

Brief documentation of BOLSIG+ version 07/2015

G. J. M. Hagelaar

Laboratoire Plasma et Conversion d'Energie (LAPLACE), Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse Cedex 9

gerjan.hagelaar@laplace.univ-tlse.fr

Last revised 23 July 2015

Contents

Introduction	3
Windows graphical user interface: bolsigplus.exe	3
Console application: bolsigminus.....	4
Main input: collision cross section data	8
Further input parameters	11
Reduced electric field E/N (Td)	11
Angular frequency / N (rad.m3/s)	11
Cosine of E-B field angle	11
Gas temperature (K)	12
Excitation temperature (K).....	12
Gas composition mole fractions	12
Ionization degree	12
Plasma density (1/m3).....	13
Ion charge parameter.....	13
Ion/neutral mass ratio	13
Electron-electron momentum effects	13
Growth model.....	13
Energy sharing model.....	14
# of grid points	14
Grid type.....	14
Precision	14
Convergence.....	14
Output parameters	14
1. Mean energy (eV).....	14
2. Mobility *N (1/m/V/s).....	15
3. Real or perpendicular mobility *N (1/m/V/s)	15
4. Imaginary or Hall mobility *N (1/m/V/s)	15
5. Bulk mobility *N (1/m/V/s)	15
6. Diffusion coefficient *N (1/m/s)	15
7. Longitudinal diffusion coefficient *N (1/m/s)	15
8. Bulk T diffusion coefficient *N (1/m/s).....	16

9. Bulk L diffusion coefficient $\ast N$ (1/m/s).....	16
10. Energy mobility $\ast N$ (1/m/V/s)	16
11. Energy diffusion coefficient $\ast N$ (1/m/s).....	16
12. Total collision frequency /N (m^3/s)	16
13. Momentum frequency /N (m^3/s)	16
14. e-i momentum frequency /N (m^3/s).....	17
15. Total ionization frequency /N (m^3/s).....	17
16. Total attachment frequency /N (m^3/s)	17
17. Townsend ionization coefficient /N (m^2)	17
18. Townsend attachment coefficient /N (m^2).....	17
19. Power /N (eV m^3/s)	17
20. Elastic power loss /N (eV m^3/s).....	17
21. Inelastic power loss /N (eV m^3/s)	18
22. Growth power /N (eV m^3/s).....	18
23. e-i power loss /N (eV m^3/s)	18
24. Rate coefficients (m^3/s).....	18
25. Inverse rate coefficients (m^3/s)	18
26. Energy loss coefficients (eV m^3/s).....	18
27. Maximum energy (eV)	18
28. # of iterations	19
29. # of grid trials	19
List of symbols	19

Introduction

This documentation gives a brief description of all BOLSIG+ options, inputs and outputs.

Before reading this documentation and using BOLSIG+, users should be familiar with the physical principles of BOLSIG+ described in the following paper:

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. Technol.* **14**, 722-733 (2005)

The current version of BOLSIG+ contains several extensions which we shall describe in a follow-up paper to be published in the near future and which are available for the moment only on a provisional basis (i.e. no support or further explanation is provided):

- Advanced transport coefficients from density-gradient expansion method, such as anisotropic diffusion coefficients.
- Electric field crossed with magnetic field at arbitrary angle.
- Options for automatic inclusion of superelastic collisions, important at low reduced electric field and near thermal equilibrium, especially in molecular gases.
- Complete two-term collision operator for electron-electron and electron-ion Coulomb collisions.

BOLSIG+ can be downloaded from www.bolsig.laplace.univ-tlse.fr in two executable forms:

- 1) Windows application with graphical user interface, named ‘bolsigplus.exe’. Recommended for most users.
- 2) Console application for Windows or Linux without graphical interface, named ‘bolsigminus’. For experienced users who prefer a console type environment.

We do not provide the BOLSIG+ source code, under any conditions. For information regarding terms of use, copyright, and how to reference BOLSIG+ in scientific publications, we refer to the above BOLSIG+ website. Please carefully check all information on this website.

Windows graphical user interface: bolsigplus.exe

Launching ‘bolsigplus.exe’ under Windows opens the BOLSIG+ main panel. Two boxes on this panel summarize the data contained in BOLSIG+:

- ‘Collisions’ box: lists all collision processes loaded from data files and taken into account in the calculations. In this box, individual collisions or a subset of collisions can be selected with the mouse for output purposes (in a similar way as selecting files in the Windows explorer). This selection does not affect the Boltzmann calculations.
- ‘Runs’ box: lists all runs performed. A run corresponds to a single solution of the Boltzmann equation for a single set of conditions. In this box, one or more runs can be selected with the mouse for the purpose of plotting or saving the corresponding conditions or results. The box can be made larger by resizing the main panel with the mouse.

The right-hand side of the main panel features a series of buttons, launching different actions:

- Read collisions: loads collision cross section data from an input file. This button can be used multiple times to load different collision sets from different files, e.g. to create a gas mixture. BOLSIG+ will show the collisions in the order they were loaded. Adding new collisions removes all previous runs.

- Plot cross sections: plots cross section data versus electron energy for collisions selected in the ‘Collisions’ box. It is recommended to do this before starting the calculations in order to check that the collision data are properly loaded. The data points shown in the plot are used directly in the calculations, assuming the cross sections to be linear functions between these points.
- Clear collisions: unloads all collision data and removes all previous runs based on this data.
- New run: performs a new run (Boltzmann calculation) or series of runs, asking first for input of physical and numerical conditions. The conditions are organized under three tabs: physical, advanced and numerical conditions. Certain conditions or options may be hidden or blocked depending on the settings for other options.
- Rerun: allows user to modify the conditions for a given run selected in the ‘Runs’ box, and run it again. This can be useful for example to fix or investigate convergence problems by readjusting numerical parameters such as maximum # of iterations or manual maximum energy (see below).
- Insert run: inserts a new run at a selected point in the ‘Runs’ box, linearly interpolating all conditions. If desired the conditions can be modified later with the ‘Rerun’ button.
- Delete runs: removes selected run(s).
- Clear runs: removes all runs.
- Show values: shows numerical values of conditions and results (transport coefficients, rate coefficients) of selected run(s).
- Plot trends: plots transport coefficients and rate coefficients for selected runs and selected collisions, as a function of reduced electric field, electron mean energy, or run number.
- Plot EEDF: plots the distribution function f_0 or the anisotropy defined as the ratio $|f_1|/f_0$, versus electron energy. See list of symbols at end of document for the exact definition of f_0 and f_1 .
- Save results: saves conditions and results in different text file formats. Some result types are available only in certain formats, e.g. distribution functions can be saved only in ‘Run by run’ format.
- Exit: saves settings and closes program.

