

# Brief documentation of MCIG

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## 1. Introduction

This documentation gives a brief description of the MCIG options, inputs and outputs, referring to the BOLSIG+ documentation in case of strong overlap.

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

G. J. M. Hagelaar, “Beyond BOLSIG+: Monte Carlo simulation of electron and ion swarms to obtain transport and rate coefficients for plasma modeling” [to appear]

MCIG can be downloaded from [www.bolsig.laplace.univ-tlse.fr](http://www.bolsig.laplace.univ-tlse.fr) in the form of a Windows application with a user-friendly graphical user interface, similar to that of BOLSIG+. Running this application under Linux or macOS requires a Windows emulator such as Wine.

The MCIG source code will not be distributed, under any conditions. For information regarding terms of use, copyright, and how to reference MCIG in scientific publications, please see the above website.

## 2. Windows graphical user interface

Launching ‘mcig.exe’ under Windows opens the MCIG main panel which is very similar to that of BOLSIG+, described in the BOLSIG+ documentation. Two boxes on this panel summarize the data contained in MCIG:

- ‘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. This selection does not affect the calculations.
- ‘Runs’ box: lists all runs performed. A run corresponds to a single Monte-Carlo simulation 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. This box also shows warnings ‘Not converged’ for runs containing significant errors in the overall power balance.

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. MCIG 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 these data.
- New run: performs a new run (Monte-Carlo simulation) or series of runs, asking first for input of physical and numerical conditions. The conditions are organized under three tabs: ‘Physics’, (physical) ‘Details’, and ‘Numerics’. Certain conditions or options may be hidden or blocked depending on the settings for other options. Unlike BOLSIG+ runs, MCIG runs take a non-negligible computation time, ranging from seconds to hours depending on the conditions. During this time, the progress of the run is shown in the top half of the main panel, and the buttons are replaced by a single ‘Stop’ button, allowing the user to abort the run (series) at any time. The duration of runs is determined by a multi-faceted stopping criterion, checking the convergence

and accuracy of the results as well as the run time itself. For more information see the ‘Stopping criterion’ section later in this document.

- Insert run: inserts a new run at a selected point in the ‘Runs’ box, linearly interpolating all conditions.
- Delete runs: removes selected run(s).
- Clear runs: removes all runs.
- Resume last: resumes the most recent Monte Carlo simulation from the point where it was left off, preserving all data sampled so far. This enables the user to temporarily interrupt a run, e.g. to check the output or modify the stopping criterion.
- Results: shows numerical values of all output parameters (transport coefficients, rate coefficients) and conditions 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 DF: plots the probability distribution functions of the particle energy and Cartesian velocity components for selected run(s), as well as the first few Legendre expansion coefficients of the velocity distribution function.
- 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.

### 3. Main input: collision cross section data

The input of electron cross section data in MCIG is exactly the same as in BOLSIG+. Please see the BOLSIG+ documentation for a description of the data format.

The cross section data format for ions involves a few extensions with respect to the BOLSIG+ format:

- Choice of label. In MCIG as well as BOLSIG+, each data set is identified by a label consisting of a single word without spaces, freely chosen by the user, used when loading the data and defining the gas composition. For electron data sets this label usually corresponds to the name of the target particle species. However, for ion data sets in MCIG, in order to avoid confusion, we recommend using a label that indicates the names of both the ion and target species, e.g.  $\text{Ar}^+_{\text{Ar}}$  for atomic argon ions in argon.
- Additional collision types. MCIG allows for two additional collision types for ions, identified by the keywords `ISOTROPIC` and `BACKSCATTER`, respectively corresponding to the isotropic and backscatter collisions used by Phelps [J. Appl. Phys. **76**, 747 (1994)].
- Ion charge and ion and neutral target particle masses. For ion data sets, the ion and neutral target particle masses must be explicitly given in a three-line block, consisting of:
  - (a) Line 1: keyword `CHARGE&MASSES` in capitals.
  - (b) Line 2: label of the data set.
  - (c) Line 3: three numerical values separated by space and/or tab characters, respectively: the ion charge number (= charge in units of elementary charge) and the ion and neutral particle masses in atomic mass units.

Example of an ion data set:

CHARGE&MASSES

He+ \_He

1. 4.0026 4.0026

(a) Keyword

(b) Label of data set

(c) Ion charge number and ion and neutral masses in a.m.u.

BACKSCATTER

He+ \_He

He+ in He: Phelps, private communication.

Qb = 1E-19\*(Erel/1000)^(-0.15)

\*[1+Erel/1000]^(-0.25)\*[1+5/Erel]^(-0.15)

UPDATED: 2011-10-30 01:03:24

COLUMNS: Energy (eV) | Cross section (m2)

(a) Keyword

(b) Label of data set

(d) Optional comment

-----

0.000000e+0 2.213880e-19

1.000000e-4 2.213880e-19

... ..

... ..

1.000000e+4 3.887040e-20

(e) Cross section table

-----

ISOTROPIC

He+ \_He

-----

-0.5d0 7.63d-20

-----

(a) Keyword

(b) Label of data set

(e) Cross section table containing power law parameters (rather than data points)

## 4. Further input parameters

### Reduced electric field E/N (Td)

This is the main control parameter in MCIG simulations, defined as the ratio of electric field strength to gas particle number density in units of 1Td = 1 Townsend =  $10^{-21}$  Vm<sup>2</sup>. One can perform either a single MCIG run for a single value of E/N, or a series of runs for linearly, quadratically or exponentially increasing E/N values over a given range. If the electric field is AC, the E/N values in MCIG are RMS field values, i.e. amplitudes divided by 2<sup>1/2</sup>.

