co-supervising 13 postgraduate research students.

His research interests include applied mechanics of solids and structures, composite structures, fracture and fatigue of materials and design optimization for additive manufacturing, wear, rail/wheel contact mechanics.

Dr Baoyu Guo  
Monash University

Dr Baoyu (Bob) Guo is a Senior Research Fellow in the Department of Chemical Engineering, Monash University since 2016. He has received his M.Eng in 1988 from Tianjin University, China and Ph.D in 2001 from The University of Sydney. Which he went on to hold a position as a Research Associate (2002-2011) and Research Fellow/Lecturer (2012-2016) in the School of Materials Science and Engineering, UNSW.

His research interests include numerical modelling of multiphase flows and transport phenomena in various processes in metallurgical, mineral, chemical and environmental engineering, particularly the iron-making blast furnace, coal preparation devices, electrostatic precipitation, spray dryers. These processes cover multiphase flows, heat/mass transfer, chemical reactions and electric field.

Prof Vladimir Strezov  
Macquarie University

Prof Vladimir Strezov is currently Professor at the Department of Environmental Sciences, Macquarie University. He has completed his PhD in 2000 from the Department of Chemical Engineering at the University of Newcastle, Australia. He is advisor for the Australian Renewable Energy Agency (ARENA) providing advice to support development and selection of projects for funding.

He has research interests in renewable and sustainable energy, industrial ecology, control of environmental pollution and designing sustainability metrics of industrial operations. He has established research links with primary industries aiming to reduce their environmental impacts and improve energy efficiency. Prof Strezov has research focus on developing and evaluating biomass processing technologies for sustainable generation of energy and bio-fuels.

Prof Cordelia Selomulya  
Monash University

Prior to joining Monash University, Professor Selomulya was a Royal Academy of Engineering Australia Postdoctoral Fellow at the University of Leeds, and an Australian Postdoctoral Fellow at the ARC Centre of Excellence for Functional Nanomaterials at UNSW. She has a PhD in Chemical Engineering from the University of New South Wales. She was recently awarded an ARC Future Fellowship (2014 – 2018) to conduct research on the manufacturing of high value particles for functional foods and pharmaceutical industries. She is an adjunct Professor of Chemical Engineering at Soochow University in China (2013 – current), and was an Australia-China Young Researcher Fellow (2013).

Prof Selomulya is leading the Biotechnology and Food Engineering group with an internationally recognised reputation in drying technology research, and the only facility in Australia for functional particle assembly via microfluidic spray drying.

Dr Shibo Kuang  
Monash University

Dr Shibo Kuang have received his PhD from Northeastern University, China. His research has focused on numerical simulation of complex multiphase and multi-field phenomena in engineering problems, which mainly include Lattice Boltzmann method (LBM), discrete element model (DEM), population balance model, and computational fluid dynamics (CFD). CFD-DEM, LBM-DEM, two-fluid model, kinetic theory, volume of fraction (VOF). The specific research topics include particle transportation (e.g. in pneumatic conveying, microchannel, non-Newtonian fluid system), particle separation (e.g. by hydrocyclone, gas cyclone, dense medium cyclone, in-line pressure jig, microchannel, nanofiltration device), multi-phase reacting flows (e.g. in metallurgical reactors for production of iron, steel, aluminium).

Dr Kailei Chu  
Monash University

Dr Kailei (Kevin) Chu is currently a Research Fellow at Monash University and UNSW Australia. He obtained his PhD (on CFD-DEM study of complex particle-fluid flow) in 2010 from UNSW Australia, BEng (on gas cyclone) in 1998 and MEng (on CFD-DEM simulation of fluidized beds) in 2001 from Xian University of Architecture and Technology (XUAT) in China.

He is specialized in the modelling and simulation of complex particle-fluid flows that are widely found in nature and many industries including mineral, metallurgical, material, environmental and chemical. He has conducted extensive pioneering work in this area by developing and applying novel simulation techniques and models (mainly combined approach of computational fluid dynamics and discrete element method (CFD-DEM)).

