Plasma Injection and Atomic Physics Models For Use In Particle Simulation Codes

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Abstract

Models of plasma injection (creation) and charged/neutral atomic physics which are suitable for incorporation into particle simulation codes are described. Both planar and distributed source injection models are considered. Results obtained from planar injection into a collisionless plasma-sheath region are presented. The atomic physics package simulates the charge exchange and impact ionization interactions which occur between charged particles and neutral atoms in a partially-ionized plasma. These models are applicable to a wide range of problems, from plasma processing of materials to transport in the edge region of a tokamak plasma.

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1 The Planar And Distributed-Source Injection Models

In order to maintain an equilibrium particle density in a plasma, it is necessary to have a particle source which balances the loss from the system. The method of particle creation or injection that is chosen for a specific system is usually determined by the means of plasma confinement. Gas puffing, frozen-gas pellet and neutral beam injection have been employed as a means of fueling magnetically confined plasmas. Cold, neutral gas is introduced across the confining magnetic field into the plasma, where it is then ionized via collisions with the plasma particles. In bounded systems, such as diodes and single-ended Q-machines, particles are emitted by one of the bounding plates and are lost via flow to the other plate or perpendicular diffusion to the walls of the device. The dominant “source” of plasma in the scrape-off layer (SOL) of a tokamak is cross-field transport of particles across the separatrix. These particles then flow along the open magnetic field lines to the divertor plate or limiter, where they are absorbed or recycled as neutral atoms. Each of these systems may be modeled through the use of the planar and distributed source injection packages in the code DIPSI [1], which are derivatives of the planar source model in Lawson’s code PDW1 [2, 3].

1.1 Methodology

Planar and distributed source algorithms are used to inject particles into a system from the left-hand boundary and a region of finite spatial extent within the system respectively. The velocities of the injected particles are chosen from a prescribed distribution function. A drift velocity v_{0s} about which the source distribution function is centered may be specified for each species s . The following subsections describe the methods that are used to determine the position and velocity of the injected particles.

1.1.1 The Distributed Source Model

The distributed source model is used to represent the volumetric production of ion-electron particle pairs. It is therefore applicable for the simulation of neutral-particle injection into magnetically confined plasmas, the ionization of neutral gas or the transport of plasma across the separatrix of a tokamak.

The velocity of each injected particle is chosen from the normalized source distribution functions $S_{\parallel,s}(z, v_{\parallel})$ and $S_{\perp,s}(z, v_{\perp})$ for each species s , which have the general forms

$$S_{\parallel,s}(z, v_{\parallel}) dv_{\parallel} = h(z) |v_{\parallel}|^{\eta_s} \exp\left(\frac{-m_s v_{\parallel}^2}{2kT_{\parallel,s}}\right) dv_{\parallel} \quad (1)$$

and

$$S_{\perp,s}(z, v_{\perp}) dv_x dv_y = h(z) \exp\left(\frac{-m_s v_{\perp}^2}{2kT_{\perp,s}}\right) v_{\perp} dv_{\perp} d\theta \quad (2)$$

where $h(z)$ is the source intensity profile in the range $[0, 1]$, k is Boltzmann's constant, and m_s , $T_{\parallel,s}$ and $T_{\perp,s}$ are the mass, parallel and perpendicular source temperatures for species s respectively. The exponent η_s allows one to choose either a Maxwellian ($\eta_s = 0$), flux ($\eta_s = 1$) or more general distribution function for the species s . The $v_{\perp}$ that follows the exponential in (2) is present because the perpendicular direction comprises two degrees of freedom (the $\hat{x}$ and $\hat{y}$ directions), such that $dv_x dv_y = v_{\perp} dv_{\perp} d\theta$, whereas $dv_z = dv_{\parallel}$.