### Angular frequency/N (rad.m3/s)

Reduced angular frequency of an AC electric field, i.e. 2π times its frequency divided by the gas particle number density. Setting this parameter to zero results in a DC electric field. Disabled when the spatial growth model has been selected (see below ‘Growth model’).

### Reduced magnetic field B/N (Hx)

Ratio of the magnetic field strength to the gas particle number density in units of 1 Hx = 1 Huxley =  $10^{-27}$  T m<sup>3</sup>. Disabled when the spatial growth model has been selected (see below ‘Growth model’).

### Angle between E & M fields (°)

Angle in degrees ∈ [0, 180] between the electric and the magnetic field vectors.

### Gas temperature T (K)

This is used to generate the target particle velocity from a Maxwellian distribution function when simulating collisions, and also to automatically set the population of excited neutral states targeted by superelastic collisions, the inverse processes of excitation collisions. MCIG calculates the fractional populations Y of the upper and lower states from Boltzmann factors:

$$Y_n = A g_n \exp(-U_n / (k_B T))$$

where the index  $n$  refers to a quantum state,  $U_n$  is energy of the state,  $g_n$  is its statistical weight, and  $A$  is a normalization constant such that the sum of fractional populations equals unity:

$$\sum_n Y_n = 1.$$

The handling of superelastic collisions in MCIG is fully consistent with that in BOLSIG+, except that it does not allow for a separate excitation temperature. See the BOLSIG+ documentation for more information.

### 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.

### Angular scattering model and screening energy

The angular scattering model is an analytical model for the probability distribution of the scattering angle in the center of mass frame of a collision, i.e. the angle between the final and initial relative velocity vectors. Different options are available:

- (1) Isotropic scattering. The default option for both elastic and inelastic collisions.
- (2) Scattering formula derived by assuming an elastic screened Coulomb interaction in the Born approximation, as given in equation (6) of [Janssen et al, Plasma Sources Sci. Technol. **25**, 055026 (2016)]. This formula involves a screening parameter  $\eta = u/(8\epsilon_{\text{rel}})$ , where  $\epsilon_{\text{rel}}$  is the relative collision energy and  $u$  is a constant screening energy, to be specified in MCIG by the user. The theoretical value of  $u$  is 1 Hartree = 27.211386 eV for a screening length equal to the Bohr radius, but other values are also used in the literature. This option is also available for inelastic collisions, in which case the screening parameter is obtained from the relative energy after the inelastic energy loss, i.e.  $\eta = (u/8)/(\epsilon_{\text{rel}} - U_n)$  [physical justification not clear to me].
- (3) Inelastic scattering formula from the Born approximation, given in equation (18) of [Janssen et al, see above].
- (4) Pure forward scattering, leaving the direction of the relative velocity vector unchanged.
- (5) Diffusive forward/backward scattering. This option changes BACKSCATTER ion collisions such as to allow for a spread of the scattering angle around 180°, depending on an adjustable parameter  $A \in [-1, 1]$ , as in equation (13) of [Skullerud, Phys. B: Atom. Mol. Phys. **6**, 728 (1973)]. For reasons of symmetry, additional ion collisions are added with a spread around 0°.

One of the options (1)-(2) must be selected for elastic collisions. This will be applied to all ELASTIC and EFFECTIVE processes loaded into MCIG. Likewise, one of the options (1)-(4) must be selected for inelastic collisions and will be used for all EXCITATION and IONIZATION processes.

### Energy sharing model and parameter

The energy sharing model determines how the remaining kinetic energy is shared between the primary and secondary electrons after ionization collisions. There are four options:

- (1) Equal sharing: each electron gets exactly half the energy. Not the most realistic option, but default for reasons of consistency with BOLSIG+.
- (2) Random sharing: one electron gets a uniformly random fraction of the energy, the other what remains.
- (3) Sharing according to an empirical model given by equation (2) of [Yoshida et al, Phys. Rev. A **27**, 2858 (1983)]. This involves a fitting parameter  $w$  of the order of 15 eV, to be specified in MCIG by the user. A table of experimental values for this parameter for common gases can be found in [Opal et al, J. Chem. Phys. **55**, 4100 (1971)].

- (4) No sharing: one electron gets all energy, the other is at rest.

N.B.: MCIG assumes that the energy sharing takes place in the laboratory frame and the two electron velocities are in the same direction (determined according to the selected angular scattering model). These are arbitrary assumptions without physical justification.

### **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. If this option is selected, the field configuration is automatically set to a DC electric field without magnetic field, and all AC and magnetic field inputs are disabled.
- (3) Not included: IONIZATION is treated as EXCITATION and ATTACHMENT is ignored.

### **Stopping criterion**

MCIG stops each run and continues with the next one of the series (if any) as soon as the following combination of three conditions [1], [2] and [3] is satisfied: (([1] AND [2]) OR [3]), with

- [1] The relative standard error in the mean energy and in any of the transport coefficients has decreased below a certain percentage, specified by the user. Note that the statistical errors decrease roughly as the inverse square root of run time, so twice smaller errors take four times longer runs, 10× smaller errors 100× longer, etcetera.
- [2] The simulated physical timespan exceeds a given number of times the characteristic relaxation time  $\tau$  (see output parameters, ‘Relaxation time unit’). Setting the minimum simulated time to 20  $\tau$  or more usually guarantees that the simulation has properly converged so that the results are free from systematic errors due to initial conditions, although they may still have large statistical errors.
- [3] The run time (measured from the computer clock) exceeds a given number of seconds.

If a run is stopped via [3], there is no guarantee whatsoever that it has converged so the results may still contain systematic errors due to initial conditions. To check this, MCIG calculates the residue of the overall power balance (power absorbed from the field minus power lost in collisions) and issues a warning ‘Not converged’ in the ‘Runs’ box of the main panel if this residue exceeds 5 times its statistical standard error, i.e. if there is significant error in the steady-state power balance.