Prof Yijiao Jiang  
Macquarie University

Yijiao is currently a Chief Investigator at Macquarie University (MQ) Energy and Environmental Research Centre and ARC Research Hub for Computational Particle Technology. After completing her PhD at University of Stuttgart (Germany), she worked as postdoc at Swiss Federal Institute of Technology (ETH Zürich) from 2008 to 2010. Yijiao was awarded UNSW Vice-Chancellor’s Postdoctoral Research Fellowship in 2011 and ARC Discovery Early Career Researcher Award in 2012.

She has secured ca. AUSD$4m in research grants from ARC Research Hub with industrial partners (Rio Tinto and JTRI), ARC DP etc. Yijiao’s research interests mainly focus on the development of better catalytic/photocatalytic systems for green chemical processes, renewable energy and environmental protection. She has developed various in situ and operando spectroscopic techniques including NMR, EPR, IR, UV-Vis and Raman for achieving breakthroughs in catalysis research.

Dr Federica Federici  
Monash University

Federica Federici is currently a Senior Research Fellow at Monash University. She obtained her PhD from the University of Exeter in 2010, followed by postdoc experience in the University of Texas at Dallas and Monash University. Federica's research focuses on the development and application of computational and experimental techniques to understand the chemical and physical processes in complex multiphase fluid flows. This research area is relevant for various applications, such as energy conversion and storage, water purification, and environmental remediation.
The contributions are reflected by a strong track record in terms of publications, research grant and synergistic activities established with leading Australian/overseas industries, including Baosteel, Rio Tinto, BlueScope Steel, Coal Energy Australia, ACARP Australian/overseas industries, including Baosteel, Rio Tinto, BlueScope Steel, Coal Energy Australia, ACARP Australian/overseas industries, including Baosteel, Rio Tinto, BlueScope Steel, Coal Energy Australia, ACARP

Dr Qin Huang is a Professor of Mechanical Engineering at UQ. He joined UQ in 2005 as a Senior Lecturer, and was promoted to Associate Professor in 2008 and Professor in 2011. Prof Huang received his PhD from The University of Western Australia in 1996. He has won a number of prestigious research accolades, including ARC Future Fellowship (2011-2015), ARC Australia and New Zealand Research Fellowship (2005-2010), JSPS Invitation Fellowship (2009), Queensland International Fellowship (2012) and Singapore National Technology Award (1999).

Professor Han Huang’s research interests are nanomanufacturing, machining technologies, mechanical characterization of nanostructured materials and nanostructures and nanoparticle based lubrication.

A/Prof Jianqiang Zhang University of New South Wales

Dr Jianqiang Zhang obtained his Master of Engineering from Zhejiang University, China in 1987 and PhD from UNSW in 2000. He joined the School of Materials Science & Engineering, UNSW as a Research Fellow/Research Associate in 2003, Senior Research Fellow in 2009, Senior Lecturer in 2012 and finally Associate Professor since 2015.

He has significant contributions in the field of gas-solid reactions at high temperature, including high temperature corrosion and processing of metallic materials. Research emphases are on the reaction thermodynamics and kinetics, phase transformation and characterisation, reaction mechanism understanding, sustainable materials processing, and new materials development.

A/Prof Yansong Shen University of New South Wales

Dr Yansong Shen is an Associate Professor (Senior Lecturer, 2016-2018, UNSW: Lecturer, 2014-2016, Monash). He obtained BEng and MEng degrees at Northeastern University and PhD degree at UNSW. He initiated and leads a vibrant research group - Smart Process Modelling and Optimisation of Reactive Flows “sProMO Group”. His research interests range from understanding fundamentals to optimising & developing new, cleaner and more efficient technologies, powered by advanced numerical and experimental approaches.