Console application: bolsigminus

The console application ‘bolsigminus’ reads a sequence of BOLSIG+ instructions from a text file and executes them. This file is to be edited by the user with an external text editor and its name to be specified as a command line argument when launching ‘bolsigminus’. The progression of execution and eventual error messages are written in a text file named ‘bolsiglog.txt’.

Each instruction consists of a block of data in fixed format, starting with a keyword in CAPITALS, corresponding (more or less) to a button or dialog of the graphical interface (described above).

Available instructions:

- READCOLLISIONS: loads collision data, similar to ‘Read collisions’ button.
- CLEARCOLLISIONS: unloads all collision data and removes all runs, similar to ‘Clear collisions’ button.
- CONDITIONS: defines complete set of physical and numerical conditions, in fixed order, to be used in subsequent calculations. Individual conditions can be marked with the keyword VAR in order to be specified later during RUN or RUN2D instructions.

- RUN: performs new run (Boltzmann calculation), requiring explicit values for previously defined VAR conditions (if these have been defined).
- RUNSERIES: performs series of runs for increasing reduced electric field or mean energy.
- RUNBACK: same as RUNSERIES except that runs are performed in reverse order; useful in order to check for bi-stable solutions.
- RUN2D: performs series of runs for combinations of two variable parameters and saves results in 2D output tables. Similar to RUNSERIES but with a second variable indicated with VAR in the conditions list.
- CLEARRUNS: removes all runs, similar to 'Clear runs' button.
- SAVERESULTS: saves conditions and results, similar to 'Save results' button.
- NOSCREEN: switches off all output to the screen terminal.
- END: terminates program.

Example of a bolsigminus script:

```
! Comment
/ Comment

/NOSCREEN

/READCOLLISIONS can be called multiple times to read from different files

READCOLLISIONS
LXCat-June2013.txt / File
Ar / Species
1 / Extrapolate: 0= No 1= Yes

READCOLLISIONS
LXCat-June2013.txt / File
N2 / Species
1 / Extrapolate: 0= No 1= Yes

CONDITIONS
10. / Electric field / N (Td)
0. / Angular field frequency / N (m3/s)
0. / Cosine of E-B field angle
300. / Gas temperature (K)
300. / Excitation temperature (K)
0. / Transition energy (eV)
0. / Ionization degree
1e18 / Plasma density (1/m3)
1. / Ion charge parameter
1. / Ion/neutral mass ratio
1 / e-e momentum effects: 0=No; 1=Yes*
1 / Energy sharing: 1=Equal*; 2=One takes all
1 / Growth: 1=Temporal*; 2=Spatial; 3=Not included; 4=Grad-n expansion
0. / Maxwellian mean energy (eV)
200 / # of grid points
0 / Manual grid: 0=No; 1=Linear; 2=Parabolic
200. / Manual maximum energy (eV)
1e-10 / Precision
1e-4 / Convergence
1000 / Maximum # of iterations
0.7 0.3 / Gas composition fractions
1 / Normalize composition to unity: 0=No; 1=Yes

RUN
```

CLEARRUNS

RUNSERIES

1 / Variable: 1=E/N; 2=Mean energy; 3=Maxwellian energy
0.1 100. / Min Max
31 / Number
3 / Type: 1=Linear; 2=Quadratic; 3=Exponential

RUNSERIES

1 / Variable: 1=E/N; 2=Mean energy; 3=Maxwellian energy
200. 1000. / Min Max
9 / Number
1 / Type: 1=Linear; 2=Quadratic; 3=Exponential

/SAVERESULTS can be called multiple times to write in different formats

SAVERESULTS

example1.dat / File
3 / Format: 1=Run by run; 2=Combined; 3=E/N; 4=Energy; 5=SIGLO; 6=PLASIMO
1 / Conditions: 0=No; 1=Yes
1 / Transport coefficients: 0=No; 1=Yes
1 / Rate coefficients: 0=No; 1=Yes
0 / Reverse rate coefficients: 0=No; 1=Yes
0 / Energy loss coefficients: 0=No; 1=Yes
1 / Distribution function: 0=No; 1=Yes
0 / Skip failed runs: 0=No; 1=Yes

!-----
! Second example: variable conditions
! In the CONDITIONS list, write VAR instead of value
! As many VARs as you like
! Specify values later, after RUN

CLEARRUNS

CONDITIONS

VAR / Electric field / N (Td)
VAR / Angular field frequency / N (m3/s)
0. / Cosine of E-B field angle
300. / Gas temperature (K)
300. / Excitation temperature (K)
0. / Transition energy (eV)
0. / Ionization degree
1e18 / Plasma density (1/m3)
1. / Ion charge parameter
1. / Ion/neutral mass ratio
1 / e-e momentum effects: 0=No; 1=Yes*
1 / Energy sharing: 1=Equal*; 2=One takes all
1 / Growth: 1=Temporal*; 2=Spatial; 3=Not included; 4=Grad-n expansion
0. / Maxwellian mean energy (eV)
200 / # of grid points
0 / Manual grid: 0=No; 1=Linear; 2=Parabolic
200. / Manual maximum energy (eV)
1e-10 / Precision
1e-4 / Convergence
1000 / Maximum # of iterations
0.99 0.01 / Gas composition fractions
1 / Normalize composition to unity: 0=No; 1=Yes

