PumpKin: A tool to find principal pathways in plasma chemical models

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In the present work we have developed a software tool called PumpKin (**p**athway red**u**ction **m**ethod for **p**lasma **kin**etic models) to find all principal pathways, i.e. the dominant reaction sequences, in chemical reaction systems. The goal was to reduce complex plasma chemistry models. Recent kinetic models of atmospheric chemistry, or any industrial application, contain thousands of chemical reactions and species. The main difficulty is that these reduced chemical pathways depend on timescales, electric field, temperature, pressure etc. PumpKin is a universal tool, which only requires from user the temporal profile of the densities of species and the reaction rates, as well the stoichiometric matrix of the system. Also, the user should specify the timescale of interest.

1. Introduction

The growing interest in plasma chemistry significantly increases the complexity of chemical models. Recent kinetic models of atmospheric chemistry [1] or of industrial applications [2] contain thousands of chemical reactions and species. Here one should take into consideration that different species have different lifetimes, reaction rates depend on externally applied electric field as well as on temperature. As a result, researchers and engineers are faced with the problem of evaluating very complex models. In some cases, it is crucial to be able to reduce the chemical reaction system to more compact chemical pathways, which will have much less reactions and will consider less species. Besides the practical and/or computational reasoning, this is very important for understanding the mechanisms of production and destruction of certain key species. For example, such techniques have been successfully applied in atmospheric chemistry to investigate ozone destruction [3].

In the present work we have developed the software PumpKin (**p**athway red**u**ction **m**ethod for **p**lasma **kin**etic models) to find all principal pathways, i.e. the important reaction sequences, in a given chemical reaction system. The user should solve first the full chemical reaction system, but only once. The output is later used as an input for PumpKin. PumpKin will analyze the full chemical reaction system, and it will automatically determine all significant pathways in the system, i.e. all pathways with a rate above a user-specified threshold.

2. Algorithm

As the problem is rather general, many different fields (atmospheric chemistry, oceanography, biological systems, genetics, plasma physics, combustion physics etc.) have their own tools and methods to deal with this problem. A general method to gain insight into a dynamical system is sensitivity analysis [4], which determines the response of the system to perturbations of individual parameters. However, it cannot determine complete pathways like, for instance, the catalytic ozone destruction cycles.

Our approach is based on the algorithm described in [5]. It starts from the basic idea of forming pathways by connecting shorter ones. Here are the key elements:

a) We assume the reaction rates are known, then we calculate the rate of each pathway.

b) In the case if a newly formed pathway includes sub-pathways, we don't simply delete it, but split it into its sub-pathways. Then its rate is fully distributed onto the sub-pathways, in order to conserve the total flux of molecules.

c) We also delete pathways with small rates, in order to avoid a too large number of pathways.

3. Software

The PumpKin package is written in object-oriented C++ language. The current version of the code reads input files in a format like the output format of the zero-dimensional plasma kinetics solver ZDPlasKin [6].

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5. References

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