His research contributions are reflected by a strong track record in terms of publication, research grant and synergistic activities established with leading Australian/overseas industries, including Baosteel, Rio Tinto, BlueScope Steel, Coal Energy Australia, ACARP, BHP Billiton, Peabody Energy, Jellinbah Resources etc.

A/Prof Haiping Zhu Western Sydney University

Dr Haiping Zhu is an Associate Professor in the School of Computing, Engineering and Mathematics at UWS. He received his PhD degree in Dynamics of Mechanical Systems from Beijing Institute of Technology in 1995. He joined UWS as a Senior Lecturer in September 2009.

Dr Zhu has been devoted to the study of multiphase flow, particulate systems, mechanical systems and related processes since 1990 and has made various contributions in both the fundamental and applied aspects of these fields. His current specific research areas/interests include modelling of particulate and multiphase processes, solids flow and segregation, fluid flow, multi-scale simulation of particulate systems, granular dynamics, powder/particle technology, processing and handling of bulk/particulate materials, heat and mass transfer in packed and fluidised beds, molecular dynamics simulation, and dynamics of mechanical systems.

Dr Qinghua Zeng specializes in nanomaterials and molecular modeling, obtaining Ph D in 2005 from University of New South Wales (UNSW). Since 2004, he has been with UNSW School of Materials Science and Engineering as a Research Associate, ARC Postdoctoral Fellow, and was promoted to Lecturer in 2009. In 2010, Dr Zeng joined University of Western Sydney (UWS) as a Lecturer in Engineering Materials and was promoted to Senior Lecturer in 2013. Dr Zeng is a member of Institution of Engineers Australia (IEAust), ARC Australian Research for Advanced Materials, and ARC Nanotechnology Network.

Dr Qinghua Zeng has been doing research in the areas of polymer composites, nanomaterials, computational materials science, and metallurgical engineering. His research on polymer nanocomposites has made a significant impact in this area with results being widely cited. His current research interests are the design, processing, characterisation, and computer modelling of various nanomaterials and nanosystems (eg. polymer nanocomposites, layered solid materials, catalysts, nanoparticle growth and self-assembly) by state-of-the-art experimental and numerical techniques.
Hub Research Programs and Research Areas

The Hub involves research at three levels:

1) Development of various new and advanced theories and computational techniques,
2) Fundamental studies of important common behaviour of particles, and
3) Application of the new theories and understanding to solve engineering problems in different industrial processes.

Program 1: “Theoretical Developments” is focused on theoretical developments or enabling science and technology for particulate research

**Area 1 - Quantification of particle-particle and particle-fluid interaction forces**

**Area 2 - Particle scale modelling of particle-fluid flow coupled with heat and mass transfer**

**Area 3 - Rheological properties of particles and techniques for process simulation**

Program 2: “Simulation, Modelling and Application” is focused on the fundamental and applied studies of different industrial processes/operations.

**Area 4 - Discrete particle simulation of particulate systems**

**Area 5 - Micro- and macro-dynamic analysis**

**Area 6 - Mathematical modelling and application**

Awards Won by Hub Postgraduate Researchers in 2018

- Two PhD students from the Hub won the best presentation (Ms Liuyimei Yang) and best poster (Mr Siddharta Shrestha) awards on The 2nd International Symposium on Computational Particle Technology, and the 13th International Conference on Computational Fluid Dynamics in the Minerals and Process Industries, 4-7 Dec 2018, Melbourne
- Ms. Yuxiang Zhu received the best Oral Presentation Award in 3rd International Symposium on Renewable Energy Technologies, Jul 19-22 2018, Gold Coast, Australia
- Mr. Aleksei Marianov and Ms. Xiaoxia Yang received the best Oral Presentation Award, in the Inaugural School HDR Conference, Macquarie University
- Ms Yuxiang Zhu received the best Poster Award in the Inaugural School HDR Conference, Macquarie University
- Mr. Aleksei Marianov and Ms Yuxiang Zhu received the 2nd and 3rd Oral Presentation Award in the 3-min Thesis Competition within the School of Engineering, Macquarie University
The 2nd International Symposium on Computational Particle Technology, & 13th International Conference on Computational Fluid Dynamics in the Minerals and Process Industries, in conjunction with Annual Hub Meeting, December 4-8, 2018, Melbourne, Australia.