The parallel and perpendicular source velocities are generated from these source distribution functions at the start of the run and are stored in arrays. The perpendicular source velocities are stored in increasing order from $v_{\min} = 0$ to $v_{\max}$, while the parallel source velocities are stored in base-2 bit-reversed order for "quiet" injection (from the planar source). (See Reference [4], pages 393-394 for a discussion of bit-reversed numbers and their application to particle simulation methods). Each of the species has an array for parallel and perpendicular source velocities. Upon injection, the index of the parallel and perpendicular velocity arrays, and hence the values of $v_{\parallel}$ and $v_{\perp}$ are chosen randomly for each particle, which tends to minimize correlations of the injected velocity components.

The source region is defined by the center location Z_{os} and the width ΔZ_s . The source intensity function that has been employed in DIPSI is $h(z) \approx 1$, although more general intensity profiles are possible. The particles are injected uniformly over the source region via

$$z_{inj} = Z_{os} + R_N \Delta Z_s \quad (3)$$

where R_N is a random number in the range $(-0.5, 0.5)$. The electrons and ions are injected at the same location. Since the electron and ion velocities are, in general, not the same, it is possible to have charge separation that will result in an electrostatic source sheath. The velocity components of the injected particles are then used to calculate the relativistic factor γ , the parallel momentum p_z and the magnetic moment μ . These quantities are

then written to the permanent particle arrays. If the number of particles injected per time step exceeds the free space at the end of the permanent particle arrays, the arrays are dynamically expanded by the input variable N_{expand} . In order to reduce the amount of time spent expanding the arrays, N_{expand} is chosen such that there are of order 100 time steps between successive array expansions.

1.1.2 The Planar Source Model

The planar source model may be used to simulate the injection of particles by the cathode of a plasma diode or single-ended Q-machine, or alternatively, may represent the flux of Maxwellian particles which is crossing a plane boundary. The planar source model is similar in many ways to the distributed source package. One major difference is the normalized source distribution function, which for particles emitted from a plane is a flux distribution

$$S_{||,s}(v_{||})dv_{||} = |v_{||}| \exp\left(\frac{-m_s v_{||}^2}{2kT_{||,s}}\right) dv_{||} \quad (4)$$

and

$$S_{\perp,s}(v_{\perp})dv_{\perp}dv_y = \exp\left(\frac{-m_s v_{\perp}^2}{2kT_{\perp,s}}\right) v_{\perp} dv_{\perp} d\theta. \quad (5)$$

The parallel and perpendicular velocity components of the injected particles are chosen in the following manner. The perpendicular velocity component is chosen randomly out of the perpendicular-velocity source array. For the parallel velocity component, the code maintains an integer counter. This counter starts at one and increases by one for each particle (of either species) that is injected. When a counter exceeds the length of the array, the counter is reset to one and then increased by one for each additional particle injected. This counter is then used as the element that is to be chosen for injection from the bit-reversed parallel-velocity source array. This method ensures that the velocity components of the injected particles are chosen uniformly from the range $[v_{min}, v_{max}]$.

The positions of the injected particles are calculated in the following way. Each particle is injected at the left boundary ($z = 0$), but its position at the end of the injection routine is related to its velocity and when it was injected during the time step. The time step Δt is divided by the number of particles of the given species that are to be injected in that time step to give the time between injections as $\tau_{inj} = \Delta t/N_{inj}$. The position of the i -th

particle at the end of the injection routine is then given by

$$z_i = v_{\parallel,i} (N_{inj} - i) \tau_{inj}. \quad (6)$$

Finally, the velocity components of the particles are used to calculate the relativistic factor γ , the parallel momentum p_z and the magnetic moment μ , which are then written into the permanent particle arrays. If necessary, the arrays are expanded via the previously described method.