### **Number of particles**

Fixed number of simulation particles in MCIG, of importance for the accuracy of the statistical error bars on the results, but not for the accuracy of the results themselves. At least 100 particles are needed for a reliable estimate of the statistical errors. The default setting for the number of particles is 1000, the maximum is  $10^5$ . Setting this the number very high can significantly increase the MCIG run time needed for the initial relaxation phase of the simulation when no steady-state output is generated.

NB: MCIG uses an original renormalization technique to handle particle production in ionization or loss in attachment without changing the number of simulation particles.

### **Relaxation time multiplier**

Scale factor for the characteristic relaxation time  $\tau$  used for the determination of diffusion coefficients, defined in the output parameter section under ‘Relaxation time unit’. The default and recommended setting for this parameter is 1. Setting this parameter to a smaller value can cause systematic errors in the diffusion coefficients, making it bigger enhances the statistical errors.

### **DF maximum energy (eV)**

Upper bound of the grid used for the diagnostics of the energy distribution function (DF). This parameter also controls the bounds of the grid for the velocity distribution functions, via the usual relation between energy and velocity. It has no influence whatsoever on the particle simulation and calculated swarm parameters.

### **DF # of velocity intervals**

Number of uniform velocity intervals (bins) used for the diagnostics of the energy and velocity distribution functions. Since these intervals are uniform, the corresponding energy intervals increase with (energy)<sup>1/2</sup>. Of no consequence for the particle simulation or swarm parameters.

### **Random number generator**

Method used to generate random numbers throughout the Monte-Carlo simulation:

- ‘NR ran’, ‘NR ran0’, ‘NR ran1’, ‘NR ran2’ : classic random number generators from the well-known ‘Numerical Recipes’ book [Press et al, Numerical Recipes in Fortran 90, Vol 2, Cambridge, 1996], by order of increasing reliability and computational cost. The first and simplest one, ‘NR ran’, is fully portable; the others involve assumptions about the computer arithmetic (checked automatically, valid on virtually all machines).
- ‘NRF77 ran0’, ‘NRF77 ran1’, etcetera: classic random number generators from an earlier version of Numerical Recipes [Press et al, Numerical Recipes in Fortran 77, 2nd edition, Cambridge, 1992], similar to those above but less efficient. All fully portable.
- ‘Intrinsic’: intrinsic random\_number() subroutine from Intel Fortran 90 compiler. Algorithm and reliability unknown (to me).

This choice is provided only for checking purposes. No effect on the results has been found so far. By default, MCIG uses the ‘NR ran2’ generator.

### **Coordinate alignment**

Choice for the definition of the three orthogonal directions ‘L’, ‘T’ and ‘X’ used to express the vector and tensor quantities in the MCIG output, in case of an oblique angle between the electric and magnetic field (i.e. a nonzero cosine of E-B field angle). By default, ‘L’ is defined as the direction of the electric field, which (for an oblique field angle) implies that the magnetic field has components along both ‘T’ and ‘L’. Alternatively one can define the ‘T’ as the direction of the magnetic field, so that the electric field has ‘L’ and ‘T’ components. For more detailed information, see box **B1** in the next section.



## 5. Output parameters

Below we give the mathematical expressions used to calculate the MCIG output parameters, as well as some brief further explanations. The mathematical symbols are defined in the list at the end of this document. All units are SI units, except that eV is used for the output of energies. The angle brackets  $\langle \rangle$  indicate ensemble averages, corresponding to averages over the particle distribution function throughout phase space. In case of an AC electric field,  $\langle \rangle$  also implies averaging over the AC oscillation period. More detailed explanations on various points are given in boxes.

### Box B1: Definition of L, T and X directions

In the MCIG output, some of the macroscopic quantities and transport coefficients are labeled with letters ‘L’ (for ‘longitudinal’), ‘T’ (for ‘transverse’) and ‘X’ (‘cross’) which refer to three directions represented by orthonormal basis vectors  $\mathbf{e}_L$ ,  $\mathbf{e}_T$  and  $\mathbf{e}_X$ . By default,  $\mathbf{e}_L$  and  $\mathbf{e}_T$  are pointing in directions along and transverse to the electric field, respectively, with  $\mathbf{e}_T$  in the plane spanned by the electric and magnetic fields, while  $\mathbf{e}_X$  is in the cross direction of the fields:

$$\mathbf{e}_L = \frac{\mathbf{E}}{E} \quad \mathbf{e}_T = \mathbf{e}_X \times \mathbf{e}_L \quad \mathbf{e}_X = \frac{\mathbf{E} \times \mathbf{B}}{|\mathbf{E} \times \mathbf{B}|} = \frac{\mathbf{E} \times \mathbf{B}}{EB \sin \psi} \quad \text{E-aligned basis – default}$$

If the angle  $\psi$  between the electric and magnetic fields is oblique ( $\psi \neq \pi/2$ ), MCIG provides an alternative option to align the basis vector  $\mathbf{e}_T$  with the magnetic field:

$$\mathbf{e}_T = \frac{\mathbf{B}}{B} \quad \mathbf{e}_L = \mathbf{e}_T \times \mathbf{e}_X \quad \mathbf{e}_X = \frac{\mathbf{E} \times \mathbf{B}}{EB \sin \psi}, \quad \text{B-aligned basis}$$

so that  $\mathbf{e}_L$  is no longer aligned with the electric field. This **B**-aligned basis is more commonly used in the general literature on magnetized plasmas, where our ‘L’ is denoted as ‘ $\perp$ ’ (perp to **B**) and ‘T’ as ‘ $\parallel$ ’ (parallel to **B**). For a right angle ( $\psi = \pi/2$ ), the above two basis vector definitions are identical. Internally in MCIG, the L, T and X directions correspond to those of the Cartesian  $x$ ,  $y$  and  $z$  coordinate axes, with the electric and magnetic fields expressed as

$$\mathbf{E} = E\mathbf{e}_x \quad \mathbf{B} = B \cos \psi \mathbf{e}_x + B \sin \psi \mathbf{e}_y,$$

or alternatively, when activating the **B**-alignment option, as

$$\mathbf{E} = E \sin \psi \mathbf{e}_x + E \cos \psi \mathbf{e}_y \quad \mathbf{B} = B\mathbf{e}_y.$$

