

## **209d Simulating the Hydrodynamics of Spouted Beds Using a Continuum Formulation**

*Dhanunjay (Jay) S. Boyalakuntla, Sreekanth Pannala, Carles E. A. Finney, and Stuart C. Daw*

Spouted beds have been prominent in the chemical industry since the 1960's, especially for processes in which solids agglomeration or coating are important objectives. Example spouted bed applications include drying and pyrolysis [Aguado et al, 2003], catalysis, gasification, and polymerization [Olazar et al, 1987, 1994, 1997], particle coating [Mathur and Epstein, 1974] and recent interest in nuclear fuel particle coating [Lowden et al, 2004]. Considerable experimental studies of spouted bed hydrodynamics have been reported over the years, including measurements of pressure drop, minimum spouting velocity, residence time, solids cycle time, spout height and width, gas and solids velocity profiles, and void fraction distribution [see for example, Mathur and Epstein, 1974]. Some studies have employed specialized probes like piezo-electric, fibre-optic probes [Olazar et al, 1995] as well as certain non-intrusive (radioactive tracer) techniques to study the spouted beds to understand better the gas-solid contact mechanisms.

More recently, there have been attempts to develop computer models capable of simulating the detailed dynamic behavior of spouted beds. Interest has grown in developing such models because they have the potential for improving our ability to account for the complex interactions of multiple simultaneous factors (e.g., the interaction of hydrodynamics and heat and mass transfer) in interpreting experimental data or in developing advanced reactor designs. Also, the detailed information available from such models offers the possibility of achieving unprecedented insights into the underlying physics.

Our specific objective here is to consider how continuum models can best be utilized for simulating spouted beds and how the resulting simulated dynamics should be compared with experimental measurements. We address these issues in the spirit of the recent discussion by Grace and Taghipour (2004), in which they rightly pointed out that many recent claims of model validation with experiments have serious deficiencies. In particular, we demonstrate that dynamical simulations need to be evaluated in terms of truly dynamic quantities in addition to time-averaged measurements from which temporal information has been removed. Temporal variations are especially important for spouted beds because they are ultimately responsible for solids circulation and mixing, which are perhaps the most critical hydrodynamic issues.

Our approach in this study has been to use a widely available continuum model (the MFIX code – <http://www.mfix.org>) to simulate the behavior of an experimental spouted bed for which time-average and dynamic measurements are available. As with all models of this type, there are several unknown physical parameters and computational assumptions required to implement the simulations. In this study, we address the impact of different choices for selected key parameters and assumptions, including [coefficient of restitution ( $e$ ), inventory size, mesh type (uniform or refined), spatial order of the numerical schemes (first-order versus second order), granular energy equation type (PDE versus algebraic), inlet pipe effect and also the effect of drag correlations used]. We assess the impact of these parameters on key temporal and spatial features in the spouted bed hydrodynamics and how these features compare with our experimental observations and the observations of other similar studies. While we do not arrive at a final set of parameters and assumptions for all spouted bed simulations, we do illustrate useful procedures for distinguishing good choices from bad ones. We also demonstrate that one of the most important physical processes in spouted beds is the energy dissipation that occurs between the spout and the outer annulus. It is clear that dissipation in this zone strongly affects global solids circulation and gas flow distribution. Assumptions about the granular stresses in regions of high solids density appear to be very important for accurately modeling this dissipation. We find that one of the most important factors in correctly predicting the observed dynamics is the way energy is transferred from gas-to-solids and subsequent dissipation for solid-solid and solid-wall interactions.

## References:

- 1.R. Lowden, J. Hunn, J. McLaughlin, J. Kelly, C. S. Daw, S. Pannala, and C. E. A. Finney, "Coated Particle Fuel for Advanced Gas Reactors", Annual Meeting of the American Ceramic Society, Indianapolis, Indiana, April 21, 2004
- 2.K. E. Mathur and N. Epstein, Spouted Beds. Academic Press, New York, USA (1974).
- 3.J. R. Grace and F. Taghipour., "Verification and validation of CFD models and dynamic similarity for fluidized beds", Powder Technology, 139: 99-110, 2004
- 4.J. Bilbao, M. Olazar, A. romero and J. M. Arandes, "Design and operation of a jet spouted bed reactor with continuous catalyst feed in the benzyl alcohol polymerization", Ind. Eng.Chem. Res., 26: 1297-1304, 1987
- 5.M. Olazar, M. J. San Jose, G. Zabala and J. Bilbao, "New reactor in jet spouted bed regime for catalytic polymerizations", Chemical Engineering Science, 49: 4579-4588, 1994
- 6.M. Olazar, M. J. San Jose, R. Llamossas, S. Alvarez and J. Bilbao, "Study of local properties in conical spouted beds using an optical fiber probe", Ind. Eng. Chem. Res., 34: 4033-4039, 1995
- 7.M. Olazar, J. M. Arandes, G. Zabala, A. T. Aguayo and J. Bilbao, "Design and Operation of a catalytic polymerization reactor in a dilute spouted bed regime", Ind. Eng. Chem. Res. 36:1637-1643, 1997
- 8.R. Aguado, M. Olazar, B. Gaisan, R. Prieto and J. Bilbao, "Kinetics of polystyrene pyrolysis in a conical spouted Bed reactor", Chemical Engineering Journal, 92: 91-99, 2003