The 2nd International Symposium on Computational Particle Technology (CPT) was held in Melbourne, Australia on 4-8 December 2018, jointly held with the 13th CSIRO International Conference on Computational Fluid Dynamics (CFD) in the Minerals and Process Industries. The CPT symposium aims to discuss the frontier and challenging problems in the modelling and simulation of complex particulate and multiphase processes, covering a wide spectrum from fundamental research to industrial application. The CFD symposium aims to cover the application of computational fluid dynamics in mineral processing, metal production, power generation, chemicals, food, oil and gas.

A total of 254 attendees including plenary speakers, keynote speakers, invited speakers, university professors and industry leaders from 13 different countries e.g. Australia, China, France, Japan, Germany, U.K and other countries attended the four-day conference. The symposium included 30 technical sessions for 300 abstracts, 6 plenary speakers, 22 keynote speakers, 212 oral presentations and 78 poster presentations, which covering 10 topics. The selected papers will be publish in a special issue of Powder Technology. The technical program included a total of 28 plenary and keynote speakers, i.e. Prof. Jennifer Curtis from University of California USA, Prof. Stefan Heinrich from Hamburg University of Technology, Germany, Prof. Charley Wu from University of Surrey, UK and Prof. Hans Kuipers from Eindhoven University of Technology, Netherlands, Prof. Raj Dave from New Jersey Institute of Technology, USA, Prof. David Pinson from Iron & Steelmaking Technology at BlueScope, Australia, Prof. Jin Ooi from the University of Edinburgh, UK, Prof. Hidehiro Kamiya from Tokyo University of Agriculture and Technology, Japan and others.

The annual hub meeting was also held in conjunction with the conference and almost all CI’s were in attendance. Most of the hub’s students and research associates have presented their research progress during the conference in either oral presentation or poster forum.

Conference Opening Ceremony, Awards Ceremony and Dinner.

Hub Annual Meeting

http://www.monash.edu/comparticletech
Hub Activities

SIMPAS saw off two visiting scholars from China

A/Prof Zhen Jiao and Prof Weifan Chen accomplished their planned work at SIMPAS, Monash University after twelve months stay with us, and are returning to their original organisations soon.

A/Prof Jiao is working in the area of Biological and Medical Nanotechnology and was awarded his PhD degree from Nanjing University in 2007. He commenced his academic career from Southeast University since then and was acting as the assistant president of the JRI (Monash-SEU Joint Institute) since 2015. Dr Jiao published over 30 papers in top journals such as Journal of Physical Chemistry B, and Fluid Phase Equilibria, focusing on nanoparticles, sustainable chemical processing, and development of premium fine chemicals.

Prof Weifan Chen joined the smart coating team at SIMPAS since Sept 2017 and was working closely with A/Prof Xuchuan Jiang and his nano team. Prof Chen is returning to School of Material & Engineering at Nanchang University.

A farewell party was organised for the visiting scholar and we wish them all the best in their new positions.

Industry Experts from Newcrest Mining visited the CPT Hub

On Oct 4th, Newcrest Mining is Australia’s leading gold mining company, and one of the top five gold companies in the world by production, reserves and market capitalisation. Last year, it produced 2.35moz gold and 78,000 ton copper. Dr Paul Griffin, the Process Manager of Newcrest with over 20 years of working experience in the mining and mineral processing industry visited the Hub and had a comprehensive discussion with the Hub director and researchers.

