Dynamic Reduced Order Models for a Bubbling Fluidized Bed Adsorber

Mingzhao Yu and Lorenz T. Biegler

Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA,

Distributed parameter first-principle models give an accurate physical description of chemical processes, but lead to large-scale models whose numerical solution is challenging and computationally expensive. The large amount of time required to solve the large-scale detailed model limits its use for process control and optimization tasks, where a large number of simulations need to be run. As a result, dynamic reduced order models with reasonable accuracy are required for advanced process control and other model based real-time applications.

In this study, we aim to build a dynamic reduced model for a bubbling fluidized-bed (BFB) adsorber, which is the essential component of an integrated carbon capture system for fossil fuel power plants. In this one-dimensional, three-region model, hydrodynamic behavior is described by partial differential and algebraic equations (PDAEs), constructed from mass and heat conservation and hydrodynamic correlations. Detailed equations for steady-state and dynamic BFB model can be found in [1, 2]. Besides, the reaction kinetic model for adsorption of CO_2 onto an amine-impregnated sorbent is developed in [3]. After spatial discretization, the model is converted to a differential and algebraic equation (DAE) system consisting of nearly 30000 equations. Solving such large-scale DAE system is computationally expensive. Thus, a reduced model of BFB adsorber is needed for simulation-based optimal design and control of the carbon capture system.

In the BFB model, where states are involved in different phases and regions, the time scale difference in differential states may lead to a high stiffness ratio and thus more integration steps. Singular perturbation is a useful tool for the reduction of models showing multiple time scale behavior. The underlying idea is the quasi-steady state approximation for fast states, which converts the differential equations describing the states with fast dynamics to algebraic equations. Eigenvalue analysis technique is used to locate fast and slow eigenvalue groups and unit perturbation spectral resolution (UPSR) matrix [4] is used to obtain a quantitative measure of the levels of association between all eigenvalues and states. Besides, we also apply the nullspace projection method [5] to the reaction kinetics of adsorption process to take advantage of the scale difference of reaction rates. The reformulated dynamic BFB model can be solved much faster while maintaining good accuracy.

Moreover, huge number of differential and algebraic equations, especially after spatial discretization, also increases the simulation time. The proper orthogonal decomposition (POD) is a powerful model reduction tool to create an accurate low dimensional approximation of large spatially distributed models. The key idea of POD is to find a low dimensional set of orthogonal basis functions, in which the spatial distribution information is captured, to represent the original high dimensional system. So POD technique is applied to identify the dominant spatial features inside the BFB adsorber and method of snapshots is used to generate POD empirical basis functions. Preliminary result shows that, instead of discretization over 100 points, only 6 to 7 basis functions are needed for each state, with an average projection error less than 0.1% , which shows great potential in further reducing the number of equations and computational cost.

[1] A. Lee and D. C. Miller. “A One-Dimensional (1-D) Three-Region Model for a Bubbling Fluidized-Bed Adsorber”. In: Ind. Eng. Chem. Res. 52 (2013), pp. 469–484.

[2] S. Modekurti, D. Bhattacharyya, and S. E. Zitney. “Dynamic Modeling and Control Studies of a Two-Stage Bubbling Fluidized Bed Adsorber-Reactor for Solid-Sorbent CO2 Capture”. In: Ind. Eng. Chem. Res. 52 (2013), pp. 10250–10260.

[3] A. Lee et al. “A model for the adsorption kinetics of CO2 on amine-impregnated mesoporous sorbents in the presence of water”. In: 28th International Pittsburgh Coal Conference, Pittsburgh, PA, USA. 2011.

[4] I. T. Cameron and A. M Walsh. “Unravelling complex system dynamics using spectral association methods”. In: Elsevier B.V., 2004. Chap. The Integration of Process Design and Control, pp. 126–145.

[5] Y. Nie, L. Biegler, C,Villa, and J, Wassick. “Reactor modeling and recipe optimization of polyether polyol processes: polypropylene glycol”. AIChE J. 2013, 59, 2515−2529