GEC16-2016-000564

Abstract for an Invited Paper
for the GEC16 Meeting of
the American Physical Society

Modeling Complex Chemical Systems: Problems and Solutions

JAN VAN DIJK, Eindhoven University of Technology

Non-equilibrium plasmas in complex gas mixtures are at the heart of numerous contemporary technologies. They typically contain dozens to hundreds of species, involved in hundreds to thousands of reactions. Chemists and physicists have always been interested in what are now called *chemical reduction techniques* (CRT's). The idea of such CRT's is that they reduce the number of species that need to be considered *explicitly* without compromising the validity of the model. This is usually achieved on the basis of an analysis of the reaction time scales of the system under study, which identifies species that are in *partial equilibrium* after a given time span. The first such CRT that has been widely used in plasma physics was developed in the 1960's and resulted in the concept of *effective* ionization and recombination rates[1]. It was later generalized to systems in which multiple levels are effected by transport[2]. In recent years there has been a renewed interest in tools for chemical reduction and reaction pathway analysis. An example of the latter is the PumpKin tool[3]. Another trend is that techniques that have previously been developed in other fields of science are adapted as to be able to handle the plasma state of matter. Examples are the Intrinsic Low Dimension Manifold (ILDM) method and its derivatives, which originate from combustion engineering, and the general-purpose Principle Component Analysis (PCA) technique[4]. In this contribution we will provide an overview of the most common reduction techniques, then critically assess the pros and cons of the methods that have gained most popularity in recent years. Examples will be provided for plasmas in argon and carbon dioxide.

[1]D.R. Bates, A.E. Kingston and R.W.P. McWhirter, *Proc. R. Soc.* **A267** 297 (1962)
[2]J. van Dijk, A. Hartgers, J. Jonkers and J.A.M. van der Mullen, *J. Phys. D* **33** 2798 (2000)
[3]A.H. Markosyan, A. Luque, F. J. Gordillo-Vázquez, U. Ebert *Comp. Phys. Comm.* **185** 2697–2702 (2014). The underlying algorithm is discussed in: Ralph Lehmann, *Journal of Atmospheric Chemistry* **47** 45–78 (2004)
[4]Peerenboom, K.S.C., Parente, A., Kozak, T., Bogaerts, A. and Degrez, G. *Plasma Sources Science and Technology* **24**(2) 025004 (2015)