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# Method for Simulation of Particle Recombination in SOL Plasma

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**Abstract.** The effect of charged particle recombination is investigated performing particle in cell (PIC) simulation of plasma in tokamak devices. For the simulation of particle collisions is used an appropriate method to account for frequencies spread in wide range of magnitude. The method was tested simulating steady state plasma in the scrape off layer (SOL). A constant density profile of deuterium atoms is assumed with sharp peaks in divertor region.

The simulation results show decreasing frequency of recombination near the plates of divertor where the ionization is dominating due to the big concentration of deuterium atoms. The recombination processes become more frequent deep in the SOL where the density of neutral particles is rather low.

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## 1 Introduction

Due to the small rate of charged particle recombination in hot plasma this process is often neglected in the simulation of particle collisions in tokamak devices. However, when the plasma has considerably higher density than the neutral component, recombination may play an important role for the balance between the charged and the neutral plasma components. A particularly important issue is to understand the role of recombination in the detachment of plasma from the divertor plates and to hamper the inward flow of impurities with puffing of gas [1].

 

Our goal here is to study the effect of the recombination using a simple model with time invariant neutral particle density. This time invariance is expected during steady state of SOL plasma.

We present a general method for simulations. The method can be applied also for models accounting for the change of the neutral component density. It can be used also for turbulent plasma during stationary edge localized mode (ELM) with small amplitude of density oscillations and invariant temperature profiles. Such ELM is a candidate scenario for performances of the international tokamak experimental reactor (ITER).

The proposed method is adopted for Monte Carlo simulation of collisions the frequencies of which are in wide range and in some cases are beyond the limits of the usual random number generator accuracy. The simulated processes are presented in Section 2, the description of the routines for simulation of collisional (three-body) and radiative (two-body) recombination processes is in Section 3, the new method for collision simulation is discussed in Section 4, statistical testing of the recombination procedures and simulation results for the profiles of plasma density and temperature in the SOL with and without recombination are presented in Section 5.

## 2 Assumptions for Particle Collisions

In the present study we consider $D$ plasma and the following processes are taken into account:

Three-body recombination

$$D^+ + e + e \;\rightarrow\; D(p) + e \tag{1}$$

One-step ionization

$$D(p) + e \;\rightarrow\; D^+ + e + e \tag{2}$$

Collisional excitation and de-excitation

$$D(p) + e \;\rightarrow\; D(q) + e \tag{3}$$

Two-step ionization

$$D(p) + e \;\rightarrow\; D(q) + e \;\rightarrow\; D^+ + e + e \tag{4}$$

Radiative recombination

$$D^+ + e \;\rightarrow\; D(p) + h\nu \tag{5}$$

Spontaneous transition

$$D(p) \ \rightarrow \ D(q) + h\nu \tag{6}$$

Ellastic collisions of electrons with atoms

$$D(p) + e \ \rightarrow \ D(p) + e \tag{7}$$

Elastic collisions of $D$ ions with $D$ atoms

$$D^+ + D(p) \ \rightarrow \ D^+ + D(p) \tag{8}$$

Charge exchange of $D$ ions with $D$ atoms.

$$D^+ + D(p) \ \rightarrow \ D(p) + D^+ \tag{9}$$

($p$ and $q$ are the principle quantum numbers of the discrete levels of $D$ atoms).

For the Coulomb collisions and electron recycling from the walls we have used the procedures in BIT1 code [4] (developed on the basis of the XPDP1 code [5]). From the BIT1 code we have used also the cross sections for elastic scattering of ions and electrons from $D$ atoms (7, 8), excitation (3) and direct ionization of atoms by electrons (2), charge exchange between atoms and $D$ ions (9).

The calculations are performed with a new code BIT1-S. BIT1-S is a new version of BIT1; it is based on an appropriate method for Monte Carlo simulation of particle collisions; it uses coefficients calculated within the general theory [2] (and verified with recent data [3]) for the rate of effective ionization combining one-step (2) and two-step (4) processes as well as for the rates of collisional (1) and radiative (5) recombination; it incorporates a procedure for effective ionization developed in an earlier paper [6] and new procedures for recombination processes presented in another paper [7].

## 3 Procedures for Monte Carlo Simulation of Recombination Processes

The procedures for charged particle recombination are developed similarly to the procedures for effective ionization in [6]. Here we use the rate coefficients $\langle \sigma_r v \rangle$ calculated by Bates *et al.* [2] for the recombination processes. In the calculations for a fixed plasma density we use an approximation of the rate coefficient as function on electron temperature (see Figure 1). The rate coefficients for recombination are calculated during the code run for the current electron temperature and density in particular grid cell.

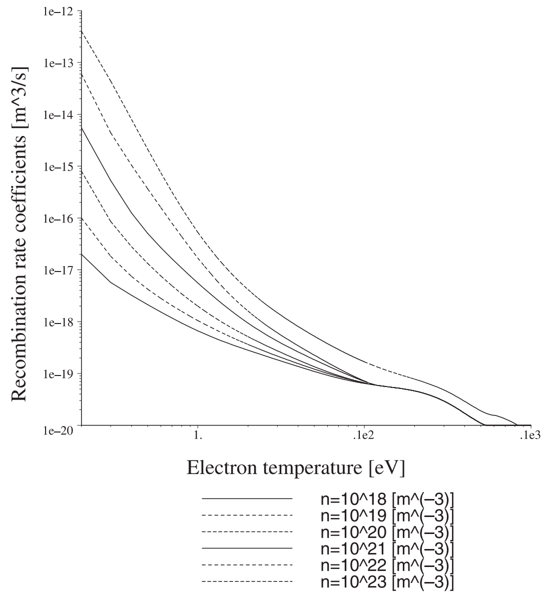


Figure 1. Approximation of the data for the recombination rate in dependence on electron temperature for fixed plasma density.

