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On Decoupling Rate Processes in Chemical Reaction Systems – Methods and Applications

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Abstract

Models of chemical reaction systems can be complex as they need to include information regarding the reactions and the mass and heat transfers. The commonly used state variables, namely, concentrations and temperatures, express the interplay between many phenomena. As a consequence, each state variable is affected by several rate processes. On the other hand, it is well known that it is possible to partition the state space into a reaction invariant subspace and its orthogonal complement using a linear transformation involving the reaction stoichiometry. This paper uses a more sophisticated linear transformation to partition the state space into various subspaces, each one linked to a single rate process such as a particular reaction, mass transfer or heat transfer. The implications of this partitioning are discussed with respect to several applications related to data reconciliation, state and rate estimation, modeling, identification, control and optimization of reaction systems.

Keywords: Chemical reaction systems, Reaction variants, Vessel extents, Data reconciliation, State and rate estimation, Modeling and identification, Control and optimization.

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1. Introduction

The chemical industry uses reaction processes to convert raw materials into desired products. The models of chemical reaction processes are typically first-principles models that describe the evolution of the total mass, the concentrations and the temperature by means of balance equations of differential nature (continuity equation, molar balances, heat balance) and constitutive equations of algebraic nature (equilibrium relationships, rate expressions). A reliable description of reaction kinetics and transport phenomena represents the main challenge in building first-principles models for chemical reaction systems.

The presence of all these phenomena, and in particular their interactions, complicates the analysis and operation of chemical reactors. The analysis would be much simpler if one could somehow separate the effect of the various rate processes and investigate each rate individually. Ideally, one would like to have a

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