RUN

100. 0.
100. 1e-16
100. 1e-15
100. 1e-14
100. 1e-13
100. 1e-12
100. 1e-11

```

RUN
100. 1e-10

RUN
1000. 1e-10
10000. 1e-10

SAVERESULTS
example2.dat / File
2 / Format: 1=Run by run; 2=Combined; 3=E/N; 4=Energy; 5=SIGLO; 6=PLASIMO
1 / Conditions: 0=No; 1=Yes
1 / Transport coefficients: 0=No; 1=Yes
1 / Rate coefficients: 0=No; 1=Yes
0 / Reverse rate coefficients: 0=No; 1=Yes
0 / Energy loss coefficients: 0=No; 1=Yes
1 / Distribution function: 0=No; 1=Yes
0 / Skip failed runs: 0=No; 1=Yes

!-----
! Third example: generate 2D tables using RUN2D
! Similar to RUNSERIES but with a 2nd variable,
! indicated with VAR in the CONDITIONS list
! RUN2D also writes output file

CLEARRUNS

CONDITIONS
10. / Electric field / N (Td)
0. / Angular field frequency / N (m3/s)
0. / Cosine of E-B field angle
300. / Gas temperature (K)
300. / Excitation temperature (K)
0. / Transition energy (eV)
0. / Ionization degree
1e18 / Plasma density (1/m3)
1. / Ion charge parameter
1. / Ion/neutral mass ratio
1 / e-e momentum effects: 0=No; 1=Yes*
1 / Energy sharing: 1=Equal*; 2=One takes all
1 / Growth: 1=Temporal*; 2=Spatial; 3=Not included; 4=Grad-n expansion
0. / Maxwellian mean energy (eV)
100 / # of grid points
0 / Manual grid: 0=No; 1=Linear; 2=Parabolic
200. / Manual maximum energy (eV)
1e-10 / Precision
1e-4 / Convergence
1000 / Maximum # of iterations
1. VAR / Gas composition fractions
1 / Normalize composition to unity: 0=No; 1=Yes

RUN2D
1 / First variable: 1=E/N; 2=Mean energy; 3=Maxwellian energy
0.1 100. 0. 1. / Min1 Max1 Min2 Max2
20 5 / Num1 Num2
2 1 / Type1 Type2: 1=Linear; 2=Quadratic; 3=Exponential
example3.dat / Output file

! In the above example, the second variable is the mole fraction of the
! second gas component N2 which is then varied from 0. to 1. in 5 steps

END

```

Main input: collision cross section data

BOLSIG+ requires input of collision cross sections forming a complete set, accounting in a consistent manner for the complete electron energy losses and momentum losses due to collisions. These input data are read from standard text files in a simple format described below, which can be edited by the user with an external text editor. Complete cross section sets for a large number of gases, compiled by different contributors and with varying levels of detail, are available directly in BOLSIG+ format from the website of the LXCat data exchange project at www.lxcat.net. With BOLSIG+ we distribute an input file with our own in-house selection of cross section sets for common gases.

Note that for the sake of traceability, publications involving BOLSIG+ calculations must always make explicit reference to the cross section data set(s) used. Instructions for this are written in the header of any BOLSIG+ output file.

The format of the cross section data file is as follows. Each collision process is defined by separate block of data, consisting of:

- (a) Line 1: keyword in CAPITALS indicating the type of the collision: ELASTIC, EFFECTIVE, IONIZATION, ATTACHMENT, EXCITATION or ROTATION.
- (b) Line 2: name of the target particle species, consisting of a single word without spaces, freely chosen by the user, used by BOLSIG+ to identify the target species when loading the data and defining the gas composition.
- (c) Line 3: one or more parameter values, depending on the collision type as described below, e.g. threshold energy for inelastic collisions.
- (d) Optionally: up to 100 lines of user comment such as reference information.
- (e) Finally: table of the cross section as a function of energy, starting and ending with a line of dashes ----- (at least 5) and otherwise containing two numerical values per line: the energy in units eV and the cross section in units m^2 , separated by space or tab characters.

Further explanation on the different collision types (keywords) is given below.

- **ELASTIC**: elastic momentum-transfer process. Line 3 specifies the ratio of the electron mass to the target particle mass. The cross section in the table is the elastic momentum-transfer cross section, rather than the total elastic cross section.
- **EFFECTIVE** or **MOMENTUM**: effective process accounting for total momentum transfer due to all collisions with the same target particle species, englobing both elastic and inelastic momentum transfer. This is used in some data sets for historical reasons, but we wish to phase it out in the future and recommend using **ELASTIC** data instead, because these are more clearly defined. Line 3 gives the ratio of electron mass to target particle mass.
- **IONIZATION**: ionization process, inelastic collision in which a new electron is created. Line 3 gives the threshold energy in units eV.
- **ATTACHMENT**: attachment process, collision in which the electron is lost. Line 3 omitted.
- **EXCITATION**: electronic, vibrational, or rotational excitation process. Optionally, on line 2, the name of the excited (upper) state can be included, separated from the target name by an arrow \rightarrow or a double arrow \leftrightarrow , e.g. $\text{Ar} \leftrightarrow \text{Ar}^*$. BOLSIG+ ignores the arrow \rightarrow and everything after it. The double arrow \leftrightarrow on the other hand activates the superelastic inverse process with the indicated excited state as a target (to be loaded as a separate target species). Line 3 specifies the threshold energy in units eV, optionally followed by the statistical weight ratio of the upper state to the lower state, used by BOLSIG+ to account for the superelastic inverse process. If the statistical weight ratio is omitted, BOLSIG+ assumes it equal to 1.

- **ROTATION:** excitation process with additional parameters to facilitate handling large numbers of transitions between excited states, well adapted for rotational excitation of molecular targets. Line 3 gives the energy in eV (with respect to the ground state) and the statistical weight of the lower state of the process. An additional line 4 is required, giving the energy and statistical weight of the upper state. BOLSIG+ automatically constructs a list of all states occurring in the ensemble of ROTATION collisions with the same target species, computes the fractional populations of these states from Boltzmann factors, normalizing the ensemble to 1, and takes into account all super-elastic inverse processes. (Since each state is identified from the numerical values of its energy and statistical weight, it is important to specify these values consistently throughout the data file; numerical differences may cause BOLSIG+ to count the same state several times.) In the BOLSIG+ output, ROTATION collisions are by default grouped into a single output item per target species, e.g. a single net energy loss coefficient for rotational excitation. This grouping can be avoided by inserting the keyword **SHOWROT** in beginning the collision data file, telling BOLSIG+ to show each ROTATION collision separately.

