# REACTIVE HYBRID EULERIAN/LAGRANGIAN TWO FLUID MODEL (TFM) SIMULATION OF INDUSTRIAL SCALE OLEFIN POLYMERIZATION FLUIDIZED BED REACTORS

Simon Schneiderbauer, Department of Particulate Flow Modelling, Johannes Kepler University, Linz, Austria
simon.schneiderbauer@jku.at
Stefan Pirker, Department of Particulate Flow Modelling, Johannes Kepler University, Linz, Austria
Pablo Aguayo, Vasileios Touloupidis, Borealis Innovation Process Technology, 4040 Linz, Austria
Alberto Martínez Joaristi, Borealis Innovation Process Technology, 2320 Schwechat-Mannswörth, Austria

Most industrial applications of particulate flows include reactive poly-disperse materials. Thus, it is important to understand the gas-solid reactions as well as the mixing, segregation and separation of the particles in the process to evaluate its efficiency.1,2 One of the most straight forward numerical methods to account for poly-disperse mixtures is DEM (discrete element method). However, since the total number of particles involved in most practically relevant gas-solid flows is extremely large, it may be impractical to solve the equations of motion for each particle. It is, therefore, common to investigate particulate flows in large process units using averaged equations of motion, i.e. two-fluid models (TFM), which include the inter-particle collisions statistically by kinetic theory based closures of the particle stresses.1–3 Even though each representative particle diameter requires an additional momentum and continuity equation, which considerably raises the computational demand with increasing number of particle diameters.4 Furthermore, the TFM approach requires considerably fine grids since the minimum stable sizes of clusters and shear bands are around ten particle diameters. Thus, due to computational limitations a fully resolved simulation of industrial scale reactors is still unfeasible. It is, therefore, common to use coarse grids to reduce the demand on computational resources. However, such a procedure inevitably neglects small (unresolved) scales, which leads, for example, to a considerable overestimation of the bed expansion in the case of fine particles. Many sub-grid drag modifications have, therefore, been put forth by academic researchers to account for the effect of small unresolved scales on the resolved meso-scales in this case (Schneiderbauer et al.5 and references cited therein).

In poly-disperse particle laden flows standard TFM approaches require a separate set of transport equations for each particle fraction under consideration. This inevitably leads to excess computational costs in particle laden flows which are characterized by broad particle size distributions. In this paper, following our previous work6 we therefore present a hybrid model for the numerical assessment of poly-disperse reactive gas-solid flows. The main idea of such a modeling strategy is to use a combination of a Lagrangian discrete phase model (DPM) and a coarse-grained TFM to take advantage of the benefits of those two different formulations. Furthermore, sub-grid drag corrections are applied to account for the impact of the small unresolved scales on the gas-solid drag force. Furthermore, this hybrid approach enables the efficient evaluation of gas-solid reactions at a particle level using the Lagrangian discrete phase model. Here, we consider the olefin polymerization accounting for the catalyst profile (activity over time),7 the pressure driven solubility of the reaction gases in the polymer particles, the particles crystallinity and the corresponding reaction masses and heats. These, in turn, appear as additional source terms in the TFM simulation.The predictive capability and numerical efficiency of this reactive hybrid modeling approach is demonstrated in the case of pilot scale olefin polymerization fluidized bed reactor. On the one hand, the model is able to predict process failures like chunking/sheeting correctly and on the other hand, the results give a closer insight about the temperatures, the local crystallinity of the polymer particles as well as the local and global particle size distributions in the reactor. It is shown that these properties are considerably affected by local injection of different process (reaction) gases.

1.Schneiderbauer, S., Puttinger, S., Pirker, S., Aguayo, P. & Kanellopoulos, V. CFD Modeling and Simulation of Industrial Scale Olefin Polymerization Fluidized Bed Reactors. *Chem. Eng. J.* 264, 99–112 (2015).
2.Aguayo, P., Schneiderbauer, S. & Kanellopoulos, V. Applications of the Euler-Granular Model for CFD Simulations of Industrial Fluidized Beds Reactors. in *Proceedings of the ANSYS Conference & CADFEM Users' Meeting 2013* (ANSYS, Inc., 2013).
3.Lun, C. K. K., Savage, S. B., Jeffrey, D. J. & Chepurniy, N. Kinetic theories for granular flow: inelastic particles in Couette flow and slightly inelastic particles in a general flowfield. *J. Fluid Mech.* 140, 223–256 (1984).
4.Schellander, D., Schneiderbauer, S. & Pirker, S. Numerical study of dilute and dense poly-dispersed gas-solid two-phase flows using an Eulerian and Lagrangian hybrid model. *Chem. Eng. Sci.* 95, 107–118 (2013).
5.Schneiderbauer, S., Puttinger, S. & Pirker, S. Comparative Analysis of Subgrid Drag Modifications for Dense Gas-Particle Flows in Bubbling Fluidized Beds. *AIChE J.* 59, 4077–4099 (2013).
6.Schneiderbauer, S., Puttinger, S. & Pirker, S. Numerical study of a bi-disperse gas-solid fluidized bed using an Eulerian and Lagrangian hybrid model. *Procedia Eng.* 102, 1539–1545 (2015).
7.Touloupidis, V. Mathematical Modelling and Simulation of an Industrial α-olefins Catalytic Slurry Phase Loop-reactor Series. (University of Thessaloniki, 2010 )