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 a number of overseas universities) to drive its research program.

In the first half of 2019, we have had visitors from Longking, which is one of our industry partners, visiting the hub in Monash University, Clayton Campus. We have had a fruitful technical seminar session between the industrial visitors and our hub researchers, and also a chance to showcase the Monash CAVE2 facility to our industrial counterpart. In June, hub staff attended the ARC Major Investments Forum held in Canberra for a discussion with ARC representatives regarding a range of topics closely related to ARC ITRPs, as well as the wonderful networking opportunity with other research entity that comes with it.

We are also kicking off six new projects with our industry partners (3 with JITRI & 3 with Baosteel) that will potentially have a high impact in terms of advancing the knowledge in the relevant fields as well as solving practical industrial problems, further information on these projects are enclosed within. The new projects attracted $200,000 in funding from Western Sydney University. A new partner of the hub, JXUST, is also on board after being approved by the ARC administration earlier this year and is bringing in $300,000 over the remaining 3 years of the hub lifecycle.

In this issue, we are excited to highlight the six new projects scheduled to start this year, our hub objectives and research areas, hub activities and research output.

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

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23 Chief Investigators
14 Partner Investigators
5 Australian Universities
6 Overseas Universities
4 Industry Partners
26 Postdoctoral Fellows
53 Postgraduate Students

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http://www.monash.edu/comparticletech
## 6 New Projects Established in 2019

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<tr>
<th>Project Title</th>
<th>Industry Partners</th>
<th>Description</th>
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<td>Averaging method of particulate system</td>
<td>A/Prof Haiping Zhu, Western Sydney University</td>
<td>Particulate systems can be described by the discrete and continuum approaches. By the use of a proper averaging procedure, the two approaches can be linked. This project aims to develop an averaging method suitable for complex flow conditions of particles to link the two approaches, and apply the new method to the simulations of the particle flows in hopper and rotating drum. Specific objectives include: 1) To develop an averaging method to link the discrete and continuum approaches for particulate systems; 2) To develop a model for continuum modelling; 3) To investigate the dynamics of particles in hopper and rotating drum and understand the governing mechanism at macro- and microscopic levels using the new averaging method.</td>
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<td>Discrete element method for industrial applications</td>
<td>Dr Kejun Dong, Western Sydney University</td>
<td>Discrete element method (DEM) is an essential tool in computational particle technology, and has been widely used in the numerical studies of particulate systems. However, to better apply DEM to simulate industrial processes, there are several aspects to be improved, including better force models for non-spherical particles, better data exchange interface for coupling and parallelizing, and more comprehensive analysing tools. The project aims to implement the latest knowledge and numerical techniques to improve the DEM model in these aspects, and hence to fortify the capability and versatility of DEM for industrial applications.</td>
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<td>PCI operation in oxygen blast furnaces: modelling and application</td>
<td>A/Prof Yansong Shen, University of New South Wales</td>
<td>Pulverized coal injection (PCI) operation is a proven ironmaking technology for cost-saving and furnace stability. Oxygen blast furnace (OBF) is a promising technology to enable zero carbon footprint in ironmaking. The in-furnace phenomena of PCI operation under OBF conditions will be very different from conventional BF operations. The project is to work with an industry partner to develop understandings of in-furnace phenomena of multiphase flow and thermochemical behaviours related to PCI operation under the OBF conditions and then optimise the PCI operations for a given OBF. This will be achieved through the use of various advanced modelling techniques and detailed process analysis. The research outcomes such as models, knowledge, database and new technology should be useful for understanding, design and optimisation of PCI technology for stable and low-cost OBF practice.</td>
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<td>Surface quality improvement of metal strips with the effect of additives/particles in lubricant</td>
<td>Prof Liangchi Zhang, University of New South Wales</td>
<td>From the perspective of Baosteel, quality rolling of metal strips has always been critical. At present, there exists two challenges: 1) it is unclear how roll deflection and lubricant additives and debris particles influence rolling stress distributions, deformation-induced temperature variation, and surface texture transfer, particularly in the regime of thin strip rolling; and 2) there is no understanding available to identify proper lubricant for metals which are prone to surface damage such as oxidation, spalling of adhesion and surface damage induced by debris particles. This project research aims to reveal the underlying mechanisms behind the challenges and in turn develop practical solutions for overcoming the relevant difficulties encountered in the production lines of Baosteel.</td>
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<td>Investigation of inclusions and precipitates in high-end gear steels</td>
<td>Prof Baojun Zhao, University of Queensland</td>
<td>This work will support our industry partner to address its product issues. Gear steels are one of the important steel products in Baosteel. For continuous improvement in the quality and properties, and development of high-end gear steels, this project aims to: 1) optimize refining conditions to improve the quality and productivity of current products; 2) develop new high-end gear steel with sophisticated MnS precipitation control; 3) provide technical support for commercial high-end gear steel products.</td>
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<td>Understanding the fracture mechanisms of high strength steel cords during manufacturing process</td>
<td>Prof Han Huang, University of Queensland</td>
<td>This project aims to investigate and understand the fracture causes of steel rods/wires during the manufacturing of high-strength steel cords through failure analysis, microstructural and structural defects characterization using innovative techniques, including computational simulation. Together with new scientific knowledge generated from the fundamental studies on microalloying of the cord steels with other solutes and on cementite dissolution and impurity, new methods to solve this long-standing problem will be proposed and initially validated. The outcomes will not only ensure the manufacturing continuity, lowering production cost, but also enable quality improvement and increase Baosteel’s competitive capacity in this market, creating economic benefits.</td>
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Industry Partner: JITRI