Further remarks on the cross section data tables:

- **Interpolation:** BOLSIG+ assumes linear variation of the cross sections vs. energy between consecutive data points given in the table, i.e. the cross section is a piecewise linear function of energy. This piecewise linear function is taken into account exactly in the collision terms of the Boltzmann equation (see equations 47-48 of our PSST paper) and is completely independent of the energy grid used to discretize the Boltzmann equation.
- **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. When loading cross section data, an option is available to 'Extrapolate cross sections'. BOLSIG+ then adds data points beyond the last data point, at energies ε increasing each time by a factor 1.5 up to $\varepsilon > 10$ keV, assuming that the cross section decreases as $\ln(\varepsilon)/\varepsilon$.
- For **IONIZATION**, **EXCITATION** and **ROTATION** collisions, a data point with zero cross section is required at or beyond the threshold energy; if this is missing BOLSIG+ adds it automatically. BOLSIG+ also removes any data points with non-zero cross section below the threshold energy.

Examples:

ELASTIC	(a) Keyword
Ar	(b) Target gas name
0.136E-04	(c) Mass ratio
COMMENT : EFFECTIVE MOMENTUM- TRANSFER CROSS SECTION	(d) Optional comment
UPDATED : 2010-03-02 16 :24 :15	
-----	(e) Cross section table
0 0.75E-19	
0.01 0.75E-19	
...	
1E5 0.49E-22	

EXCITATION

Ar

11.5 6.

11.5 0.

12.7 7.0E-22

... ..

EXCITATION

Ar -> Ar*

11.5

... ..

EXCITATION

Ar <-> Ar*

11.5 6.

... ..

ROTATION

N2

0. 1.

0.0015 5.

N2 (J=0) <-> N2 (J=2)

Gerjouy and Stein, Phys. Rev.
97, 1671 (1954)

... ..

ROTATION

N2

0.0015 5.

0.0050 9.

N2 (J=2) <-> N2 (J=4)

... ..

(a)

(b)

(c) Threshold energy and statistical weight ratio

(e) Cross section table

Data point at threshold energy with zero cross section

(a)

(b) Last part -> Ar* is ignored

(c) Threshold energy, stat weight ratio assumed 1

(e)

(a)

(b) Enable superelastic process for target Ar*

(c) Threshold energy and statistical weight ratio

(e)

(a)

(b)

(c) Lower state energy and statistical weight

Upper state energy and statistical weight

(d) Comment

(e)

(a)

(b)

(c) Lower state energy and statistical weight

Upper state energy and statistical weight

(d) Comment

(e)

Further input parameters

Reduced electric field E/N (Td)

This is the main control parameter for BOLSIG+ calculations, defined as the ratio of electric field strength to gas particle number density in units of $1\text{Td} = 1\text{ Townsend} = 10^{-21}\text{ Vm}^2$.

Different options are available to specify this:

- Single run for a single value of E/N .
- Series of runs for linearly increasing E/N , for given initial and final E/N values and given number of runs. A typical E/N range for standard conditions is from 1 Td to a few 1000 Td.
- Series of runs for quadratically increasing E/N .
- Series of runs for exponentially increasing E/N .
- Series of runs where E/N is automatically increased such that the mean electron energy increases linearly over a given energy range. This option can be very useful but it requires more computation time than the previous options and it sometimes fails for non-standard conditions such as AC electric field or electron-ion Coulomb collisions.
- Calculation of transport and rate coefficients assuming a Maxwellian electron energy distribution function for a series of linearly increasing energy mean energies, without solving the Boltzmann equation, where each mean energy value corresponds to $3/2$ times the Maxwellian electron temperature in eV.

NB: In case of an AC electric field, the E/N values correspond to the RMS field values, i.e. the AC field amplitude divided by $2^{1/2}$. Using this definition, the AC results tend exactly to the DC results for the same E/N as the AC frequency is decreased to zero. This does not hold for earlier BOLSIG+ versions (before 2014) and our 2005 PSST paper, which defined E/N as the AC field amplitude.

NB: Under certain conditions, the steady-state solution of the Boltzmann equation is not unique due to nonlinear mechanisms, e.g. bi-stable solutions may arise due to Coulomb collisions. The BOLSIG+ results then depend on the initial conditions for the iterative procedure used to handle nonlinearities. When executing a series of runs for increasing E/N , BOLSIG+ estimates these initial conditions from the previous run in the series, and bi-stable solutions may be found by repeating the E/N series in reverse order. BOLSIG+ includes a special 'Run backwards' option for this purpose.

Angular frequency / N (rad.m³/s)

This parameter corresponds to the reduced angular frequency of an AC electric field or to the angular cyclotron frequency of magnetized electrons, using

$$\omega / N = (e / m_e)(B / N)$$

i.e. (angular frequency ω/N in units m^3/s) = $1.7588 \times 10^{-16} \times$ (reduced magnetic field B/N in units of 1 Huxley = 1 Hx = 10^{-27} T m^3). Setting this parameter to zero imposes a DC electric field without magnetic field.

NB: Some advanced options, such as spatial growth (SST) or anisotropic diffusion coefficients, are not available for AC or magnetic fields.

Cosine of E-B field angle

Cosine of the angle between the electric field and the magnetic field. Used only if a non-zero value has been specified for the angular frequency above. If this parameter is zero (90° angle) then the two-term Boltzmann equation for $E \times B$ fields has exactly the same form as that for an AC electric field, and BOLSIG+ does not make the distinction. Hence, in the console version of BOLSIG+, an AC field is modeled by setting this parameter to zero.

Gas temperature (K)

Used for elastic collisions and for superelastic collisions (as explained below).