1.2 Simulation Results

The planar source injection model is used to simulate a flux of Maxwellian particles which cross a specified plane in space, and proceed to flow to an electrostatically floating, conducting plate. This absorbing wall is the system boundary on the right side, while the “injection” plane is the left side boundary. It is assumed that there is a collisional, distributed source located to the left of the computational domain, where particles of species s are created and maintained in a Maxwellian velocity distribution of characteristic temperature kT_s . As these particles enter the system across the left system boundary, the electrons are, in general, travelling faster than the ions. As a result, a source sheath is generated which attempts to equilibrate the particle fluxes in the region just to the right of the left system boundary. Particles which exit the system across the left system boundary are reflected, with a velocity chosen from an untruncated half-Maxwellian of temperature kT_s travelling to the right. This boundary condition is included to replicate the collisional relaxation processes which take place in the region to the left of the system.

The model assumes that the plasma is unmagnetized and collisionless (except for the re-thermalization process which takes place at the left system boundary). Equal numbers of electrons and ions per time step are “injected” across the source plane $z = 0$ with parallel velocity distribution functions that are half-Maxwellian travelling to the right and perpendicular velocity distributions that are Maxwellian. Hence, the model is 1-D (one spatial coordinate) and 2-V (two velocity space coordinates). For the results presented below, the system length $L = 2.0\text{cm}$ corresponds to approximately $26.6\lambda_{De}$ for the equilibrium density n_e and source temperature kT_e . The source temperature ratio is $kT_e/kT_i = 1$ and the mass ratio is $m_i/m_e = 100$. The drift velocity of both the electrons and ions is $v_{0e} = v_{0i} = 0$.

The equilibrium phase space scatter plots for the electrons and ions are shown in Figures 1 and 2 respectively. The corresponding potential profile along the z axis is given in Figure 3. Since the system is unmagnetized and collisionless, there are no forces present in the model to change the perpendicular velocity distribution of the particles. This is borne out by Figures 1b and 2b, which show that the perpendicular-velocity phase space for each of the species remains Maxwellian as the particles traverse the system.

Figure 3 indicates that there is source sheath on the left side and a collector sheath on the right side of the system. Each of these sheaths have formed over four to five electron Debye lengths, which is a typical distance over which deviations from quasineutrality (due to the injection of particles at the left boundary and the net negative charge on the collector plate) are shielded out in a plasma. The parallel-velocity phase space plot (Figure 1a) shows electrons that apparently form a cut-off or truncated Maxwellian distribution function. This structure is a consequence of the equilibrium potential profile. Only electrons that are energetic enough to climb over the collector sheath potential hill are absorbed on the plate. The remaining electrons are reflected by the collector sheath. Since the electron distribution function to the left of the collector sheath region is essentially a right-going half-Maxwellian (the electron distribution function is modified by the source sheath to some extent), the reflected electrons form a left-going, truncated half-Maxwellian distribution function. The velocity cut-off is due to the electrons that were energetic enough to traverse the collector sheath and impinge upon the absorbing plate. The ion parallel-velocity phase space plot (Figure 2a) shows that the ions are accelerated towards the plate by the monotonically decreasing potential. Therefore, all of the ions that are injected across the plane at $z = 0$ will reach the absorbing plate. The number of electrons that reach the plate is such that the electron and ion currents at that location are equal, which is necessary to maintain a steady-state plate charge and collector sheath drop.

The distributed source model has been used in to study the effect of the source distribution function $S(z, v)$ on the width and magnitude of the collisionless source and collector sheaths [5], to investigate the effect of Coulomb collisions on the potential structure and plasma transport in the plasma-sheath region [6], and to study the effect of charge-exchange and ionization of recycled neutral particles on the presheath potential variation in the SOL of a high-recycling diverted tokamak [7].

(a) Electron parallel-velocity phase space scatter plot.

(b) Electron perpendicular-velocity phase space scatter plot.

Figure 1: Electron (a) parallel-velocity and (b) perpendicular-velocity phase space scatter plots for the case of Maxwellian particle injection into the plasma-sheath region adjacent to a floating, absorbing conductor. The species mass and source temperature ratios are $m_i/m_e = 100$ and $kT_e/kT_i = 1$.

(a) Ion parallel-velocity phase space scatter plot.