Industry Partner: BAOSTEEL
### Hub Objectives and Research Areas

#### Hub Objectives

| **Objective 1** | To develop novel and comprehensive theories and techniques to study and quantify not only the interaction forces but also the heat and mass transfer between particles (including nanoparticles), and between particle and fluid under various conditions |
| **Objective 2** | To develop generic theories and corresponding computational technology for particle scale simulation of complex particulate and multiphase processes which may have wide distributed particle sizes and shapes, and multiphase flow strongly coupled with heat and mass transfer |
| **Objective 3** | To develop and generalise an effective method to link the discrete and continuum approaches, and formulate, based on the particle scale results, the governing equations, constitutive relations and boundary conditions that can be implemented in continuum-based process modelling and optimisation |
| **Objective 4** | To apply the developed theories and simulation/modelling techniques to solve challenging problems associated with various processes or operation in the minerals, metallurgical and materials industries |
| **Objective 5** | To establish an advanced research platform to train postdoctoral fellows and research students in computational particle technology |

#### Hub Research Areas

- **Area 1:** Nanoparticle synthesis and application
- **Area 2:** Particle packing and agglomeration
- **Area 3:** Flow of fly ash and dusts
- **Area 4:** Particle flow, mixing and segregation
- **Area 5:** Particle-fluid flows
- **Area 6:** Metallurgical processes

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ARC Major Investments Forum

The ARC Major Investments Forum was held on 12-13th June at The Canberra Rex Hotel, Canberra City, ACT. Directors and COO/Managers from various ARC Training Centres, Research Hubs and Centres of Excellence were invited to participate in the event. The purpose of the event is to showcase research progress as well as facilitate discussions and exchange of ideas amongst the attendees. Some of the topics covered in the forum includes research highlights, building partnerships, succession planning, equality & diversity and future research workforce. The forum also serves as a valuable platform for networking not only among researchers for potential collaboration, but also for COO/Managers to get together and exchange ideas/tips and to provide feedback/having discussions with ARC staff regarding management of the ARC large investment initiatives.

