Short users' guide to BOLSIG+ - version 1.2
23/09/2010

REFERENCES

The physical principles of BOLSIG+ are described in:
G. J. M. Hagelaar and L. C. Pitchford, "Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models", Plasma Sources Sci. Techn. **14** (2005) 722-733.

This users' guide frequently refers to this paper as 'our PSST paper'.

Cross section data in BOLSIG+ format can be downloaded for user-selected gases from the LXCat website: http://www.lxcat.laplace.univ-tlse.fr/.

INPUT OF COLLISION DATA

All collision data are read from text files, created and edited by the user with an external text editor. To read the data into BOLSIG+, press the 'Read collisions' button, specify the file name, and select a species from the list; this loads all collisions with the selected species. For gas mixtures (or mixtures of excited species), repeat the procedure. The loaded collisions are listed in the 'Collisions' box. To unload all collisions and start again, press 'Clear collisions'.

Two different file formats are supported: the old format, used by previous versions of BOLSIG, and a more flexible new format, which we recommend for BOLSIG+. In the old format, collision data are defined per target species, and collision cross sections and the corresponding the electron energies are given in separate tables. In the new format, each collision process is defined by separate block of data, consisting of :

(a) 1st line: Keyword in CAPITALS (case sensitive!) indicating the type of the collision. Possible collision types (keywords) are `MOMENTUM`, `ELASTIC`, `EXCITATION`, `IONIZATION`, and `ATTACHMENT`. For the use of `MOMENTUM` and `ELASTIC` see remark* below.

(b) 2nd line: Name of the target particle species, e.g. `Ar` for ground-state argon gas. This name must be one word, freely chosen by the user, and is used by the BOLSIG+ interface when reading in the data and when defining the gas composition. Optionally for excitation processes, the name of the corresponding excited (upper) state can be specified on the same line, separated from the target name by an arrow `->` or a double arrow `<->` , e.g. `Ar <-> Ar*`. BOLSIG+ ignores the arrow `->` and everything after it. The double arrow `<->` on the other hand activates the definition of the inverse super-elastic process with the indicated excited state as target; see remark** below.

(c) 3rd line, depending on collision type: For `ELASTIC` or `MOMENTUM` collisions, the ratio of the electron mass to the target particle mass. For `EXCITATION` or `IONIZATION`, the threshold energy in units eV. For `ATTACHMENT`, the 3rd line is missing. In case of an `EXCITATION` process where a double arrow and upper state have been indicated on the

2nd line (e.g. `Ar <-> Ar*`), the 3rd line must specify also ratio of the statistical weights of the upper state to the lower state.**

(d) Optionally: up to 100 lines of lines of user comment such as reference information.

(e) Finally: table of the cross section as a function of energy. The table starts and ends with a line of dashes '------' (at least 5), and has otherwise two numbers per line: the energy in units eV and the cross section in units m^2.***

Examples:

```
ELASTIC                          (a)
Ar                               (b)
0.136E-04                        (c) Mass ratio m/M
COMMENT: EFFECTIVE MOMENTUM-     (d)
TRANSFER CROSS SECTION
UPDATED: 2010-03-02 16:24:15
------------------               (e)
0     0.75E-19
0.01  0.75E-19
…     …
1E5   0.49E-22
---------------------
```

```
EXCITATION                       (a)
Ar                               (b) Alternatively: Ar -> Ar* (-> and further text ignored)
13.6                             (c) Threshold energy
------------------               (e)
…     …
---------------------
```

Remarks:

* Elastic vs. total momentum transfer. For each target species, the momentum-transfer cross section can be specified using either the keyword `ELASTIC` or the keyword `MOMENTUM`. `ELASTIC` refers to the elastic momentum-transfer cross section; BOLSIG+ will then construct the total momentum transfer cross-section by adding the inelastic cross sections; see equation (7) of our PSST paper. `MOMENTUM` indicates the total momentum-transfer cross section including both elastic and inelastic collisions. Note that the old data file SIGLO.SEC (old format) did not distinguish between elastic and total momentum transfer and contained some inconsistencies in this respect.

