

The Use of Time-scale based methods for reducing the complexity of chemical reaction systems.

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Detailed chemical sub-systems are computationally expensive because of both the large number of coupled species and the large range in time-scales leading to stiff systems of equations. The presence of stiffness makes the use of implicit numerical methods difficult due to the need for extremely small time steps and often, even efficient stiff ODE solvers require significant computational resources. In chemical-transport models either model resolution or chemical detail is often sacrificed in order to make computational savings. Methods are therefore required for reduced chemical modelling within transport codes without loss of complexity or accuracy.

One method of reducing the complexity within a chemical sub-model is to make use of the range of time-scales present in the model by assuming that the fastest time-scales have equilibrated or collapsed onto a slow manifold. In this way the long time dynamics of a chemical reaction system can be described not in full species phase space, but on a lower dimensional or slow manifold. The fast modes are then described as functions of slow modes ( i.e. locally equilibrated) and effectively removed from the ODE system. Highly reduced variable sets can often be achieved which adequately represent the long time dynamics of the system, and computational savings of up to 1000 can be made over stiff ODE solvers.

The presentation will cover an introduction to time-scale methods and low dimensional manifolds. It will outline the use of locally linear perturbation methods for the investigation of system time-scales and will explore the relationship between chemical species couplings and time-scale modes. It will present a simple method for estimating errors resulting from the application of low dimensional manifolds and therefore estimating the local system dimensionality. Several methods for the application of time-scale methods for model reduction will be discussed including i) the Quasi-Steady State Approximation (QSSA), ii) the ILDM (intrinsic low dimensional manifold) method iii) repro-modelling.