Manual for the script MonteCarlo_run.m

Example: Ar/N2 (30%/70%) mixture at E/N=100 Td. The script "/Ar_N2_mixture/MonteCarlo_single_run" can be tested without any modifications.

For new gases, the following steps have to be followed to **perform a single simulation** (one E/N value):

1. Download the cross section files from LXcat: http://www.lxcat.net/data and **save each cross section .txt-file for each gas separately in a directory**. E.g. for the Ar/N2 mixture: / N2_Biagi/xsections.txt and/ Ar_Biagi/ xsections.txt. The name of the .txt-file (here: xsections) is not important.
2. create a directory where to perform the simulation, e.g. "/Ar_N2_mixture"
3. copy the script MonteCarlo_run.m into the directory and open it
4. set paths for the following two directories correctly:
   - **functionsDir**: path of the directory "_functions" (should be already correct).
   - **gasDir**: directories of the cross section input *.txt files of the gases, here:

   gasDir = {'.._Xsection\Ar_Biagi','.._Xsection\N2_Biagi'}

5. set the following **important parameters** for the simulation:
   - **gas**: sum formulas of the gas components as a cell array, here:

   gas = {'Ar','N2'}

   - **mix**: mixing ratio of the gas components as a vector, here:

   mix = [0.3 0.7]

   - **EN**: reduced field E/N in Townsend, here:

   EN = 100;

6. set the following **additional parameters** for the simulation (in general do not have to be changed to obtain steady-state transport data. For more information, type "doc MonteCarlo" into the command window):
   - **p**: pressure
   - **Temp**: temperature
   - **N0**: number of start electrons
   - **Ne_max:** maximum allowed electron number
   - **W**: energy sharing factor in interval [0,1]
   - **w_err**: relative error tolerance for flux drift velocity
   - **DN_err**: relative error tolerance for flux diffusion constant
   - **col_equ**: minimum number of collisions before steady-state
   - **col_max**: maximum number of collisions of simulation
   - **conserve**: conserve electron number (=1) or not (=0)
   - **interactive**: plots the temporal data (=1 or not (=0)
7. **run** the script **MonteCarlo_run.m**

The results are saved during the simulation in the file **results.mat.** The development of the results (mean energy, drift velocities, diffusion constants and effective ionization rate constants) during the simulation can be followed in the command window as well as in the file **temporal.txt**. The simulation can be stopped at any time without losing the results.

The **results.mat** file is a matlab-structure and contains:

1. the input parameters **E/N**, **gas**, **mix** and the **dir** (directories of the cross sections)
2. **energy data E**: mean energy **E_mean**, electron energy distribution function **EEDF** and electron energy probability function **EEPF** with the corresponding **energy**
3. **transport data bulk:** drift velocities **w** in x-,y- and z-direction, density reduced diffusion constants **DN** in x,y and z-direction
4. **transport data flux:** drift velocities **w** in x-,y- and z-direction, density reduced diffusion constants **DN** in x,y and z-direction
5. **reaction rate constants**:
    a. calculated via counting of ionization/attachment events: **count**
    b. calculated via convolution of cross sections with EEDF: **conv**

    Both methods contain the total ionization rate constant **ion_tot**, total attachment rate constant **att_tot** and effective ionization rate constant **eff**