** There are two ways to define a super-elastic collision process. Firstly, it can be defined explicitly as an `EXCITATION` process with a negative threshold energy on the 3rd line (c). Secondly, it can be defined together with the corresponding forward `EXCITATION` process. In this case, the 2nd line (b) must contain the names of two species (corresponding to the upper and lower state of the transition) separated by a double arrow `<->`; the 3rd line (c) must specify both the transition energy u and the statistical weight ratio g (upper/lower). BOLSIG+ then constructs the super-elastic cross section σ_{inverse} vs. energy ε from the excitation cross section σ by detailed balancing:

$$\sigma_{\text{inverse}}(\varepsilon) = \frac{(\varepsilon + u)}{g\varepsilon}\sigma(\varepsilon + u).$$

Example:

```
EXCITATION
Ar <-> Ar*
13.6  6.
------------------
…      …
------------------
```

(a)
(b) Double arrow `<->` activates definition of inverse process
(c) Threshold energy and statistical weight ratio *g* upper/lower
(e)

*** Interpolation. BOLSIG+ assumes linear variation of the cross sections vs. energy between consecutive data points of the table (e), i.e. the cross section is a piecewise linear function of energy. All data points are taken into account exactly in the collision terms of the Boltzmann equation, equations (47)-(48) of the PSST paper.

Extrapolation. Below the first data point and beyond the last data point, BOLSIG+ assumes that the cross-section is constant at the values of these data points. Optionally, when reading in the cross section data, the user can check 'Extrapolate cross sections'. BOLSIG+ will then add data points beyond the last point of the table (e), at energies ε each time increasing by a factor 1.5, up to $\varepsilon > 10$ keV, assuming that the cross section decreases as $\ln(\varepsilon)/\varepsilon$.

For `EXCITATION` or `IONIZATION` collisions, a data point with zero cross-section is required at or beyond the threshold energy (c); if this is missing, BOLSIG+ will add it. BOLSIG+ will also remove any data points with non-zero cross-section below the threshold energy.

PERFORMING CALCULATIONS

To perform calculations, press the 'New run' button in the main window, specify the desired physical and numerical parameters in the conditions window, and press 'Run'. The main parameter in the conditions window is the reduced electric field E/N. In the menu in the top right corner of the conditions window, one can choose to

- perform a single calculation for a single value of E/N;
- perform a series of calculations for linearly increasing E/N;
- perform a series of calculations for quadratically increasing E/N;
- perform a series of calculations for exponentially increasing E/N;
- perform a series of calculations where E/N is automatically increased such that the mean electron energy increases approximately linearly over a given energy range; this option is very useful but sometimes fails when combined with some non-standard conditions such as high-frequency field oscillations;
- assume a Maxwellian energy distribution and calculate the electron properties and rate coefficients for a series linearly increasing electron mean energies, without solving the Boltzmann equation.

When using AC electric fields, the specified E/N values are reduced field amplitudes.

Other physical parameters specified in the conditions window are the gas temperature (only important for very low E/N values where the electrons may gain energy in elastic collisions

with gas particles), the fractional concentrations of the different target species (only in case there are more than one), the reduced field frequency (only for AC fields), and the ionization degree and electron density (only when accounting for electron-electron collisions). Some more advanced physical parameters (growth model and energy sharing model) are accessible by pressing the 'Details' button. For the meaning of these physical parameters see our PSST paper.

Numerical parameters can be accessed by pressing the 'Numerics' button in the conditions window. For most conditions the default numerical settings lead to optimal calculation results, but sometimes the user might want to try different settings. Increasing the number of grid points improves the accuracy of the results, but strongly reduces the calculation speed. Whenever a calculation fails to converge, the user can try to increase the maximum number of iterations or to use a fixed linear or quadratic computational grid with a fixed maximum energy, which must be estimated a priori.

The performed calculations are listed in the 'Runs' box in the main window. For each run the reduced electric field and the calculated mean energy are indicated. Pressing the 'Insert run' button inserts a calculation into a series, interpolating all physical and numerical conditions. Selected runs / all runs can be removed from the interface by pressing 'Delete run' / 'Clear runs'.

RESULTS

In addition to the EEDF, BOLSIG+ calculates numerous transport coefficients and rate coefficients for fluid models, which can be read from tables by pressing the 'Results' button, viewed in graphs by pressing 'Plot trends', or written in text files by pressing 'Save results'. Most of these coefficients are discussed in our paper in PSST. Below we list the coefficients the way they appear in the BOLSIG+ interface and output files. We indicate the corresponding equations in the PSST paper and give some additional definitions and remarks. The used symbols are defined as in the paper; N is the total gas density.