(b) Ion perpendicular-velocity phase space scatter plot.

Figure 2: Ion (a) parallel-velocity and (b) perpendicular-velocity phase space scatter plots for the case of Maxwellian particle injection into the plasma sheath region adjacent to a floating, absorbing conductor. The species mass and source temperature ratios are $m_i/m_e = 100$ and $kT_e/kT_i = 1$.

Figure 3: Potential profile for the case of Maxwellian particle injection into the plasma-sheath region adjacent to a floating, absorbing conductor. The species mass and source temperature ratios are $m_i/m_e = 100$ and $kT_e/kT_i = 1$.

2 The Atomic Physics Models

The heat load on and plasma-induced sputtering of the surface of a divertor plate in a tokamak is strongly dependent upon the amount of energy that is transferred from the incoming charged particles to the neutral atoms which are located in the vicinity the plate [8]. These cold neutral particles are formed by reflection or "recycling" of the plasma ions from the divertor plate, which supplies the electrons which are required to neutralize the incident charged particles. The plasma particles undergo charged-neutral collisions with the background gas. These collisions can be either elastic (the combined kinetic energy of the particles remains constant, but the trajectories are changed), inelastic (the charged particle provides energy to place the bound electrons of the neutral particle in an excited state) or ionizing (where the energy transferred in the collision is large enough to remove the orbital electron from the neutral particle) in nature. In addition, a warm plasma ion may exchange an electron with a cold neutral particle, producing a cold ion and a warm neutral atom. In an attempt to model some of these atomic physics processes, an impact ionization and

charge exchange package has been incorporated into the code DIPSI [1].

2.1 Methodology

The atomic physics package in the code DIPSI is used to simulate the effects of charged particles interacting with a background neutral gas. The atomic physics models that are incorporated into DIPSI are similar to those in the “PD” series of bounded particle codes from the University of California at Berkeley [12, 13], which are used to model the low-ionization plasmas employed in semiconductor processing. The neutral gas in a tokamak SOL is produced as plasma interacts with the divertor plate. As plasma ions impact a material surface, they undergo both elastic collisions with the nuclei, and inelastic collisions with the electrons of the plate atoms, leading to a reduction in their kinetic energy. Collisions with the atomic nuclei also lead to changes the direction of the flight path. A fraction of these ions will undergo sufficient pitch-angle scattering to exit from the plate and reenter the plasma. These reflected or recycled particles may have either positive, neutral or negative charge states (having obtained electrons from the plate material). The fraction of these “prompt” reflected particles, their average reflected energy and energy distribution, and their charge state depend upon the energy of the incident ions, the angle of incidence and the atomic charges and masses of the incident and target particles [9]. The plasma ions that come to rest (thermalize) in the atomic lattice of the plate material are another source of neutral particles. These monatomic and/or molecular particles will diffuse towards the surface of the plate, where they may be released by physical (photon or plasma impact) or chemical desorption processes [10, 11].

The code DIPSI treats the neutral particles in an ad hoc manner by assuming that the neutral density decays exponentially with increasing distance from the divertor plate. This density profile is obtained if one represents the divertor plate as a planar source of reflected neutral particle flux. The neutral density e-folding length $\mathcal{L}_n$ is taken to be the average ionization mean-free-path length $\langle\lambda_{ion}\rangle$, such that

$$n_n(z) = \hat{n}_n \exp(-[L - z]/\mathcal{L}_n) \quad (7)$$

where L is the location of the divertor plate (system length), and $\hat{n}_n$ is the peak neutral density adjacent to the divertor plate. The average ionization mean-free path ($\langle\lambda_{ion}\rangle$) and

the peak neutral density ($\hat{n}_n$) are treated as input parameters in this model.