Excitation temperature (K) and Transition energy (eV)

These parameters are used to calculate the population of excited neutral states in order to account for superelastic collisions, the inverse processes of excitation collisions. BOLSIG+ calculates the fractional populations y of the upper and lower states from bi-Maxwellian Boltzmann factors, with a transition from the gas temperature T_g to an excitation temperature T_{exc} occurring around a transition energy U_{tr} :

$$y^{(n)} = Ag^{(n)} \exp(-U^{(n)}e / (k_B T_{\text{exc}})) \quad U_{\text{tr}} = 0 \text{ or } T_{\text{exc}} = T_g$$

$$y^{(n)} = Ag^{(n)} \left[\exp((U_{\text{tr}} - U^{(n)})e / (k_B T_g)) + \exp((U_{\text{tr}} - U^{(n)})e / (k_B T_{\text{exc}})) \right] \quad T_{\text{exc}} > T_g$$

$$y^{(n)} = \frac{Ag^{(n)}}{\exp((U^{(n)} - U_{\text{tr}})e / (k_B T_g)) + \exp((U^{(n)} - U_{\text{tr}})e / (k_B T_{\text{exc}}))} \quad T_{\text{exc}} < T_g$$

where the upper index n refers to a quantum state, $U^{(n)}$ is energy of the state in eV, $g^{(n)}$ is its statistical weight, and A is a normalization constant such that the sum of fractional populations equals unity:

$$\sum_n y^{(n)} = 1.$$

For EXCITATION collisions, the normalization condition is applied to each process separately, with only two states $U^{(1)} = 0$ and $U^{(2)} = U = \text{threshold energy}$. For ROTATION collisions, normalization is done more rigorously over the ensemble of states within the same target species. The two temperatures can be used for example to model a typical ro-vibrational distribution, setting T_{exc} to the vibrational temperature and U_{tr} near the first vibrational threshold.

Given the population fractions y , the collision operator applied by BOLSIG+ for each excitation process k together with its superelastic inverse process is

$$\tilde{C}_{0,k=\text{exc}} = -\gamma x_k y_k^{\text{low}} \left[\varepsilon \sigma_k(\varepsilon) \left(f_0(\varepsilon) - \frac{y_k^{\text{up}} g_k^{\text{low}}}{y_k^{\text{low}} g_k^{\text{up}}} f_0(\varepsilon - U_k) \right) - (\varepsilon + U_k) \sigma(\varepsilon + U_k) \left(f_0(\varepsilon + U_k) - \frac{y_k^{\text{up}} g_k^{\text{low}}}{y_k^{\text{low}} g_k^{\text{up}}} f_0(\varepsilon) \right) \right] \quad U_k = U_k^{\text{up}} - U_k^{\text{low}}$$

where the superelastic cross section is assumed to obey the principle of detailed balancing:

$$\sigma^{\text{inv}}(\varepsilon) = \frac{g^{\text{low}}}{g^{\text{up}}} \frac{\varepsilon + U}{\varepsilon} \sigma(\varepsilon + U).$$

The statistical weights g have only a minor influence on this net collision operator, affecting it only indirectly through the lower state fractional population, so that it is often reasonable to assume $g = 1$.

If the excitation temperature is set to zero, BOLSIG+ neglects all superelastic collisions. This was the default setting in earlier versions of BOLSIG+, but often it is not appropriate for low reduced electric fields ($E/N < \text{few Td}$), causing unphysical artifacts such as the electrons cooling down below the gas temperature.

Gas composition mole fractions

Fractions of the total neutral gas particle number density N carried by the different particle species composing a gas mixture, i.e. ratios of the species densities to the total gas density.

Ionization degree

Main control parameter for Coulomb collisions, defined as the ratio of the electron number density to the neutral particle number density. However, in case electron-electron collisions are switched off, this

parameter is rather the ratio of the ion number density to the neutral particle number density. Setting this parameter to zero suppresses all Coulomb collisions.

Plasma density (1/m3)

Plasma electron number density used to calculate the Coulomb logarithm in the binary Coulomb collision operator. Has only a weak effect on the results, so an order to magnitude estimate of the plasma density is sufficient.

Ion charge parameter

Parameter controlling the importance of electron-ion Coulomb collisions with respect to electron-electron collisions, defined as

$$Z = \frac{1}{n_e} \sum_i Z_i^2 n_i$$

where n_e is the electron density and the sum is over different ions species with charge numbers Z_i and densities n_i . For quasineutral electropositive low-temperature plasmas this parameter is usually close to 1, for electronegative plasmas it can be much larger. In the console version of BOLSIG+, this parameter can be used to switch off one Coulomb collision type but not the other: $Z = 0$ removes electron-ion collisions (while keeping electron-electron collisions); $Z = -1$ removes electron-electron collisions (while keeping electron-ion collisions).

Ion/neutral mass ratio

Parameter used to calculate the average ion mass from the average gas particle mass, in order to be able to account for electron energy losses in electron-ion Coulomb collisions. For mixtures defined as

$$\frac{\langle m_i \rangle}{\langle M \rangle} = \frac{\sum_i Z_i^2 n_i}{\sum_i Z_i^2 n_i / m_i} \sum_n x_n / M_n$$

where the sums are over different ion species i with charge numbers Z_i , densities n_i and masses m_i and over different neutral species n with mole fractions x_n and masses M_n . By default BOLSIG+ assumes this parameter equal to 1, i.e. ion mass = gas particle mass.

Electron-electron momentum effects

Advanced option to account for diffusion of momentum in energy space due to electron-electron Coulomb collisions (as in classical Spitzer resistivity), based on the work of Rosenbluth [Rosenbluth et al, Phys. Rev 107, 1-6 (1957)]. This will be described in a future publication.

Growth model

Method to account for the effects of production or loss of electrons in ionization or attachment, based on different assumptions for the evolution of the electron density in time and space. Different options are available:

- 1) Exponential temporal growth, as in Pulsed Townsend (PT) experiments. Default option.
- 2) Exponential spatial growth, as in Steady State Townsend (SST) experiments. This option is sensitive to numerical convergence issues, as yet unresolved.
- 3) Not included: IONIZATION is treated as EXCTATION and ATTACHMENT is ignored.
- 4) Density gradient expansion: classical method to obtain transport coefficients without a priori assumptions on the density evolution [Kumar et al, Aust. J. Phys. **33**, 343-448 (1980)]. This option gives access to advanced transport coefficients for the analysis of swarm data, such as anisotropic diffusion coefficients.

Options 2) and 4) are not available in combination with AC or magnetic fields or with the advanced option for momentum effects in e-e collisions.

