A Scaling Approach for CFD-DEM Modelling of Thermochemical Behaviours in Moving Bed Reactors and Its Application

Qinfu Hou^{1,*}, Dianyu E.^{1,2}, Shibo Kuang¹ and Aibing Yu^{1,3}

¹ARC Research Hub for Computational Particle Technology, Department of Chemical Engineering, Monash University, Clayton, VIC 3800, Australia.

²International Research Institute for Minerals, Metallurgy and Materials, Jiangxi University of Science and Technology, Nanchang, 330013, China.

³Centre for Simulation and Modelling of Particulate Systems, Southeast University - Monash University Joint Research Institute, Suzhou, 215123, China.

*Corresponding Author: Qinfu Hou. Email: qinfu.hou@monash.edu.

Abstract: Intensive heat and mass transfer between continuum fluids and discrete particulate materials plays a critical role in many chemical reactors [1]. For example, the shaft furnace and the blast furnace in ironmaking are operated with continuous charge and discharge of solid materials, and it takes hours for the solid materials moving from the furnace top to the bottom. To understand and improve the operation of these reactors, discrete particle models are very helpful when combined with flow, heat and mass transfer, and chemical reaction models [2-6]. However, due to the high computational cost with such discrete particle models, it is very challenging until now to study these slow and transient processes.

First, a scaling approach is established for the combined computational fluid dynamics (CFD) and discrete element method (DEM) modelling of thermochemical behaviours in moving bed reactors [7]. The scaled model is derived based on the governing equations of mass, momentum and energy and then applied to a moving bed reactor. The results in terms of flow, heat and mass transfer and chemical reactions with different scaling factors demonstrate that two-order acceleration can be achieved merely by the scaling approach.

Then, the scaling approach is applied to a complicated moving bed reactor, a blast furnace (BF) to be specific, with significant variations of material properties. The results demonstrate that the scaled virtual BF model can reasonably predict infurnace flow state, temperature distribution, iron ore reduction and the characteristics of the cohesive zone. More importantly, the scaling approach makes its practical to track the whole process of iron ore reduction from burden charge to the cohesive zone [8].

It is a critical step forward towards establishing virtual real-time thermochemical reactors with discrete particle models.

References

- 1. Kuang, S. B., Li, Z. Y., Yu, A. B. (2018). Review on modeling and simulation of blast furnace. *Steel Research International*, *89*, 1700071.
- 2. Hou, Q. F., E, D. Y., Kuang, S. B., Li, Z. Y., Yu, A. B. (2017). DEM-based virtual experimental blast furnace: a quasi-steady state model. *Powder Technology*, *314*, 557-566.
- 3. Hou, Q. F., Zhou, Z. Y., Yu, A. B. (2012). Micromechanical modeling and analysis of different flow regimes in gas fluidization. *Chemical Engineering Science*, *84*, 449-468.

- 4. Hou, Q. F., Zhou, Z. Y., Yu, A. B. (2012). Computational study of the heat transfer in bubbling fluidized beds with a horizontal tube. *AIChE Journal*, *58*, 1422-1434.
- 5. Hou, Q. F., Zhou, Z. Y., Yu, A. B. (2016). Gas-solid flow and heat transfer in fluidized beds with tubes: Effects of material properties and tube array settings. *Powder Technology*, 296, 59-71.
- 6. Zhou, Z. Y., Yu, A. B., Zulli, P. (2009). Particle scale study of heat transfer in packed and bubbling fluidized beds. *AIChE Journal*, *55*, 868-884.
- 7. Hou, Q. F., E, D. Y., Kuang, S. B., Yu, A. B. (2019). A scaling approach for CFD-DEM modelling of thermochemical behaviours in moving bed reactors (To be published).
- 8. Hou, Q. F., E, D. Y., Kuang, S. B., Yu, A. B. (2019). A transient discrete element method-based virtual experimental blast furnace model (To be published).