Newcrest is dedicated to exploring innovative technologies which could extract valuable products from the waste stream worth of $750m. The Hub’s significant experience in modelling and simulation of the mineral processing, such as grinding, screening, hydro-cyclone, etc., could be a great help in this initiative. The tools developed in the Hub regarding the analysis of forces between particles and the interactions between particles and fluid will provide more scientific insights and an effective approach to test new ideas and optimise operations in their current operations. Technical discussions for specific issues will be followed up in a few weeks.

Senior delegation from Longking visited the CPT Hub

A senior delegation from Longking visited the Hub on Oct 5th and had a constructive discussion with the researchers and students of the Hub. Longking is focused in flue gas clean-up, water treatment, soil remediation and material convey which are generally aligned with the research area of the Hub. Longking is one of the industry partners of the Hub with an annual output of over US$1.2 billion, and over 7000 employees, it is a leading environmental engineering company in China and has operations in both China and overseas. The collaboration of Longking with SIMPAS can be traced back years ago when Prof Yu established a cooperative research centre with local partners. Several postgraduates from SIMPAS joined Longking and they are playing important roles of the company.
**Research Output Highlight**

**Advances on tungsten oxide based photochromic materials: strategies to improve their photochromic properties**

Shufen Wang, Weiren Fan, Zichuan Liu, Aibing Yu and Xuchuan Jiang*

Photochromic materials have been extensively studied because they are quite attractive and promising for many applications. Tungsten oxide (WO₃), a typical photochromic material, has attracted considerable attention. So far, many advances have been achieved in different subfields of WO₃ photochromism, mainly focused on the enhancement of WO₃ photochromic properties, which depends not only on the chemical features but also on the microstructures, interface and hybrid components. This review aims to summarize recent progress in different advanced strategies to improve WO₃ photochromic properties, such as a fast photoresponse (within 1 min), strong and stable photochromism, visible-light coloration and reversible photochromism. However, it is still challenging to achieve these properties for large-scale commercial applications. In addition, many previous studies have been limited to lab research purposes, although some photochromic WO₃-based devices have been fabricated. To address the above-mentioned issues clearly, this review will provide a discussion of the following aspects. First, the fundamental photochromism of WO₃ is described. Secondly, various advances towards improving its photochromic properties will be summarized. Thirdly, the optical applications of WO₃-based photochromic materials will be reviewed and discussed. And finally, a perspective on the development trends in WO₃-based photochromic materials and devices is proposed.


**Discrete particle simulation of food grain drying in a fluidised bed**

Jannatul Azmir, Qinfu Hou*, Aibing Yu

Drying is a common practice for post-harvest processing of food grains. Fluidised beds are often adopted for this purpose. It is of importance to understand the fluidised bed drying process for improving its energy efficiency. This work establishes a numerical drying model based on the combined approach of computational fluid dynamics and discrete element method for describing heat and mass transfer in the gas-solid flow system. Water evaporation is modelled in resemblance to a chemical reaction, thereby requiring fewer model parameters. The model is first described in detail. Then it is tested by comparing model predictions with those experimental data of corn kernel from the literature. General drying characteristics including grain and air moisture contents are reproduced qualitatively. The predicted drying rate curves are quantitatively comparable with those of experimental data. Finally, the effects of inlet air velocity and temperature are examined. The model predictions confirm that the drying rate increases with both the inlet air velocity and temperature. However, the drying product quality, here represented by the standard deviation of grain moisture distribution, increases with increasing air velocity or decreasing air temperature. This grain scale model would be useful to the design and control of the drying process.


**Contact us**

Dr Bernard Xu, Hub Manager
ARC Hub for Computational Particle Technology (CPT)
Ph: + 61 3 9905 1789, Email: Bernard.xu@monash.edu
Simpas: www.monash.edu/engineering/simpas
CPT: www.monash.edu/comparticletech

**Location**

The Research hub is located at Monash University (Clayton Campus) within the Lab for Simulation and Modelling of Particulate Systems (SIMPAS) (24 Research Way, Monash University).