Energy sharing model

Model for how the energy is shared between primary and secondary electrons in ionization collisions. Two options: 1) equal energy sharing or 2) primary takes all energy, secondary at rest.

of grid points

Number of points of the numerical energy grid used to discretize the electron distribution function and Boltzmann equation. Increasing this number increases the accuracy of the results but also very strongly the computation time. Usually 100 grid points is an appropriate choice, but sometimes more points (200, 400, 800) are needed to eliminate numerical discretization errors, depending also on the type of result being considered, e.g. the longitudinal diffusion coefficient is more sensitive to numerical errors than the ionization rate coefficient. This parameter is completely independent of the discretization of the cross sections in the input data tables.

Grid type and Maximum energy (eV)

Parameters determining the spacing of the energy grid points used to discretize the distribution function and Boltzmann equation. Available grid type options:

- 1) Automatic determination of maximum energy and grid stretching.
- 2) Manual maximum energy (fixed by user) and linear grid.
- 3) Manual maximum energy and quadratic grid.

Precision

Parameter controlling the truncation of the distribution function at the high energy end, defined as the ratio of the minimum to maximum f_0 values over the energy grid domain. This parameter should never be smaller than the machine precision.

Convergence and Maximum # of iterations

Parameters to terminate the iterative procedure used by BOLSIG+ to handle nonlinear terms due to the growth model or Coulomb collisions. The ‘convergence’ parameter is used in different convergence criteria on the relative change of f_0 between iterations and the fractional residue of the overall energy balance. If these criteria cannot be met within the specified maximum number of iterations, an error flag is set.

Output parameters

Below we give the mathematical expressions used to calculate the BOLSIG+ output parameters, as well as some brief further explanations. The mathematical symbols are defined in the list at the end of this document; most definitions (but not all) are the same as in our 2005 PSST paper. All units are SI units except that energies are in eV; following a common convention in low-temperature plasma literature (e.g. Lieberman’s book) we use $1 \text{ eV} = 1 \text{ V}$ rather than $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$ (i.e. the variable ϵ has the dimension of voltage rather than energy).

All transport coefficients in the BOLSIG+ output have been multiplied or divided by the total gas density N such as to obtain ‘reduced’ coefficients which are independent of N , indicated below in brackets (). The unreduced transport coefficients for a specific value of N are found by applying the inverse operation, dividing or multiplying the reduced coefficients by this specific N value, e.g. the mobility μ at $N = 3.2 \times 10^{22} \text{ m}^{-3}$ (pressure of 1 Torr & room temperature) is $(\mu N) / (3.2 \times 10^{22} \text{ m}^{-3})$.

1. Mean energy (eV)

$$\langle \epsilon \rangle = \int_0^{\infty} \epsilon^{3/2} f_0 d\epsilon$$

2. Mobility *N (1/m/V/s)

$$(\mu N) = -\frac{\gamma}{3} \int_0^\infty \frac{\varepsilon}{Q} \frac{\partial f_0}{\partial \varepsilon} d\varepsilon$$

Mobility corresponding to DC transport, even in case an AC electric field is set for the electron heating. In case of magnetic field: mobility along magnetic field lines.

3. Real or perpendicular mobility *N (1/m/V/s)

$$(\mu_{\text{Re}} N) = (\mu_{\perp} N) = -\frac{\gamma}{3} \int_0^\infty \frac{Q\varepsilon}{Q^2 + q^2} \frac{\partial f_0}{\partial \varepsilon} d\varepsilon$$

In case of AC electric field: real part of mobility, in phase with the field, determining power absorption. In case of magnetic field: mobility component for classical collisional transport across the magnetic field lines. Not calculated for DC electric field without magnetic field.

4. Imaginary or Hall mobility *N (1/m/V/s)

$$(\mu_{\text{Im}} N) = (\mu_{\times} N) = -\frac{\gamma}{3} \int_0^\infty \frac{q\varepsilon^{1/2}}{Q^2 + q^2} \frac{\partial f_0}{\partial \varepsilon} d\varepsilon$$

In case of AC electric field: absolute value of imaginary part of electron mobility, out of phase with the field, determining reactive power. In case of magnetic field: absolute value of electron mobility component for magnetic drift in $\mathbf{E} \times \mathbf{B}$ direction. Not calculated for DC electric field without magnetic field.

NB: From the above mobility components, the electron current density due to an AC electric field or due to DC crossed electric and magnetic fields is

$$\mathbf{j}_{\text{AC}} = en_e \mu_{\text{Re}} \mathbf{E} - en_e \frac{\mu_{\text{Im}}}{\omega} \frac{\partial \mathbf{E}}{\partial t}$$

$$\mathbf{j}_{\text{ExB}} = en_e \mu (\mathbf{E} \cdot \mathbf{b}) \mathbf{b} + en_e \mu_{\perp} (\mathbf{E} - (\mathbf{E} \cdot \mathbf{b}) \mathbf{b}) - en_e \mu_{\times} \mathbf{E} \times \mathbf{b} \quad \text{with } \mathbf{b} = \mathbf{B}/B$$

5. Bulk mobility *N (1/m/V/s)

$$(\mu' N) = (\mu N) + \frac{1}{(E/N)} \int_0^\infty \tilde{C}_0[g_0] d\varepsilon$$

Apparent mobility which arises when deriving the drift-diffusion-continuity equation through the density gradient expansion method, useful for analysis of swarm data but not recommended for general plasma modeling (due to ambiguous description of ionization), e.g. see [Petrovic et al, J. Phys. D: Appl. Phys. **42**, 194002 (2009)].

6. Diffusion coefficient *N (1/m/s)

$$(DN) = (D_{\text{T}} N) = \frac{\gamma}{3} \int_0^\infty \frac{\varepsilon}{Q} f_0 d\varepsilon$$

Standard expression for diffusion coefficient, corresponding to transversal diffusion coefficient from density gradient expansion method with density gradient perpendicular to electric field. Used in swarm data analysis, but relevance for general plasma modeling is not clear.

7. Longitudinal diffusion coefficient *N (1/m/s)

$$(D_{\text{L}} N) = (D_{\text{T}} N) + (E/N) \frac{\gamma}{3} \int_0^\infty \frac{\varepsilon}{Q} \frac{\partial g_0}{\partial \varepsilon} d\varepsilon - (\mu' N) (E/N)^2 \frac{1}{3} \int_0^\infty \frac{\varepsilon^{1/2}}{Q^2} \frac{\partial f_0}{\partial \varepsilon} d\varepsilon$$

Longitudinal diffusion coefficient from density gradient expansion method with density gradient parallel to electric field. Used in swarm data analysis, but relevance for general plasma modeling is not

clear. Available only for standard swarm conditions; not calculated in case of AC electric field, magnetic field, SST growth or Coulomb collisions.