The peak neutral density is adjusted in time so as to maintain a constant ionization source term S_{ion} . At the start of a simulation, the initial source term is calculated via

$$S_{ion}^0 \equiv \int_{z'=z_{min}}^L n_e(z') n_n(z') \{\sigma_{ion}(E_e) v_e\} dz' \quad (8)$$

$$\simeq \sum_{j=j_{min}}^{NG+1} n_{e,j} \hat{n}_{n,j} \sigma_{ion}(\bar{E}_{e,j}) \bar{v}_{e,j} \quad (9)$$

where j is the grid point index, $n_e(z)$ is the electron density profile, σ_{ion} is the electron-impact ionization cross section, E_e is the local electron kinetic energy and v_e is the local electron velocity. This source term is reevaluated every NT_{nd} time steps (where NT_{nd} is an input parameter), using quantities that have been averaged over the previous NT_{nd} time steps

$$S_{ion}^T = \sum_{j=j_{min}}^{NG+1} \bar{n}_{e,j} \bar{n}_{n,j} \sigma_{ion}(\bar{E}_{e,j}) \bar{v}_{e,j} \quad (10)$$

where T is an integer multiple of NT_{nd} . The peak neutral density is then adjusted via

$$\hat{n}_n^T = \hat{n}_n^0 \left(\frac{S_{ion}^0}{S_{ion}^T} \right) \quad (11)$$

where $\hat{n}_n^0$ is initial peak neutral density that is input by the user.

Many of the physical aspects of neutral particle recycling from a divertor plate are included in this constant-ionization model. The flux of neutral particles reflected from the plate increases with the flux of plasma incident upon the plate. The flow of warm plasma to the plate is inhibited by the charged/neutral interactions which occur in the region adjacent to the plate. As the fraction of plasma ions recycled from the plate increases, the neutral density and charged/neutral interaction rates will also increase, thereby reducing the recycled neutral flux and neutral particle density. In the proposed model, as the plasma density adjacent to the plate increases (as a result of impact ionization events), the neutral density is decreased accordingly. If the plasma density in this region decreases, the neutral density is increased. Note that the model also includes a dependence on the energy of the plasma in this region through the ionization reaction rate $\sigma_{ion}(\bar{E}_{e,j}) \bar{v}_{e,j}$.

The time history of the peak neutral density during the simulation of transport in a high-recycling divertor SOL is shown in Figure 4. Warm plasma ($kT_e \simeq 100\text{eV}$) flows collisionally towards the plate, undergoing interactions with cold neutral particles ($kT_n = 5\text{eV}$). The

Figure 4: The time history of the peak neutral density in a high-recycling divertor scrape-off layer in a tokamak. The peak density is adjusted every $NT_{nd} = 25$ time steps in order to maintain a constant ionization rate.

peak density was adjusted every $NT_{nd} = 25$ time steps. The peak density decreases over the first 5000 time steps of the simulation as the plasma density adjacent to the plate increases due to (i) the influx of warm plasma from upstream and (ii) the ionization of cold neutral particles. The neutral density approaches a steady-state value at approximately the half-way point in the simulation. The high-frequency fluctuations occur on the NT_{nd} time scale.

2.1.1 The Impact Ionization Model

Neutral atoms may be ionized via collisions with the charged particles of the plasma. If the charged particles strike the atoms with sufficient force, one or more electrons will be stripped from the neutral atom. For atoms which are isotopically identical to the plasma ions, this process results in an increase in the plasma electron and ion density.

Since the electron/neutral collision model in the code DIPSI is intended to simulate plasma recycling from a plasma-facing component, such as a divertor plate or limiter, only ionization events arising from electron/neutral interactions are considered. Elastic-

scattering and excitation collisions between electrons and fusion-relevant neutral atoms (hydrogen, deuterium, tritium and helium) are neglected, as are ion-impact-ionization events, since the cross sections for these processes are much smaller than that for electron-impact ionization [14]. This model borrows from the previous efforts of I. J. Morey and M. Surendra at the University of California at Berkeley [12].

