Plasma diagnostics and simulations

Zero-dimensional plasma kinetics with ZDPlasKin

Introduction

The dynamics of species density $[N_i]$ is described by kinetic equation

$$\frac{d[N_i]}{dt} = \sum_j S_{ij}, \tag{1}$$

where the source term for specie i consists of a sum of corresponding reaction sources S_{ij} . For example, the source term for reaction

$$aN_i + bN_l + [\delta\epsilon] \rightarrow a'N_i + cN_m + [\delta\epsilon] \tag{2}$$

can be expressed using reaction rate R_j and reaction constant rate k_j as follows:

$$R_j = k_j[N_i]^a[N_l]^b, \tag{3}$$

$$S_{ij} = (a' - a)R_j. \tag{4}$$

The evolution of the gas temperature can optionally be taken into account, through energy loss/gain terms $[\delta\epsilon]$. Solution of the heat transport equation under adiabatic isometric approximation in the form

$$\frac{N_{gas}}{\gamma - 1}\frac{dT_{gas}}{dt} = \sum_j \pm\delta\epsilon_j \cdot R_j + P_{pelast} \cdot [N_e] + Q_{src} \tag{5}$$

gives for known specific gas heat ratio γ the evolution of gas temperature T_{gas}. The second term in the right side $P_{pelast} \cdot [N_e]$ is Joule heating due to the electron current and corresponds to elastic election-neutral collisions. The third term Q_{src} represents other heat sources.

ZDPlasKin and Bolsig+

ZDPlasKin 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 described by model equations above. 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. ZDPlasKin is now available as freeware and can be downloaded from the following address: `www.zdplaskin.laplace.univ-tlse.fr`.

BOLSIG+ is a free and user-friendly computer program for the numerical solution of the Boltzmann equation for electrons in weakly ionized gases in uniform electric fields, conditions which occur in swarm experiments and in various types of gas discharges and collisional low-temperature plasmas. Under these conditions the electron distribution function is non-Maxwellian and determined by an equilibrium between electric acceleration and momentum and energy losses in collisions with neutral gas particles.

The main utility of BOLSIG+ is to obtain electron transport coefficients and collision rate coefficients from more fundamental cross section data, which can then be used as input for fluid models.

The principles of BOLSIG+ can be summarized as follows:

- Electron-neutral collision cross sections versus electron energy are read from input files.
- It is assumed that the electric field and collision probabilities are constant in space and time and that there are no boundaries.
- Angular dependence of the electron velocity distribution is approximated by two-term Legendre expansion. Electron production/loss due to ionization/attachment is assumed to result in exponential growth/decay of the electron number density.

Under the above assumptions, the Boltzmann equation reduces to a convection-diffusion equation with non-local source term in energy space, which is then discretized by an exponential scheme and solved for the electron energy distribution function by a standard matrix inversion technique. Various electron transport coefficients and rate coefficients are calculated and accessible in different numerical/graphical forms and output file formats. Additional options are provided for AC electric fields, crossed electric and magnetic fields, electron-electron and electron-ion collisions.

Linking of BOLSIG+ with ZDPlasKin is done automatically wia BOLSIG+ module distributed within ZDPlasKin package.

BOLSIG+ as a separate executable program can be downloaded at `https://www.bolsig.laplace.univ-tlse.fr/`

Cross section data

Cross section data can be found at `www.lxcat.net` (pronounced "elecscat"), an open-access website for collecting, displaying, and downloading electron and ion scattering cross sections, swarm parameters (mobility, diffusion coefficient, etc.), reaction rates, energy distribution functions, etc. and other data required for modeling low temperature plasmas. The available data bases have been contributed by members of the community and are indicated by the contributor's chosen title. All download from this site data is compatible with ZDPlasKin package. Use of the data from this site in publications should be accompanied by proper references. Original references should be used where possible and reference should be made to the specific database(s) from which data were retrieved, the LXCat site address, and the retrieved date.

Tasks

1. Download and find out how to use ZDPlasKin and BOLSIG+.
2. Download cross section files for Ar from `www.lxcat.net`.
3. Run test case corresponding to an Ar plasma consisting of electrons, atomic ions, and neutrals. The charged particles are supposed to be generated by direct electron impact ionization and lost by 3-body recombination

$$\mathrm{e} + \mathrm{Ar} \rightarrow \mathrm{e} + \mathrm{e} + \mathrm{Ar}^+, \quad k_1 \tag{6}$$

$$\mathrm{e} + \mathrm{Ar}^+ + \mathrm{Ar} \rightarrow \mathrm{Ar} + \mathrm{Ar}, \quad k_2 \tag{7}$$

   The recombination rate coefficient assumed to be constant $k_2 = 10^{-25}$ cm^6/s, and the reduced field strength, E/N = 50 Td, is also constant. This system has a simple asymptotic solution.
4. Using BOLSIG+ separately, plot electron energy distribution function for Ar at E/N = 50 Td.
5. Using BOLSIG+ create tables for transport parameters and reactions rates as a function of E/N from 10 to 1500 Td.