The expressions for the transport coefficients below thus are given in terms of  $x$ ,  $y$ , and  $z$  coordinates. This is irrelevant for the usage of the transport coefficients: via the basis vectors, the MCIG transport coefficients can be applied to arbitrary field orientation cases as explained in boxes **B4** and **B5**.

### Box B2: Meaning of standard errors

For each of the output parameters, MCIG estimates a standard error (SE) which is a measure for its statistical uncertainty, to be interpreted as follows: there is a 15.9% probability that the statistical error of the MCIG result (i.e. its difference with respect to the exact expectation value) is larger than +SE and another 15.9% that it is smaller than –SE; 2.275% probability that it is larger/smaller than  $\pm 2 \times \text{SE}$ ; 0.135% probability that it is larger/smaller than  $\pm 3 \times \text{SE}$ ; 0.00317% probability that it is larger/smaller than  $\pm 4 \times \text{SE}$ ; and only 0.000029% probability that it is larger/smaller than  $\pm 5 \times \text{SE}$ . The estimated standard errors themselves have a relative SE of the order of  $(2 \times \text{number of simulation particles})^{-1/2}$ . NB: The validity of the SE estimated by MCIG can be checked by running the same case a large number of times, using the  $E/N$  series option with identical initial and final  $E/N$  values, and then comparing the standard deviation of the results with the estimated SE. MCIG does this comparison automatically when writing the results of a series of identical runs in the ‘Run by run’ format.

### Box B3: Scaling with gas density N

All transport coefficients in the MCIG 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  $\mu$  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)

$$\bar{\varepsilon} = \frac{1}{2} m \langle v^2 \rangle$$

#### 2. Mean velocity – L, T, X (m/s)

$$W_L = \langle v_x \rangle \quad W_T = \langle v_y \rangle \quad W_X = \langle v_z \rangle$$

Zero in case of an AC electric field.  $W_X$  is nonzero only if there is a magnetic field,  $W_T$  only if the magnetic field is oblique.

#### 3. Temperature – L, T, X, LT, LX, TX (eV)

$$k_B T_L = m \left( \langle v_x^2 \rangle - \langle v_x \rangle^2 \right) \quad k_B T_T = m \left( \langle v_y^2 \rangle - \langle v_y \rangle^2 \right) \quad k_B T_X = m \left( \langle v_z^2 \rangle - \langle v_z \rangle^2 \right)$$

$$k_B T_{LT} = k_B T_{TL} = m \left( \langle v_x v_y \rangle - \langle v_x \rangle \langle v_y \rangle \right)$$

$$k_B T_{LX} = k_B T_{XL} = m \left( \langle v_x v_z \rangle - \langle v_x \rangle \langle v_z \rangle \right)$$

$$k_B T_{TX} = k_B T_{XT} = m \left( \langle v_y v_z \rangle - \langle v_y \rangle \langle v_z \rangle \right)$$

Components of the temperature tensor, defined as the space-averaged kinetic pressure tensor divided by the space-averaged particle number density. The LX and XL components are nonzero only if there is a magnetic field; the LT, TL, TX and XT if there is an oblique magnetic field. Related to mean energy via:

$$\bar{\varepsilon} = \frac{1}{2} (k_B T_L + k_B T_T + k_B T_X) + \frac{1}{2} m (W_L^2 + W_T^2 + W_X^2)$$

#### 4. Mobility\*N – L, T, X (1/m/V/s)

In case of a DC electric field, defined as the ratio of absolute mean velocity to reduced electric field:

$$(\mu_L N) = \frac{|\langle v_x \rangle|}{(E/N)} \quad (\mu_T N) = \frac{|\langle v_y \rangle|}{(E/N)} \quad (\mu_X N) = \frac{|\langle v_z \rangle|}{(E/N)}$$

This corresponds to the ‘flux’ mobility defined in the swarm literature (as opposed to ‘bulk’ mobility). In case the electric field is AC, real (in-phase) part of complex mobility:

$$(\mu_{\text{Re}}^{L/T/X} N) = \frac{\sqrt{2} \text{sgn}(q)}{(E/N)} \langle v_{x/y/z} \cos \omega t \rangle \quad \text{NB: } E_{\text{AC}}(t) = \sqrt{2} (E/N) N \cos(\omega t)$$

The mobility for the X direction is nonzero only if there is a magnetic field; that for the T direction only if there is an oblique magnetic field. When using the SST (Steady State Townsend) growth model for electrons, the mobility is defined from the mean velocity (as above), ignoring diffusion due to the exponential density profile; this definition is arbitrary and not consistent with that used in BOLSIG+ (also arbitrary) but it does not affect the characteristic energy  $D/\mu$ , due to the way the SST diffusion coefficients are defined (see below).

## 5. Imaginary mobility\*N – L, T, X (1/m/V/s)

$$(\mu_{\text{Im}}^{\text{L/T/X}} N) = \frac{\sqrt{2} \text{sgn}(q)}{(E/N)} \langle v_{x/y/z} \sin \omega t \rangle \quad \text{NB: Sign convention: } E_{\text{AC}}(t) \propto e^{-i\omega t}$$

Imaginary (out-of-phase) part of complex mobility, only for AC field. The sign convention for the exponential notation is such that this parameter is positive if the drift velocity has a delayed response to the electric field, which is usually the case (due to inertia).