8. Bulk T diffusion coefficient *N (1/m/s)

$$(D_T' N) = (D_T N) + \int_0^{\infty} \tilde{C}_0[h_0] d\varepsilon$$

Apparent transversal diffusion coefficient which arises when deriving the drift-diffusion-continuity equation through the density gradient expansion method [Petrovic, see 5 above]. Useful for analysis of swarm data but not recommended for general plasma modeling (due to ambiguous description of ionization).

9. Bulk L diffusion coefficient *N (1/m/s)

$$(D_L' N) = (D_L N) + \int_0^{\infty} \tilde{C}_0[h_0] d\varepsilon$$

Apparent longitudinal diffusion coefficient which arises when deriving the drift-diffusion-continuity equation through the density gradient expansion method [Petrovic, see 5 above]. Useful for analysis of swarm data but not recommended for general plasma modeling (due to ambiguous description of ionization).

10. Energy mobility *N (1/m/V/s)

$$(\mu_\varepsilon N) = -\frac{\gamma}{3\langle\varepsilon\rangle} \int_0^{\infty} \frac{\varepsilon^2}{Q} \frac{\partial f_0}{\partial \varepsilon} d\varepsilon$$

Transport coefficient for DC convective electron energy flux used by some authors in the electron energy equation. This coefficient multiplied by the mean electron energy $\langle\varepsilon\rangle$ is sometimes called ‘thermoelectric coefficient’ [W. P. Allis, *Electrons Ions and Waves*, p. 173 (MIT Press, Cambridge, 1967)]. Its relevance for general plasma modeling is not clear.

11. Energy diffusion coefficient *N (1/m/s)

$$(D_\varepsilon N) = \frac{\gamma}{3\langle\varepsilon\rangle} \int_0^{\infty} \frac{\varepsilon^2}{Q} f_0 d\varepsilon$$

Transport coefficient for diffusive electron energy flux used by some authors in the electron energy equation. This coefficient multiplied by the mean electron energy $\langle\varepsilon\rangle$ is sometimes called “heat diffusivity” [Allis, see above]. Its relevance for general plasma modeling is not clear.

12. Total collision frequency /N (m³/s)

$$(\nu_{\text{tot}} / N) = \gamma \int_0^{\infty} \sum_{k=\text{all}} x_k \sigma_k \varepsilon f_0 d\varepsilon$$

Collision frequency summed over all electron-neutral collisions, without Coulomb collisions.

13. Momentum frequency /N (m³/s)

$$(\nu_m / N) = \frac{e}{m_e (\mu N)} - (\nu_{ei} / N)$$

Effective frequency for DC momentum transfer in electron-neutral collisions, without electron-ion Coulomb collisions.

14. e-i momentum frequency /N (m³/s)

$$(\nu_{ei} / N) = -\frac{2ex_i}{3m_e(\mu N)} \int_0^\infty \sigma_{ei} \frac{\varepsilon^{3/2}}{Q} \frac{\partial f_0}{\partial \varepsilon} d\varepsilon$$

Effective frequency for momentum transfer in electron-ion Coulomb collisions.

15. Total ionization frequency /N (m³/s)

$$(\nu_{iz} / N) = \gamma \int_0^\infty \sum_{k=\text{ionization}} x_k \sigma_k \varepsilon f_0 d\varepsilon$$

Total ionization frequency, number of electrons created per unit time.

16. Total attachment frequency /N (m³/s)

$$(\nu_{at} / N) = \gamma \int_0^\infty \sum_{k=\text{attachment}} x_k \sigma_k \varepsilon f_0 d\varepsilon$$

Total attachment frequency, number of electron lost per unit time.

17. Townsend ionization coefficient /N (m²)

$$(\alpha / N) = \frac{(E / N)(\nu_{iz} / N)}{(P / N)}$$

First Townsend ionization coefficient, total number of electrons created per unit length.

18. Townsend attachment coefficient /N (m²)

$$(\eta / N) = \frac{(E / N)(\nu_{at} / N)}{(P / N)}$$

First Townsend attachment coefficient, total number of electrons lost per unit length.

19. Power /N (eV m³/s)

Energy per unit time absorbed by the electrons from the electric field, calculated from different expressions depending on the field configuration, as follows.

DC electric field with temporal growth (PT) or without growth:

$$(P / N) = (\mu N)(E / N)^2$$

DC electric field with spatial growth (SST):

$$(P / N) = (\mu N)(E / N)^2 \left(\frac{1}{2} + \frac{1}{2} \left(1 - \frac{4(DN)((\nu_{iz} - \nu_{at}) / N)}{(\mu N)^2 (E / N)^2} \right)^{1/2} \right)$$

AC electric field:

$$(P / N) = (\mu_{Re} N)(E / N)^2$$

DC electric field crossed with magnetic field under angle β :

$$(P / N) = ((\mu_{Re} N) \sin \beta + (\mu N) \cos \beta)(E / N)^2$$

20. Elastic power loss /N (eV m³/s)

$$(P_{el} / N) = \sum_{k=\text{elastic}} \gamma x_k \frac{2m_e}{M_k} \int_0^\infty \left[\sigma_k \left(\varepsilon^2 f_0 + \frac{k_B T}{e} \frac{\partial f_0}{\partial \varepsilon} \right) \right] d\varepsilon$$

Total net energy loss rate due to elastic electron-neutral collisions, without electron-ion Coulomb collisions.

21. Inelastic power loss /N (eV m3/s)

$$(P_{\text{inel}} / N) = \sum_{k=\text{inel}} U_k x_k (y_k^{\text{low}} k_k - y_k^{\text{up}} k_k^{\text{inv}})$$

Total net energy loss rate due to inelastic collisions, including superelastic collisions.

22. Growth power /N (eV m3/s)

Apparent energy loss rate due to electrons appearing or disappearing in ionization or attachment.

