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Modelling and simulation of reactive transport phenomena

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Abstract

Mathematical modelling and numerical simulation of chemical transport phenomena are very challenging due to large numbers of species and reactions involved. Reactive transport models for such systems have high degrees of freedom, and therefore, are computationally expensive to solve. In this discussion, we present and numerically analyse stoichiometric decoupling method for reducing the high degrees of freedom and hence, cost of simulation. This method is a model reduction procedure that is based on some key properties of chemical systems. A multi-scale model of a passive treatment method for acidic mine effluents is used to test the efficacy of the reduction procedure. Moreover, reduced models are characteristically non-linear and stiff, thus, we used numerical techniques to study the reduction error in order to establish compatibility/efficiency of the reduction procedure.

Keywords: Modelling, simulation, chemical transport, model reduction, nonlinear, numerical techniques.

2000 MSC: 92E20, 80A30, 92F05

1. Introduction

Multi-scale modelling of reactive transport phenomena can enhance our understanding of chemical processes and also provide useful quantitative information for policy-making and for improving engineering designs.

However, due to the presence of many chemical species in most chemical systems, multi-scale models for reactive transport phenomena usually have high degrees of freedom and therefore, are computationally expensive to analyse or solve. Thus, it is necessary for model reduction techniques to be developed for such systems. Model reduction techniques have been developed and applied to many biochemical systems that do not involve transport phenomena. The reduction techniques and resulting approximations are in general, based on a partial equilibrium assumption, a quasi steady state assumption and a computational singular perturbation analysis of the system of interest [1, 2, 3].

Quasi steady state approximations (QSSAs) are common reduction techniques that have been successfully applied in biochemical systems for many years [1, 4]. The QSSAs reduce large systems by replacing derivatives of some species (in the system which are assumed to be in quasi equilibrium) with algebraic functions. However, it is reported

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