## 6. Bulk mobility\*N – L, T, X (1/m/V/s)

$$(\mu_{\text{L}}^{\text{b}} N) = \frac{1}{(E/N)} \left| \frac{d\langle x \rangle}{dt} \right| \quad (\mu_{\text{T}}^{\text{b}} N) = \frac{1}{(E/N)} \left| \frac{d\langle y \rangle}{dt} \right| \quad (\mu_{\text{X}}^{\text{b}} N) = \frac{1}{(E/N)} \left| \frac{d\langle z \rangle}{dt} \right|$$

Ratio of the absolute ‘bulk’ mean velocity to reduced electric field. Characterizes the spatiotemporal evolution of the swarm particle density rather than flux. Different from the above ‘flux’ mobility due to ionization or attachment. Zero for AC electric field. See box **B5** below on how to use.

### Box B4: How to calculate the drift velocity vector

Using the mobility components and the basis vectors defined above in box **B1**, the drift velocity due to constant electric and magnetic fields can be obtained from:

$$\mathbf{W} = \text{sgn}(q)E(\mu_{\text{L}}\mathbf{e}_{\text{L}} + \mu_{\text{T}}\mathbf{e}_{\text{T}}) + \mu_{\text{X}}E\mathbf{e}_{\text{X}}$$

In case of AC electric field, the fundamental harmonic of the drift velocity is:

$$\mathbf{W}_{1\omega} = \text{sgn}(q) \left( \mu_{\text{Re}} E - \frac{\mu_{\text{Im}}}{\omega} \frac{\partial E}{\partial t} \right) \mathbf{e}_{\text{L}} + \text{sgn}(q) \left( \mu_{\text{Re}}^{\text{T}} E - \frac{\mu_{\text{Im}}^{\text{T}}}{\omega} \frac{\partial E}{\partial t} \right) \mathbf{e}_{\text{T}} + \left( \mu_{\text{Re}}^{\text{X}} E - \frac{\mu_{\text{Im}}^{\text{X}}}{\omega} \frac{\partial E}{\partial t} \right) \mathbf{e}_{\text{X}}$$

**NB:** Since the mobility components are positive by definition, the sign of the particle charge must be included explicitly in the longitudinal (L) and transverse (T) terms, but not in the E×B (X) term.

## 7. Diffusion coefficient\*N – L, T, X, LT, TL, LX, XL, TX, XT (1/m/s)

$$(D_{\text{L}} N) = N \left( \langle v_x x \rangle - \langle v_x \rangle \langle x \rangle \right)$$

$$(D_{\text{T}} N) = N \left( \langle v_y y \rangle - \langle v_y \rangle \langle y \rangle \right)$$

$$(D_{\text{X}} N) = N \left( \langle v_z z \rangle - \langle v_z \rangle \langle z \rangle \right)$$

$$(D_{\text{LT}} N) = N \left( \langle v_x y \rangle - \langle v_x \rangle \langle y \rangle \right)$$

$$(D_{\text{TL}} N) = N \left( \langle v_y x \rangle - \langle v_y \rangle \langle x \rangle \right)$$

$$(D_{\text{LX}} N) = N \left( \langle v_x z \rangle - \langle v_x \rangle \langle z \rangle \right)$$

$$(D_{\text{XL}} N) = N \left( \langle v_z x \rangle - \langle v_z \rangle \langle x \rangle \right)$$

$$(D_{\text{TX}} N) = N \left( \langle v_y z \rangle - \langle v_y \rangle \langle z \rangle \right)$$

$$(D_{\text{XT}} N) = N \left( \langle v_z y \rangle - \langle v_z \rangle \langle y \rangle \right)$$

Components of the ‘flux’ diffusion tensor, each characterizing diffusion flux in a certain direction due to a density gradient in a certain (possibly different) direction. The LX and XL components are nonzero only if there is a magnetic field; the LT, TL, TX and XT components only if there is magnetic field under an oblique angle. See box **B5** below for explanation on how to use.

When using the spatial (SST) growth model, the T and X diffusion coefficients are calculated in a different way, in order to reproduce the characteristic energy  $D/\mu$  as measured in SST experiments:

$$(D_{\text{T}}^{\text{SST}} N) = (\mu_{\text{L}}^{\text{SST}} N) \left| \frac{E}{2} \frac{d}{dx} \langle y^2 \rangle \right| \quad (D_{\text{X}}^{\text{SST}} N) = (\mu_{\text{L}}^{\text{SST}} N) \left| \frac{E}{2} \frac{d}{dx} \langle z^2 \rangle \right| \quad (\mu_{\text{L}}^{\text{SST}} N) = \frac{\langle v_x \rangle}{(E/N)},$$

where the definition of  $\mu$  is arbitrary. Other diffusion coefficients are not calculated in this case.

### 8. Bulk diffusion coefficient\* $N - L, T, X, LT+TL, LX+XL, TX+XT$ (1/m/s)

$$\begin{aligned} (D_L^b N) &= \frac{N}{2} \frac{d}{dt} (\langle x^2 \rangle - \langle x \rangle^2) & (D_{LT+TL}^b N) &= N \frac{d}{dt} (\langle xy \rangle - \langle x \rangle \langle y \rangle) \\ (D_T^b N) &= \frac{N}{2} \frac{d}{dt} (\langle y^2 \rangle - \langle y \rangle^2) & (D_{LX+XL}^b N) &= N \frac{d}{dt} (\langle xz \rangle - \langle x \rangle \langle z \rangle) \\ (D_X^b N) &= \frac{N}{2} \frac{d}{dt} (\langle z^2 \rangle - \langle z \rangle^2) & (D_{TX+XT}^b N) &= N \frac{d}{dt} (\langle yz \rangle - \langle y \rangle \langle z \rangle) \end{aligned}$$

Components of the ‘bulk’ diffusion tensor, characterizing the evolution of swarm particle density along the electric field. Different from the above ‘flux’ diffusion coefficients due to ionization or attachment. See box **B5** below for explanation on how to use.

