Plasma Parameter Calculator

This web tool calculates many parameters for electron-ion plasmas from one to five ion species. In this document example usage is given as well the formulary for the calculations.

**Input**

The required inputs for the calculator are,
- first, the number of species in the system,
- then the types of ions, given by the charge and mass of each ion type,
- and finally the total density and the temperature of the system.

In addition if the system has more than one species, the concentration of each species must be given. And optionally for simulation cell information a total number of ions in the simulation may be given.

**Examples**

In the examples to the right the input usage can be seen.

Top  Here a single species is considered. In this case aluminum with only 3 valence electrons is to be calculated, fully ionized aluminum by contrast would have an input ion charge of 13.

Middle  Next is a binary mixture, and a concentration must now be given. Shown here the mixture is given by the relative number of ions, that is 12 hydrogen atoms to 4 carbon atoms. Note a fractional number of ions can be used also.

Bottom  Lastly the ion mixture concentrations may also be given by mass percentage by molar percentage. If these methods are used the last species will be calculated so the total is 100%.

In all of these examples the total density is given in g/cm³, and the temperature is given in eV, but other options are available. Also 128 total atoms are selected for total number of ions in the simulation unit cell, but this may be left blank if not desired.

System

<table>
<thead>
<tr>
<th>Number of ion species:</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species Ion Charge, Atomic Mass</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Total density</td>
<td>3.5</td>
</tr>
<tr>
<td>System temperature</td>
<td>5</td>
</tr>
</tbody>
</table>

Optional (for cell parameters):
Total ions in simulation | 128 |

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System

<table>
<thead>
<tr>
<th>Number of ion species:</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specify ion concentrations by number of ions</td>
<td></td>
</tr>
<tr>
<td>Species Ion Charge, Atomic Mass, Concentration</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1.0078</td>
</tr>
<tr>
<td>2</td>
<td>1.0078</td>
</tr>
<tr>
<td>Total density</td>
<td>3</td>
</tr>
<tr>
<td>System temperature</td>
<td>10</td>
</tr>
</tbody>
</table>

Optional (for cell parameters):
Total ions in simulation | 128 |

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System

<table>
<thead>
<tr>
<th>Number of ion species:</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specify ion concentrations by percent by mass</td>
<td></td>
</tr>
<tr>
<td>Species Ion Charge, Atomic Mass, Concentration</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1.0078</td>
</tr>
<tr>
<td>2</td>
<td>1.0078</td>
</tr>
<tr>
<td>3</td>
<td>15.9999</td>
</tr>
<tr>
<td>Total density</td>
<td>3</td>
</tr>
<tr>
<td>System temperature</td>
<td>10</td>
</tr>
</tbody>
</table>

Optional (for cell parameters):
Total ions in simulation | 128 |
Units and conversion factors

1 amu = 1.66053892 × 10^{−24} g = 1822.8884 \, m_e
1 Ang = 10^{−8} \, cm = 1.88972599 \, bohr
1 Ha = 27.211385 \, eV = 27.211385 \, k_B \, K
\quad k_B = 8.617332 \times 10^{-5} \, eV/K
\quad a_B = 1 \, bohr
1 s = 10^{15} \, fs = 4.134137 \times 10^{16} \, \hbar/\text{Ha}

Electron parameters

Electron density:
\quad n_e = N_e/V = < Z > n
Wigner-Seitz radius:
\quad a_e = (3/4\pi n_e)^{1/3}
Wigner-Seitz radius (dimensionless):
\quad r_s = (3/4\pi n_e)^{1/3}/a_B
Fermi wave number:
\quad k_F = (3\pi^2 n_e)^{1/3}
Fermi energy:
\quad E_F = \hbar^2 k_F^2/2m_e
Fermi degeneracy (dimensionless):
\quad \Theta = k_B T/E_F
Coulomb coupling (dimensionless):
\quad \Gamma = e^2/ak_B T
Relativistic parameter (dimensionless):
\quad x_r = \hbar k_F/m_e c
Thermal de Broglie wavelength:
\quad \lambda_{dB} = (2\pi \hbar^2/m_e k_B T)^{1/2}
Plasma frequency:
\quad \omega_{pe} = (4\pi n_e e^2/m_e)^{1/2}
Thomas-Fermi screening length (at \Theta = 0):
\quad \lambda_{TF}^{\Theta=0} = (\hbar^2 \pi/4e^2 m_e k_F)^{1/2}
Debye length (TF screening for \Theta \gg 1):
\quad \lambda_D = (k_B T/4\pi e^2 n_e)^{1/2}

Ion Parameters

Most quantities averaged over species.

Ion density:
\quad n = n_{total} = \sum_i n_i = N_{total}/V
Ion averages:
\quad <M> = \sum_i M_i n_i/n
\quad <Z^\alpha> = \sum_i Z_i^\alpha n_i/n
Wigner-Seitz radius:
\quad a = (3/4\pi n)^{1/3}
Wigner-Seitz radius (dimensionless):
\quad R_s = (3/4\pi n)^{1/3}/a_B
Fermi wave number:
\quad k_F = (6\pi^2 n)^{1/3}
Fermi energy:
\quad E_F = \hbar^2 k_F^2/2 <M>
Fermi degeneracy (dimensionless):
\quad \Theta = k_B T/E_F
Coulomb coupling (dimensionless):
\quad \Gamma = e^2/ak_B T
Coulomb coupling effective:
\quad \Gamma_{eff} = <Z^{5/3}> <Z>^{1/3} \Gamma
Relativistic parameter (dimensionless):
\quad x_r = \hbar k_F/ <M> c
Thermal de Broglie wavelength:
\quad \lambda_{dB} = (2\pi \hbar^2/ <M> k_B T)^{1/2}
Plasma frequency:
\quad \omega_p = (4\pi n <Z>^2 e^2/ <M>)^{1/2}