In case of temporal (PT) growth model:

$$(P_{\text{growth}} / N) = ((v_{\text{iz}} - v_{\text{at}}) / N) \langle \varepsilon \rangle$$

In case of spatial (SST) growth model:

$$(P_{\text{growth}} / N) = ((\alpha - \eta) / N) \left[((\alpha - \eta) / N) (D_{\varepsilon} N) - (E / N) (\mu_{\varepsilon} N) \right] \langle \varepsilon \rangle - (E / N) (DN)$$

23. e-i power loss /N (eV m3/s)

$$(P_{ei} / N) = \gamma x_i \frac{2m_e}{\langle m_i \rangle} \int_0^{\infty} \left[\sigma_{ei} \left(\varepsilon^2 f_0 + \frac{k_B T}{e} \frac{\partial f_0}{\partial \varepsilon} \right) \right] d\varepsilon$$

Total net energy loss rate due to electron-ion Coulomb collisions.

NB: BOLSIG+ checks numerical convergence from the balance of the above five power outputs:

$$(P / N) = (P_{\text{el}} / N) + (P_{\text{inel}} / N) + (P_{\text{growth}} / N) + (P_{ei} / N) + \text{numerical errors}$$

24. Rate coefficients (m3/s)

$$k_k = \gamma \int_0^{\infty} \varepsilon \sigma_k f_0 d\varepsilon$$

Rate coefficient for each individual collision process k.

25. Inverse rate coefficients (m3/s)

$$k_k^{\text{inv}} = \gamma \int_0^{\infty} \varepsilon \sigma_k^{\text{inv}} f_0 d\varepsilon = \gamma (g^{\text{low}} / g^{\text{up}})_k \int_0^{\infty} (\varepsilon + U_k) \sigma(\varepsilon + U_k) f_0(\varepsilon) d\varepsilon$$

Rate coefficient for superelastic inverse process of each individual excitation process k.

26. Energy loss coefficients (eV m3/s)

Coefficient for net energy loss per unit time in each individual collision process k.

For elastic collisions:

$$K_k = \frac{2m_e}{M_k} \gamma \int_0^{\infty} \left[\sigma_k \left(\varepsilon^2 f_0 + \frac{k_B T}{e} \frac{\partial f_0}{\partial \varepsilon} \right) \right] d\varepsilon$$

For inelastic collisions without superelastics:

$$K_k = U_k k_k$$

For excitation collisions with superelastic inverse process: net energy loss rate including quantum state population fractions:

$$K_k = U_k (y_k^{\text{low}} k_k - y_k^{\text{up}} k_k^{\text{inv}})$$

27. Maximum energy (eV)

Upper boundary of numerical grid in energy space, automatically determined and/or readjusted during iterative solution procedure.

28. # of iterations

Total number of iterations performed during solution procedure.

29. # of grid trials

Number of different energy grid configurations used during solution procedure, 1 + number of grid adjustments needed.

List of symbols

Symbol	Unit	Description
\mathbf{B}, B	T	Magnetic field vector and strength
$\tilde{C}_0[]$	$\text{eV}^{1/2}\text{m}^3\text{s}^{-1}$	Collision operator for isotropic part of distribution function.
e	C	Elementary charge
E	V/m	Electric field
ε	eV	Electron energy
f_0	$\text{eV}^{-3/2}$	Isotropic part of electron distribution function, corresponding to zeroth-order term of spherical harmonics expansion in velocity space, sometimes called “electron energy probability function” (EEPF) e.g. in [Lieberman and Lichtenberg, “Principles of plasma discharges and materials processing” (Wiley, New York, 2005)].
g_0	$\text{eV}^{-3/2}\text{m}^{-2}$	First-order component of density-gradient expansion of distribution function; perturbation of f_0 due to electron density gradient.
γ	$\text{C}^{1/2}\text{kg}^{-1/2}$	Constant coefficient: $\gamma = (2e / m_e)^{1/2}$
h_0	$\text{eV}^{-3/2}\text{m}^{-4}$	Second-order component of density-gradient expansion of distribution function; perturbation of f_0 due to curvature of electron density profile.
N	m^{-3}	Total gas particle number density
$n_{e,i}$	m^{-3}	Electron and ion number density
Q	m^2	Effective total momentum-transfer cross section, including superelastics and electron-ion Coulomb collisions, if activated. In case of PT growth model, including also effects of creation or loss. $Q = \sum_{k=\text{all}} x_k y_k^{\text{low}} \sigma_k + \sum_{k=\text{exc}} x_k y_k^{\text{up}} \sigma_k^{\text{inv}} + x_i \sigma_{ei} + ((\nu_{iz} - \nu_{at}) / N) / (\gamma \varepsilon^{1/2})$
q	m^2	Equivalent cross section for AC field oscillations or cyclotron motion of magnetized electrons. $q = (\omega / N) / (\gamma \varepsilon^{1/2}) = (e / m_e)(B / N) / (\gamma \varepsilon^{1/2})$
m_e	kg	Electron mass
$\langle m_i \rangle$	kg	Average ion mass: $\langle m_i \rangle = \sum_i (Z_i^2 n_i) / \sum_i (Z_i^2 n_i / m_i)$
M_k	kg	Particle mass of target particles of collision process k .
σ_k	m^2	Cross section of electron-neutral collision process k . For inelastic processes this is the total cross section, for elastic processes the momentum-transfer cross section.

σ_k^{inv}	m^2	Cross section of superelastic inverse process of excitation process k , calculated automatically from detailed balancing.
σ_{ei}	m^2	Momentum-transfer cross-section for electron-ion Coulomb collisions.
U_k	eV	Threshold energy of inelastic collision process k .
ω	rad/s	Angular frequency of AC field or cyclotron motion (angular gyrofrequency)
x_i	1	Ratio of ion density to gas particle density: $x_i = Zn_e / N = \sum_i Z_i^2 n_i / N$
x_k	1	Fractional particle number density of target gas species of collision process k .
y_k^{low}	1	Fractional population of lower quantum state of excitation process k , set to 1 for other collision types.
y_k^{up}	1	Fractional population of upper quantum state of excitation process k , set to 0 for other collision types
Z_i	1	Ion charge number = ratio of ion particle charge to elementary charge