#### Box B5: How to use ‘flux’ and ‘bulk’ transport coefficients

Via the basis vectors defined above in box **B1**, the MCIG transport coefficients can be applied to arbitrary field orientation cases as follows. The ‘flux’ transport coefficients should be used to calculate the particle flux vector from:

$$\begin{aligned} \Gamma &= [\text{sgn}(q)\mu E n - D_L \nabla_L n - D_{LT} \nabla_T n - D_{LX} \nabla_X n] \mathbf{e}_L \\ &+ [\text{sgn}(q)\mu_T E n - D_T \nabla_T n - D_{TL} \nabla_L n - D_{TX} \nabla_X n] \mathbf{e}_T \\ &+ [\mu_X E n - D_X \nabla_X n - D_{XT} \nabla_T n - D_{XL} \nabla_L n] \mathbf{e}_X \end{aligned}$$

where the  $\nabla$  operator has been decomposed as:

$$\nabla = \mathbf{e}_L \nabla_L + \mathbf{e}_T \nabla_T + \mathbf{e}_X \nabla_X \quad \nabla_L = \mathbf{e}_L \cdot \nabla \quad \nabla_T = \mathbf{e}_T \cdot \nabla \quad \nabla_X = \mathbf{e}_X \cdot \nabla.$$

The ‘bulk’ transport coefficients, on the other hand, are measurable swarm parameters that enter directly into the following equation for the spatiotemporal evolution of the particle density:

$$\begin{aligned} \frac{\partial n}{\partial t} + \text{sgn}(q)E(\mu^b \nabla_L n + \mu_T^b \nabla_T n) + \mu_X^b E \nabla_X n - D_L^b \nabla_L^2 n - D_T^b \nabla_T^2 n - D_X^b \nabla_X^2 n \\ - D_{LT+TL}^b \nabla_L \nabla_T n - D_{LX+XL}^b \nabla_L \nabla_X n - D_{TX+XT}^b \nabla_T \nabla_X n + \dots = (\bar{\nu}_{iz} - \bar{\nu}_{at})n, \end{aligned}$$

where  $\bar{\nu}_{iz}$  and  $\bar{\nu}_{at}$  are the mean ionization and attachment frequencies defined below. The electron bulk transport coefficients may be different from their flux counterparts due to ionization and attachment effects; see the literature on swarm data analysis e.g. [Petrovic et al, J. Phys. D: Appl. Phys. **42**, 194002 (2009)]. For general plasma modeling purposes, we recommend working primarily with the flux transport coefficients. The above equations simplify considerably if the magnetic field is transverse to the electric field ( $\psi = \pi/2$ ):

$$\begin{aligned} \Gamma &= [\text{sgn}(q)\mu E n - D_L \nabla_L n - D_{LT} \nabla_T n - D_{LX} \nabla_X n] \mathbf{e}_L \\ &- [D_T \nabla_T n] \mathbf{e}_T + [\mu_X E n - D_X \nabla_X n - D_{XL} \nabla_L n] \mathbf{e}_X, \\ \frac{\partial n}{\partial t} + \text{sgn}(q)E\mu^b \nabla_L n + \mu_X^b E \nabla_X n - D_L^b \nabla_L^2 n - D_T^b \nabla_T^2 n - D_X^b \nabla_X^2 n \\ &- D_{LX+XL}^b \nabla_L \nabla_X n + \dots = (\bar{\nu}_{iz} - \bar{\nu}_{at})n, \end{aligned} \quad \left. \vphantom{\begin{aligned} \Gamma \\ \frac{\partial n}{\partial t} \end{aligned}} \right\} \mathbf{B} \text{ transverse to } \mathbf{E}$$

because

$$\mu_T = \mu_T^b = D_{LT} = D_{TL} = D_{TX} = D_{XT} = D_{LT+TL}^b = D_{TX+XT}^b = 0.$$

Without magnetic field, they simplify even further:

$$\begin{aligned} \Gamma &= [\text{sgn}(q)\mu E n - D_L \nabla_L n] \mathbf{e}_L - [D_T \nabla_T n] \mathbf{e}_T - [D_X \nabla_X n] \mathbf{e}_X \\ \frac{\partial n}{\partial t} + \text{sgn}(q)\mu^b E \nabla_L n - D_L^b \nabla_L^2 n - D_T^b (\nabla_T^2 + \nabla_X^2) n + \dots &= (\bar{\nu}_{iz} - \bar{\nu}_{at})n, \\ D_X = D_T \quad \mu_X = \mu_X^b = D_X = D_{XL} = D_{LX} = D_X^b = D_{LX+XL}^b &= 0. \end{aligned} \quad \left. \vphantom{\begin{aligned} \Gamma \\ \frac{\partial n}{\partial t} \end{aligned}} \right\} \mathbf{B} = 0$$

### 9. Collision frequency/N (m3/s)

$$(\bar{\nu} / N) = \sum_k X_k Y_k K_k$$

Mean total collision frequency, summed over all real collision types.

### 10. Momentum transfer frequency/N (m3/s)

Effective frequency for momentum transfer in neutral collisions, deduced from mobility diagnostics.