JXUST joined as new partner and extra fundings secured

A new partner, Jiangxi University of Science and Technology (JXUST), applied to join the ARC Hub and has been approved by ARC administration in early 2019. JXUST was founded in 1958 and is currently offer a range of curriculum ranging from science, engineering, materials, IT, economics, management, arts and law. Specifically, it has established a set of highly competitive programs (both undergraduate and graduate) in mining, metallurgy, mineral processing and material engineering. JXUST is jointly sponsored by the Ministry of Education, Ministry of Industry and Information Technology, as well as Jiangxi Provincial Government. It is also one of the top five ranking university in Jiangxi province, with leading research capabilities and facilities in the fields of tungsten, copper, rare earth metals and lithium batteries in China.

JXUST brought $300,000 cash to the hub for collaborative research activities over the next three years. Extra fundings were also secured by A/Prof Haiping Zhu and Dr Kejun Dong, $100,000 each, from their university, WSU, for the newly established projects highlighted in this newsletter.

Visiting student returning to Italy

A visiting student, Filippo Marchelli is returning to Free University of Bozen-Bolzano, Italy, after 4 months (Feb - May) stay with us as a visiting student. During his stay, he has been working closely with ARC DECRA Fellow, Dr Qinifu Hou, who acted as his supervisor while completing his work here. His work here focused on the effects of various drag force models in predicting spouted bed characteristics with the combined computational fluid dynamics and discrete element method (CFD-DEM) approach. He realized the study with user-defined functions (UDF) in the commercial software, Fluent, and prepared a draft on this topic to be published before he left. This study is connected to the drag force model proposed in our hub’s previous study using the Lattice Boltzmann Method (LBM) and showed that the drag force model is better than other models in low gas velocities.

A farewell lunch was organised and we wish Filippo all the best in his future endeavours.

17 delegates from Longking visited the hub

17 delegates from Longking visited the hub on 2nd May and had a fruitful technical seminar session with our hub researchers, various researchers from the hub presented their recent work which are of interest to the industry. Longking is one of our industry partners which focusses on environmental protection technologies, specific interests include flue gas dust collection, flue gas desulphurisation, selective non-catalytic reduction, bulk materials conveying and electrical control equipments. The delegates were also brought on a campus tour, as well as experiencing the state-of-the-art Monash CAVE2 facility.
Research Output Highlight

**Review on Modeling and Simulation of Blast Furnace**

Shibo Kuang*, Zhaoyang Li, Aibing Yu*

The design and control of blast furnace (BF) ironmaking must be optimized in order to be competitive and sustainable, particularly under the more and more demanding and tough economic and environmental conditions. To achieve this, it is necessary to understand the complex multiphase flow, heat and mass transfer, and global performance of a BF under different conditions. Mathematical modeling, often coupled with physical modeling, plays an important role in this area. This paper reviews the recent developments in this direction. The emphasis is given to mathematical models for different BF regions from the top charging system, body, and finally down to raceway and hearth. The needs for the further research and developments are also discussed.


**Lattice Boltzmann Investigation of the Wake Effect on the Interaction Between Particle and Power-Law Fluid Flow**

Zhang Qi, Shibo Kuang*, Liangwen Rong, Aibing Yu

The wake behind a particle, namely particle wake, affects the interaction between particle and fluid. This effect of either single or two interactive particles is established for Newtonian fluid flow but not clear for non-Newtonian fluid flow. In this study, the particle wake behaviors and related particle-fluid forces in a power-law fluid flow are studied by a parallel three-dimensional lattice Boltzmann (LB) model over wide ranges of Reynolds number (0.1 < Re < 500) and power-law index (0.6 < n < 1.4). These ranges are well beyond those reported before. A new calibration model is proposed to reduce the discretization effects on the results analysis to most extents. The validity of the LB model with the calibration step is first examined by comparing the calculated fluid drag forces on a single particle against the measurements for different power-law fluid flows. On this basis, the model is used to study the flow and force characteristics resulting from the interaction of non-Newtonian fluid flow with a single particle or two interactive particles with fixed locations. From the simulation data, a new correlation is formulated to predict the drag coefficient of a single particle in power-law fluid flows. Also, the effect of placement distance between two particles is examined. The numerical results reveal the dynamic characteristics of the particle wake and particle-fluid forces, as well as their dependence on the power-law index, Reynolds number, and particles placement.