Recent developments on PLASMAKIN – a software package to model the kinetics in gas discharges

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PLASMAKIN is a software package for handling physical and chemical data used in plasma physics modeling and for computing gas-phase and gas-surface kinetics data: particle production and loss rates, photon emission spectra and energy exchange rates. It can handle an unlimited number of chemical species and reactions, is independent of problem dimensions, and can be used in both steady-state and transient problems. The package supports a large number of species properties and reaction types, namely: gas or electron temperature dependent collision rate coefficients, vibrational and cascade levels, evaluation of branching ratios, superelastic and other reverse processes, three-body collisions, radiation imprisonment and photoelectric emission. Support of non-standard rate coefficient functions can be handled by a user-supplied shared library.

The library has been expanded to (a) include a module to compute the electron kinetics; (b) allow the simulation of emission spectra in the chemical kinetics module; (c) simplify data input and (d) develop a Python interface [1].

Presently, the electron kinetics is limited to the case of zero magnetic field. The electron velocity distribution function (evdf) can be obtained under two different sets of assumptions:

a) Spatially homogeneous electron density with the angular dependency on velocity represented by a two-term spherical harmonic expansion; and

b) Non-constant electron density with the electrons moving in the hydrodynamic regime. The evdf is represented by a density gradients expansion.

The first case can be used to study DC and HF discharges at relatively low reduced field (E/N) and solves the Boltzmann equation following the treatment in [2]. The second case is useful for moderate to high constant E/N, when non-conservative processes are important or high precision values of transport coefficients are needed. In this case the Boltzmann equation is solved following the treatment in [3].

The chemical kinetics module now includes the simulation of emission spectra in two idealized situations: infinite slab and infinite cylinder. In mixtures with atomic vapours,

radiation trapping is taken into account assuming complete frequency redistribution in the laboratory rest frame [4].

The data input file, characterizing the species and reactions considered on a given discharge model, has been simplified with the use of a database of species properties.

The interface of procedures in the package has been engineered to allow the use from either Fortran or C programs. To allow prototyping or rapid development of programs using an interpreted language, a Python module providing function interfaces and classes has been developed [1] allowing access to the package when it has been compiled as a shared library.

Several examples of applications centered on the new capabilities will be presented.

[1] N.R. Pinhão 2007 *The Python Papers*, **2** (4) 35-47

[2] J. Loureiro, 1993 *Phys. Rev. E* **47** 1262

[3] P. Segur, P. M. Yousfi and M. C. Bordage 1984 *J. Phys. D: Appl. Phys.* **17** 2199-214

[4] A. F. Molish and B. P. Oehry 1998 *Radiation Trapping in Atomic Vapors*, Clarendon Press, Oxford.