In case of a DC field:

$$(\bar{\nu}_m / N) = \frac{|q|}{m} \frac{(\mu N)^2}{(\mu N)^2 + (\mu_x N)^2}$$

In case of an AC field:

$$(\bar{\nu}_m / N) = \frac{|q|}{m} \frac{(\mu_{Re} N)}{(\mu_{Re} N)^2 + (\mu_{Im} N)^2 + (\mu_{Re}^H N)^2 + (\mu_{Im}^H N)^2}$$

NB: In case of a magnetic field and/or AC electric field, this definition of the momentum transfer frequency is different from that in BOLSIG+ which characterizes only non-magnetized DC transport; see the BOLSIG+ documentation.

### 11. Total ionization frequency /N (m<sup>3</sup>/s)

$$(\bar{\nu}_{iz} / N) = \sum_{k=\text{ionization}} X_k Y_k K_k$$

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

### 12. Total attachment frequency /N (m<sup>3</sup>/s)

$$(\bar{\nu}_{at} / N) = \sum_{k=\text{attachment}} X_k Y_k K_k$$

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

### 13. Townsend ionization coefficient /N (m<sup>2</sup>)

$$(\alpha / N) = \frac{(\bar{\nu}_{iz} / N)}{\langle v_x \rangle}$$

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

### 14. Townsend attachment coefficient /N (m<sup>2</sup>)

$$(\eta / N) = \frac{(\bar{\nu}_{at} / N)}{\langle v_x \rangle}$$

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

### 15. Power /N (eV m<sup>3</sup>/s)

Energy per unit time absorbed from the electric field, for a DC field given by:

$$(P / N) = q \langle v_x \rangle (E / N)$$

For an AC electric field:

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

### 16. Elastic power loss/N (eV m3/s)

$$(P_{el} / N) = \frac{1}{N} \sum_{k \neq \text{attachment}} \frac{m M_k}{(m + M_k)^2} \left\langle \left\langle v_k (m \mathbf{v} + M_k \mathbf{V}) \cdot (\mathbf{v} - \mathbf{V}) (1 - \beta \cos \chi) \right\rangle \right\rangle_{\mathbf{v}, \chi}$$

$$\text{where } \beta = \sqrt{1 - \frac{m + M_k}{mM_k} \frac{2U_k}{|\mathbf{v} - \mathbf{V}|^2}}$$

Rate of net kinetic energy transfer to the background gas by the ensemble of elastic and inelastic collisions, causing gas heating in the translational mode. The average is taken not only over the ensemble of particles, but also over distributions of the gas particle velocity  $\mathbf{V}$  (Maxwellian) and the scattering angle  $\chi$  (in the center of mass frame). For inelastic collisions, the factor  $\beta$  takes into account the effect of inelastic energy loss on the transfer of kinetic energy; for elastic collisions  $\beta = 1$ . NB: For isotropic collisions,  $\cos\chi$  averages out to zero so that  $\beta$  is of no importance.

### 17. Inelastic power loss /N (eV m3/s)

$$(P_{\text{inel}} / N) = \sum_{k=\text{inelastic}} \frac{M_k}{m + M_k} X_k Y_k K_k U_k + \frac{m}{2N} \sum_{k=\text{attachment}} \langle \langle v_k v^2 \rangle \rangle_{\mathbf{v}}$$

Total net rate of electron or ion energy loss due to quantum state transitions in inelastic collisions, including superelastic collisions for which  $U_k$  is negative (= minus threshold energy of the corresponding excitation process). Also includes the kinetic energy of electrons lost by attachment. Excludes the contribution of the gas particle energy to the inelastic processes, given by a similar formula but with complementary mass factor  $m/(m + M_k)$  rather than  $M_k/(m + M_k)$ .

### 18. Growth power /N (eV m3/s)

In case of temporal (PT) growth model:

$$(P_{\text{growth}} / N) = \left( (\bar{v}_{\text{iz}} / N) - (\bar{v}_{\text{at}} / N) \right) \frac{1}{2} m \langle v^2 \rangle$$

In case of spatial (SST) growth model:

$$(P_{\text{growth}} / N) = \frac{m}{2N \langle v_x \rangle} \left( \sum_{k=\text{ionization}} \langle \langle v_k v_x v^2 \rangle \rangle_{\mathbf{v}} - \sum_{k=\text{attachment}} \langle \langle v_k v_x v^2 \rangle \rangle_{\mathbf{v}} \right)$$

Apparent energy loss rate that appears when renormalizing the particle distribution function, via a “growth model”, to compensate for particle production by ionization and/or particle loss by attachment (for electrons). For ionization this can be loosely interpreted as the power needed to “heat new electrons up to the mean energy”.

### 19. Power residue (%)

$$\left( 1 - \frac{(P_{\text{el}} / N) + (P_{\text{inel}} / N) + (P_{\text{growth}} / N)}{(P / N)} \right) \times 100\%$$

Percentage deviation from overall steady state power balance. Once in steady state, this parameter is nonzero only due to statistical errors so its absolute value should be smaller than 5 times its standard error (with 99.99994% probability). If not so, this indicates that either the simulation has not yet sufficiently relaxed to steady state, in which case it needs to run for a longer time, or there is some systematic error e.g. due to the MCIG growth-renormalization technique. In each of these cases the results cannot be trusted, so MCIG sets an error flag and shows a warning in the ‘Runs’ box.

### 20. Mean energy 2f oscillations (eV)

$$m \sqrt{\langle v^2 \cos(2\omega t) \rangle^2 + \langle v^2 \sin(2\omega t) \rangle^2}$$

Amplitude of second harmonic oscillations of the mean energy, in case of an AC electric field.

### 21. Number density 2f oscillations (%)

$$2 \sqrt{\langle \cos(2\omega t) \rangle^2 + \langle \sin(2\omega t) \rangle^2} \times 100\%$$

Relative amplitude of second harmonic oscillations of the number of particles, due to ionization or attachment processes in case of an AC electric field. Note that the angle brackets indicate averaging over particles as well as time, so the cosine and sine functions in the above expression are implicitly weighted by the number of particles.