Since the model does not include excitation collisional processes, it is not entirely applicable for the simulation of impurity particle (carbon, oxygen, iron, nickel, etc.) transport. The emission of line radiation by excited orbital electrons (as they make a transition to a lower energy state), and bremsstrahlung by free electrons (as they are accelerated by plasma ions) are major energy loss mechanisms in a low to moderate temperature SOL plasma. The power emitted in the form of line radiation increases with the number of available orbital-electron energy states, which in turn rises with the atomic number of the particle, and the bremsstrahlung power emission increases as the square of the effective atomic number of the plasma. Therefore, even small quantities of impurity particles can lead to a significant amount of energy loss via radiative processes. Models for these radiative processes should be added to the present atomic physics package if one wishes to simulate impurity particle transport.

The probability of the k -th plasma electron having an ionizing collision with a neutral particle during a given time step is a function of the local neutral density $n_n(z)$ (defined on the grid points), the kinetic energy (and hence the velocity of the electron) $E_e \equiv \frac{1}{2}m_e(v_{\parallel e}^2 + v_{\perp e}^2)$ and the length of the time step Δt

$$P_{ion,k} = [1 - \exp\{-n_n(z)\sigma_{ion}(E_{e,k})v_{e,k}\Delta t\}] \quad (12)$$

where k is the electron index. The probability $P_{ion,k}$ is calculated for each electron in a given grid cell. An ionizing collision occurs if a random number R_N (chosen from the range $(0, 1)$) is less than $P_{ion,k}$. (If the argument of the exponential in (12) is $\ll 1$, such that $P_{ion,k} \ll 1$, it is possible to sample every N_{skip} electrons, and multiply the right side of (12) by N_{skip} to provide a reasonable ionization probability per sampled electron per time step.)

The electron-impact ionization cross section has the following energy dependence

$$\sigma_{ion}(E_e) = \begin{cases} 0 & , E_e < E_{th} \\ \delta_{ion} \left(\frac{E_e - E_{th}}{E_{pl,min} - E_{th}} \right) & , E_{th} \leq E_e < E_{pl,min} \\ \delta_{ion} & , E_{pl,min} \leq E_e < E_{pl,max} \\ \delta_{ion} \left(\frac{E_{pl,max}}{\ln(E_{pl,max})} \right) \left(\frac{\ln(E_e)}{E_e} \right) & , E_e \geq E_{pl,max} \end{cases} \quad (13)$$

where δ_{ion} is the peak ionization cross section, E_{th} is the minimum or threshold kinetic energy required to ionize a neutral particle, and $E_{pl,min}$ and $E_{pl,max}$ are the limits of kinetic energy for which the cross section has a constant, peak (plateau) value. All of these quantities are input parameters in the present model. The energy dependence of the ionization cross section for electrons colliding with monatomic hydrogen ($1H^1$) is shown in Figure 5. Figure 5a shows experimentally measured values [15], while Figure 5b shows the values obtained from (13) for $\delta_{ion} = 7.15 \times 10^{-17} \text{ cm}^2$, $E_{th} = 13.6 \text{ eV}$, $E_{pl,min} = 40.0 \text{ eV}$ and $E_{pl,max} = 80.0 \text{ eV}$. The simple model described by (13) provides reasonable agreement with measured values over the energy range $0.1 \text{ eV} \lesssim E \lesssim 1.0 \text{ keV}$.

Once it has been determined that a given electron will ionize a neutral particle, the energy available for the scattered electron (E_{e1}), and the new electron (E_{e2}) and ion (E_i) pair are obtained via an energy balance

$$\Delta E = E_{e1} + E_{e2} + E_i = E_e + E_n - E_{th} \quad (14)$$

where the energy of the neutral particle E_n is chosen from an isotropic Maxwellian distribution of temperature kT_n via the relation

$$E_n = kT_n \ln \left(\frac{1 + \delta}{1 + \delta - R_N} \right) \quad (15)$$

where $\delta = 10^{-8}$ and R_N is a random number in the range (0, 1). The argument of the logarithm ranges in value from 1 to 10^{-8} , representing the limits on the value of the normalized distribution function $\hat{f}(v)$.

