

ZDPLASKIN: A NEW TOOL FOR PLASMACHEMICAL SIMULATIONS

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Abstract. ZDPlasKin (Zero-Dimensional Plasma Kinetics) is a Fortran 90 module designed to follow the time evolution of the species densities and gas temperature in non-thermal plasmas with an arbitrarily complex chemistry. A Boltzmann equation solver (BOLSIG+) incorporated in ZDPlasKin provides values of electron transport and rate coefficients when the electron energy distribution function is non-Maxwellian. In this communication, we present an overview of ZDPlasKin and an example of its application in high-pressure argon plasmas.

1. INTRODUCTION

In this work we present ZDPlasKin (Zero-Dimensional Plasma Kinetics), a freeware utility which was developed for a wide range of complex plasmachemical simulations in various gas mixtures. Our approach is based on a local approximation of the evolution of species densities obtained by solving the conservation equations. In a first step a pre-processor is used to translate a list of species, reactions and corresponding rate constants in a simple flexible and user-friendly text format into a FORTRAN 90 module. This automatically generated module contains the definition of the problem, an interface to the DVODE_F90 ODE solver and a set of supplementary routines. It includes as well an automated link to BOLSIG+ [1], a Boltzmann equation solver based on the two-term approximation, which provides the electron transport rates and the rates of electron-neutral collisions. In a second step, execution of the code yields the time evolution of the species densities and the reaction rates. A simple acquisition algorithm allows tracing of time-averaged species densities and corresponding source terms and reaction rates for sensitivity analyses. ZDPlasKin is now available as freeware and can be downloaded from the following address: <http://www.zdplaskin.univ-tlse.fr/>.

2. PHYSICAL MODEL

The time evolution of the species densities in a plasma can be formulated as a set of coupled rate equations. In ZDPlasKin, the time evolution of $[N_i]$, density of species $i = 1 \dots i_{\max}$, as represented in eq. (1), is determined by numerical integration, starting with some initial conditions defined by the user. The source terms Q_{ij} corresponding to the contributions from different processes $j = 1 \dots j_{\max}$ are constructed automatically from information provided by the user in the input data file. The source terms corresponding to reaction (2), for example, are constructed using reaction rate k_j (3) (which is given by the user in the initial file, along with the reaction definition). The source terms are shown explicitly in eq. (4).

$$\frac{d[N_i]}{dt} = \sum_{j=1}^{j_{\max}} Q_{ij}(t) \quad (1)$$



$$R_j = k_j [A]^a [B]^b \quad (3)$$

$$Q_A = (a' - a)R, \quad Q_B = -bR, \quad Q_C = cR \quad (4)$$

$$\frac{N_{gas}}{\gamma - 1} \frac{dT_{gas}}{dt} = \sum_{j=1}^{j_{\max}} \pm \delta\varepsilon_j \cdot R_j + P_{clast} \cdot [N_e] \quad (5)$$