## 22. Relaxation time unit (s/m3)

$$(\tau N) = C \left( \frac{10}{(\bar{v}_m / N)} + \frac{m \langle v^2 \rangle}{(P_{el} / N) + (P_{inel} / N)} \right)$$

Characteristic relaxation time used for the diagnostics of diffusion coefficients and the suppression of systematic errors due to the initial conditions. The pre-factor  $C$  is 1 by default but can be adjusted by the user via the ‘Relaxation time multiplier’ entry (not recommended). In AC cases,  $\tau$  is rounded up to the next higher multiple of the AC period:

$$(\tau N)_{AC} = \frac{2\pi}{(\omega / N)} \left\lceil \frac{(\omega / N)}{2\pi} (\tau N) \right\rceil$$

## 23. Relaxation time count

Simulated timespan (for each particle) expressed in units of the relaxation time  $\tau$  defined just above. Proper convergence to steady state cannot be expected for relaxation time counts lower than 10 or so. This parameter also corresponds to the average number of samples per particle taken for the calculation of the bulk transport coefficients. The number of simulated collisions per particle can be found by multiplying this parameter by  $(\tau N)$  and by the collision frequency  $(\bar{v}/N)$ .

## 24. Run time (s)

Run time in seconds as measured by the computer system clock.

## 25. Error code

0 = No problem detected.

1 = Significant error in steady state power balance (> 5 times statistical standard error).

2 = Power balance OK but simulated timespan possibly too short for proper relaxation (<10  $\tau$ ), needs to run longer.

3 = Runaway, particle energy exceeds 10000 eV.

4 = Number of cross section data points too large for allocated memory.

5 = Averages OK but unreliable estimation of standard errors, due to strong growth/renormalization.

In case of an AC field, this flag is set whenever the average number of ionization or attachment collisions per AC period is greater than one.

## 26. Rate coefficient (m3/s)

$$K_k = \frac{1}{NX_k Y_k} \langle \langle v_k \rangle \rangle_{\mathbf{v}} = \langle \langle \sigma_k | \mathbf{v} - \mathbf{V} | \rangle \rangle_{\mathbf{v}}$$

Rate coefficient for an individual collision process  $k$ . The average is also taken over the distribution function of the gas particle velocity  $\mathbf{V}$ .

## 27. Inverse rate coefficient (m3/s)

Rate coefficient for a superelastic inverse excitation process. Same as ‘Rate coefficient’, except that the cross section  $\sigma$  is not taken directly from the input file but generated by MCIG from the excitation cross section and statistical weight ratio, using the Klein-Rosseland relation from detailed balancing (see BOLSIG+ documentation). Only available when superelastic collisions are activated.

## 28. Energy distribution function & Legendre coefficients $F_0, F_1, F_2, F_3$ (eV-3/2)

First four Legendre expansion coefficients of the velocity distribution, expressed as a function of energy:

$$F_l(\varepsilon) = \frac{2l+1}{\sqrt{\varepsilon}} \left\langle P_l(\cos \theta) \delta\left(\frac{1}{2}mv^2 - \varepsilon\right) \right\rangle \quad \cos \theta = (\mathbf{v}/v) \cdot (\mathbf{E}/E) = v_x/v$$

$$l = 0, 1, 2, 3$$

where  $P_l$  is the  $l$ <sup>th</sup>-order Legendre polynomial,  $\theta$  is the velocity angle with respect to the electron field direction, and  $\delta$  is the Dirac-delta function.  $F_0$  and  $F_1$  are defined the same as in BOLSIG+.  $F_0$  is identical to the energy probability function (EPF), normalized as

$$\int_0^\infty \sqrt{\varepsilon} F_0(\varepsilon) d\varepsilon = 1 .$$

Determined using a fixed number of gradually increasing energy bins (approximating the delta function by a boxcar function), see ‘DF # of velocity intervals’ input parameter.

## 29. 1D velocity distribution functions – L, T, X (s/m)

$$f_L(u_x) = \langle \delta(v_x - u_x) \rangle \quad f_T(u_y) = \langle \delta(v_y - u_y) \rangle \quad f_X(u_z) = \langle \delta(v_z - u_z) \rangle$$

Distribution functions of single Cartesian velocity components in the directions defined in box **B1** above.

## List of symbols

Symbol	Unit	Description
$\mathbf{B}, B$	T	Magnetic field vector and strength
$E$	V/m	Electric field
$K_k$	$\text{m}^3\text{s}^{-1}$	Rate coefficient of collision process $k$
$N$	$\text{m}^{-3}$	Total gas particle number density
$q$	C	Electron or ion particle charge
$m$	kg	Electron or ion particle mass
$M_k$	kg	Particle mass of target particles of collision process $k$
$\sigma_k$	$\text{m}^2$	Total (integral) cross section of collision process $k$
$U_k$	eV	Threshold energy of inelastic collision process $k$
$v_x$	m/s	Particle velocity along the electric field direction
$v_y$	m/s	Particle velocity along the magnetic field direction
$v_z$	m/s	Particle velocity along the cross direction of electric and magnetic fields
$\mathbf{v}$	m/s	Electron or ion particle velocity
$\mathbf{V}$	m/s	Target particle velocity, sampled from Maxwellian distribution function
$\omega$	rad/s	Angular frequency of AC electric field
$x$	m	Particle position along the electric field direction
$y$	m	Particle position along the magnetic field direction
$z$	m	Particle position along the cross direction of electric and magnetic fields
$X_k$	1	Fractional particle number density of target gas species of collision process $k$
$Y_k$	1	Fractional population of initial quantum state of excitation process $k$ , set to 1 for other collision types