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Invariant based modeling and control of multi-phase reactor systems☆

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ABSTRACT

We propose a modeling framework for stable simulation of multi-phase reactor systems operating at thermodynamic equilibrium. The model framework can be used to determine system characteristics, explore parameter sensitivity and test control system strategies. The thermodynamic equilibrium assumption and the use of reaction invariants make it computationally inexpensive. We show that the feedback control approach based on the overall inventories of the system can be effectively used for improved performance of such reactor systems. Two multi-phase reactor systems – the vapor recovery reactor used in carbothermic aluminum reduction and the gasification reactor used in IGCC are considered to demonstrate the efficacy of the proposed modeling and control approach.

1. Introduction

Multi-phase reactor systems are used in a wide range of applications such as in power plants, petrochemical and chemical industries and in various other fields [1]. The multi-phase technology is gaining attention because of its flexibility and ability to perform reaction and separation in one process. In order to quantify the performance and optimize these reactor systems in the absence of any appropriate experimental technique to measure a specified parameter in the multi-phase region or for any expensive/harmful experiments, computational modeling is the key.

Multi-phase reactor systems are difficult to model or to be visualized because of complex phenomena like phase change, significant variation in physical properties and chemical reaction interactions. Also, the characteristics of such systems rely mostly on different processes at different scales. Hence, a consolidated analysis of all the processes at different scales and at different phases is not straightforward and can be of major challenge. Low order models are often employed to help in process development, scale-up, validation and process control.

Multi-phase systems are often modeled based on isothermal assumption with either a pseudo-homogeneous [2] or a heterogeneous model [3] along with plug flow for gas and liquid phases. There are other studies [4] where the non-isothermal behavior is modeled by implementing a one-dimensional pseudo-homogeneous energy balance.

Khadilkar et al. [5] developed a model for unsteady-state operation that captures the effect of multi-component transport, multiple reactions, phase change, intra-reactor wet-dry transition. Pellegrini et al. [6] modeled a hydrocracking Fischer Tropsch unit based on vapor–liquid equilibrium. Jarungthammachote and Dutta [7] used Gibbs energy minimization method to predict the composition of the gas produced by gasifying a solid fuel in a spouted bed.

One of the challenges of multi-phase reactors is numerical complexity due to changing number of components and phases. One of the applications we study is coal gasification where slag formation is an unwanted side reaction. It is difficult to model slag formation due to complex chemistry and phase change [8,9]. In this paper, we overcome these challenges by using a model based on thermodynamic equilibrium and representing the state with variables that do not depend on the number of phases or components present in the system.

We propose an invariant based modeling framework and control scheme for process systems operating at thermodynamic equilibrium. We identify a particular class of states of the process systems called invariant inventories. These invariant inventories are closely related to the concept of reaction invariants.

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