The energy of the scattered electron E_{e1} is calculated via the energy-differential cross section [16]

$$\sigma_{ion}(E_e, E_{e1}) = \frac{\alpha(E_e)}{E_{e1}^2 + 1^2} \quad (16)$$

(a) Experimentally measured ionization cross section [11].

(b) Ionization cross section calculated by the simple model (4.13).

Figure 5: Ionization cross section as a function of energy for collisions between electrons (e) and monatomic hydrogen (H¹) from (a) experimental measurements [11] and (b) from the simple model (4.13).

where Γ is the energy-level width of the cross section. Since the maximum energy available for the scattered electron is $E_{e1,max} = (E_e + E_n - E_{th})/2$, it is possible to integrate the energy-differential cross section as [12, 13]

$$\sigma_{ion}(E_e) = \int_0^{E_{e1,max}} \sigma_{ion}(E_e, E_{e1}) dE_{e1} \quad (17)$$

such that one obtains

$$\alpha(E_e) = \frac{\sigma_{ion}\Gamma}{\arctan\left(\frac{E_e + E_n - E_{th}}{2\Gamma}\right)}. \quad (18)$$

Since the energy-differential cross section is normalized as

$$\int_0^{E_{e1,max}} \frac{\sigma_{ion}(E_e, E_{e1})}{\sigma_{ion}} dE_{e1} = 1 \quad (19)$$

it is possible to choose a random number R_N in the range (0,1) to determine the kinetic energy of the scattered electron E_{e1} , such that

$$R_N = \int_0^{E_{e1,max}} \frac{\Gamma dE_{e1}}{(E_{e1}^2 + \Gamma^2) \arctan\left(\frac{E_e + E_n - E_{th}}{2\Gamma}\right)}, \quad (20)$$

or rearranging

$$E_{e1} = \Gamma \tan\left(R_N \arctan\left(\frac{E_e + E_n - E_{th}}{2\Gamma}\right)\right). \quad (21)$$

The kinetic energy of the new electron and ion are then determined by a mass-energy balance relation

$$\begin{aligned} E_{e2} &= (\Delta E - E_{e1}) \left(\frac{m_i}{m_i + m_e} \right) \\ E_i &= (\Delta E - E_{e1}) \left(\frac{m_e}{m_i + m_e} \right), \end{aligned} \quad (22)$$

where m_e and m_i are the masses of the electron and ion respectively. Note that this method does *not* conserve kinetic energy, since the threshold energy (E_{th}) is required to remove the bound electron from the atom.

The velocity components ($v_{||}$ and $v_{\perp}$) of the scattered electron, and the new electron and ion are all chosen randomly

$$\begin{aligned} v_{||} &= \sqrt{\frac{2E}{m}} \cos(\pi R_N) \\ v_{\perp} &= \sqrt{\frac{2E}{m}} \sin(\pi R_N) \end{aligned} \quad (23)$$

where R_N is a random number in the range $(0,1)$. This implies that the incident electron velocity is scattered isotropically during the ionizing collision. These velocity components are then used to calculate the parallel momentum p_z and magnetic moment μ of the new electron and ion. The spatial location of the new electron/ion pair is assumed to be the same as that of the incident electron. By placing the new electron and ion at the same position, there is no net contribution to the net charge density $\rho(z)$ and the electric field $E(z)$ arising from the ionization event.

2.1.2 The Charge Exchange Model

A charge exchange event occurs when a neutral atom transfers one or more electrons to an adjacent ion. This process results in a change in the kinetic energy of the charged and neutral species, with the ion and neutral particle densities remaining constant. Charge exchange is the most probable interaction between ions and fusion-relevant neutral particles [14]. Therefore, it is the only ion/neutral collision process simulated by the code DIPSI.