- Mean energy: $\bar{\varepsilon}$ from equation (58).
- Mobility × N (1/m/V/s): in case of a DC field, equation (55); in case of an AC field, the real part of equation (69).
- Diffusion coefficient × N (1/m/s): equation (56).
- Energy mobility × N (1/m/V/s): equation (61).
- Energy diffusion coefficient × N (1/m/s): equation (62).
- Imaginary mobility × N (1/m/V/s): in case of a AC field, the imaginary part of equation (69); otherwise zero.
- Cross-B diffusion coefficient × N (1/m/s). BOLSIG+ can also be used to calculate the EEDF in crossed DC electric and magnetic fields. Realize that the effect of the magnetic field is mimicked by making the electric field oscillate at the Larmor frequency $\omega = eB/m$. The mobility across the magnetic field is then given by the real part of equation (69). The diffusion coefficient across the magnetic field is:

  $$DN = \frac{\gamma}{3}\int_0^\infty \frac{\varepsilon\tilde{\sigma}_m}{\tilde{\sigma}_m{}^2 + q^2} F_0 \mathrm{d}\varepsilon ;$$

  the diffusion coefficient along the magnetic field is given by equation (56).

- Total collision frequency / N (m^3/s): sum over all collision processes, of the target species mole fraction x_k × rate coefficient k_k from equation (63).
- Effective momentum frequency / N (m^3/s): in case of a DC field,
  $$\frac{\bar{\nu}_{\text{eff}}}{N} = \frac{e}{m_e \mu N}$$
  with μN from equation (55); in case of a AC field, equation (70).
- Effective momentum transfer fraction: equation (71).
- Temporal growth coefficient (m^3/s): $\bar{\nu}_i / N$ from equation (10).
- Spatial growth coefficient (m^2): for the spatial growth model, α / N from equation (21); for the temporal growth model, $\alpha / N = (\bar{\nu}_i / N) / (\mu E)$.
- Power / N (eV m^3/s): in case of a DC field, mobility × N × $(E/N)^2$; in case of an AC field, 1/2 × the real part of the complex mobility of equation (69) × N × $(E/N)^2$.
- Elastic power loss / N (eV m^3/s):
  $$\sum_{k\ =\ \text{elastic}} x_k \frac{2m}{M_k} \gamma \int_0^\infty \sigma_k \varepsilon^2 F_0 \mathrm{d}\varepsilon \,.$$
- Inelastic power loss / N (eV m^3/s): sum over all inelastic collision processes, of the target species mole fraction x_k × threshold energy u_k × rate coefficient k_k from equation (63).
- Rate coefficients (m^3/s): equation (63). Note that these coefficients do not include the mole fractions of the target species and are calculated even if the target mole fraction is set to zero.
- Townsend coefficients / N (m^2): depending on the growth model, equation (66) or (67). Note that these coefficients do not include the mole fractions of the target species.
- Energy loss coefficients (eV m^3/s): for elastic collisions,
  $$\frac{2m}{M_k} \gamma \int_0^\infty \sigma_k \varepsilon^2 F_0 \mathrm{d}\varepsilon \,;$$
  for inelastic collisions, the threshold energy u_k × rate coefficient k_k from equation (63). Note that these coefficients do not include the mole fractions of the target species.
- Energy loss fractions: energy loss coefficients × target species mole fraction x_k × N / power. In contrast to the above collision coefficients, the energy loss fractions depend directly on the composition of the gas mixture. Note also that the sum of the energy loss fractions can be significantly smaller than unity due to growth effects, depending on the growth model.

Remark: When viewing or saving data, BOLSIG+ shows only calculations that are selected (highlighted) in the ‘Runs’ box in the main window. Similarly, the collision coefficients (rate coefficient, Townsend coefficient, etc) are shown only for processes that are selected in the ‘Collisions’ box in the main window. The selections can be changed with the mouse (hold down the ‘Shift’ key if necessary) even when a graphics window is open at the same time; the graph is then automatically updated. The collision selection has no effect on calculations: all collisions are always taken into account.