The algorithm for the charge exchange model is similar to that described above for the impact ionization model. The probability of the k -th plasma ion exchanging at least one electron with a neutral particle during a given time step is also a function of the local neutral density $n_n(z)$ (defined on the grid points), the ion kinetic energy and velocity $E_i \equiv \frac{1}{2} m_i (v_{ji}^2 + v_{1i}^2)$ and the time step duration Δt

$$P_{cx,k} = [1 - \exp(-n_n(z)\sigma_{cx}(E_{i,k})v_{i,k}\Delta t)]. \quad (24)$$

The probability $P_{cx,k}$ is calculated for each ion in a given grid cell. A charge exchange event occurs if a random number R_N in $(0,1)$ is less than $P_{cx,k}$. (As above, if the argument of the exponential in (24) is very small compared to unity, (i. e. $P_{cx,k} \ll 1$, it is possible to sample every N_{skip} ions, and multiply the right side of (24) by N_{skip} to provide a reasonable probability per sampled ion per time step.)

The charge-exchange cross section for hydrogenic particles has been fit to measured data by Riviere [17, 14]. This empirical fit has the following dependence on the ion kinetic energy

$$\sigma_{cx}(E_i) = \hat{\sigma}_{cx} \left(\frac{\{1 - 0.155 \log(E_i)\}^2}{1 + 1.112 \times 10^{-15} E_i^{3.3}} \right) \quad (25)$$

where $\hat{\sigma}_{cx}$ is the maximum charge-exchange cross section, and E_i is the ion kinetic energy in units of eV. This fit is used in the present model. Therefore, the energy dependence of

the cross section is assumed to be the same for various ion/neutral particle combinations, but the magnitude may be changed via the input parameter σ_{cx} . The energy dependence of the charge-exchange cross section for protons interacting with monatomic hydrogen ($1H^1$) is shown in Figure 6. Figure 6a shows experimentally measured values [18], while Figure 6b presents the values obtained from (25) for $\sigma_{cx} = 0.94 \times 10^{-15} \text{ cm}^2$. The empirical fit (25) provides excellent agreement with measured values over the energy range $0.1\text{eV} \lesssim E_i \lesssim 1.0\text{MeV}$ (even though Figure 6b only covers the range $0.1\text{eV} \leq E_i \leq 2.0\text{keV}$).

The velocity components $v_\perp$ and $v_\parallel$ of the ion are modified as a result of the charge exchange event. However, the positions of the initial and final ions are the same. The velocity components of the new ion are dependent upon the temperature of the neutral atoms kT_n . This thermal spread is assumed to be isotropic and Maxwellian in Cartesian velocity space, such that the speed of the new ion is given by

$$v'_i = \left[(2kT_n/m_n) \ln \left(\frac{1+\delta}{1+\delta-R_N} \right) \right]^{1/2} \quad (26)$$

where $\delta = 10^{-8}$, R_N is a random number in $(0,1)$ and $m_n = m_i + Zm_e$ is the mass of the neutral atom of atomic number Z . The same method was used to determine the kinetic energy of the neutral particle in the impact ionization model described above. The velocity components are then chosen randomly by $v'_{\parallel,i} = v'_i \cos(\pi R_N)$ and $v'_{\perp,i} = v'_i \sin(\pi R_N)$, where R_N is a random number in the range $(0,1)$. These velocity components are then used to calculate the parallel momentum p_z and magnetic moment μ of the new ion.

The impact ionization and charge exchange models have been used in [7] to study the interaction of cold, recycled, neutral gas and warm plasma, and its effect on the transport of particles and energy through the scrape-off layer to the divertor plate in a tokamak.

(a) Experimentally measured charge-exchange cross section [14].

(b) Charge-exchange cross section calculated by the empirical fit (4.25).

Figure 6: Charge-exchange cross section as a function of energy for protons ($_1p^1$) interacting with monatomic hydrogen ($_1H^1$) from (a) experimental measurements [14] and (b) from the empirical fit (4.25).

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