Two recombination processes are considered: for two-body radiative recombination (5) and three-body collisional processes (1) of $D$ ion and two electrons. In the first case an electron recombines with a bare $D^+$ nucleus in the absence of any third body. The incident energy is carried out by the emitted radiation. The second case (of three-body recombination) appears for sufficiently dense plasma at low temperature. The incident energy of the electron striking the bare nuclear is randomly shared among the emerging new atom and a neighboring electron.

The type of the recombination process is chosen in correspondence to the instant plasma temperature during the code run. A distributive procedure is calling one of the two – radiative or collisional recombination procedure function. In accordance with the general theory [2] the following rule was used: if the temperature is below a threshold $T_c = 0.086$ eV at which the rate for radiative recombination is vanishing to $0$ ($\langle \sigma_r v \rangle^{rad} = 0$) three-body recombination subroutine is called. In the present calculations the released energy for ionization (above $13.6$ eV) is given to the neighboring electron according to [3]. If the temperature is above another threshold, $T_r = 0.86$ eV at which the rate for collisional recombination vanishes ($\langle \sigma_r v \rangle^{col} = 0$) then two-body procedure is called. In this case the energy of incoming electron and the released energy for ionization are carried out by the emitted radiation. It is a complete loss of energy in the conditions of a thin plasma in the SOL.

For plasma temperature between $T_c$ and $T_r$ the type of collision is chosen with Monte Carlo procedure over the linear approximations of the rate distributions of both reactions. Approximation parameters are defined from the rates for the boundary temperature values, $T_c$ and $T_r$.

## 4 Method for Collision Simulation

In the present calculations is used Particle-In-Cell (PIC) method according to which the simulated volume is presented as a grid of cells.

To save computer time in the original XPDP1 code there is used the null-collision method [8]. For collision simulation of a particle instead to use the probability $P = 1 - exp(-\nu\,\Delta t)$ there is used the collision frequency $\nu = \sigma\,v\,n_t$ normalized to the maximum value $\nu^{\max}$. The latter could reach $10^7$ s$^{-1}$ but since the time for collision in PIC simulation is very small ($\Delta t$ is about $10^{-12}$ s) such $O(\Delta t^2)$ approximation seems to be satisfactory.

A problem arises when the rates of the collisions and particle densities drop (for recombination in hot plasma it is about $10^{-20}$ m$^3$s$^{-1}$ and the density of ions could drop below $10^{18}$ m$^{-3}$) so that the normalized frequencies could become less than the limit of random number generator which is $2^{-31}$. The number of simulated collisions with small frequency is underestimated despite the re-normalization with maximum number of experienced collisions. It motivates the opinion that the recombination does not play an important role at temperature above few eV [3].

In our method we estimate the number of collisions using the average values of plasma characteristics (electron temperature, plasma and neutral gas densities) in the calculation of the total probability for electron collisions

$$P_{\text{tot.},e} = 1 - \exp\left\{-[\bar{n}_0\langle\sigma v\rangle_e^* + \bar{n}_i\langle\sigma_r v\rangle]\Delta t\right\} \tag{10}$$

and for ion collisions

$$P_{\text{tot},e} = 1 - \exp\left\{-[\bar{n}_0\langle\sigma v\rangle_i]\Delta t\right\}, \tag{11}$$

where

$$\langle\sigma v\rangle_e^* = (\sigma_{el.coll.}^e + \sigma_{excit.} + \sigma_{ioniz.})\bar{v}, \tag{12}$$

and for the ion collisions

$$\langle\sigma v\rangle_i^* = (\sigma_{elas} + \sigma_{ch.ex.})\bar{v} \tag{13}$$

($\bar{n}_0$ and $\bar{n}_i$ are the averaged densities of $D$ atoms and ions respectively for time $\Delta t$).

The electron velocity $\bar{v}$ is calculated from the temperature of electrons averaged on all grid cells during $\Delta t$

$$\bar{v} = \sqrt{\frac{3.\bar{T}.k}{m_e}}$$

($k = 1.6 \times 10^{-19}$ j/eV, $m = 9.1 \times 10^{-31}$ kg). Thus the total number of simulated collisions is exactly the sum of collisions from the call of corresponding Monte Carlo procedures:

$$N_{\text{tot},e} = P_{\text{tot},e} N_e = \sum_{j=1}^{4} N_j^{e\ coll}$$

$$N_{\text{tot},ion} = P_{\text{tot},ion} N_{ion} = \sum_{j=1}^{2} N_j^{ion\ coll}.$$

The choice of collision is made between all collisions that the simulated particle could suffer. For this purpose a random number is compared with the particular probabilities normalized to their sum. In the case of SOL plasma the use of the approximation $O(\sigma^2)$ could decrease essentially the time of simulation.

The rate of plasma decay due to the recombination processes was checked with a numerical test similar to the check for the effective ionization procedure in our previous work [6]. The decay of plasma was simulated in a closed box and compared with the analytically calculated rate. A very good agreement is obtained confirming the efficiency of the method for collision simulation.

## 5 Statistical Testing and Simulations

To perform strict statistical testing we run the code in conditions of hot plasma within a wide range of temperature variations. The temperature and density profiles of the neutral particles are assumed constant (computed with Monte Carlo Codes [Nimbus, Eirene] [9], Figure 2 presents the density profile). An outward flow from the crossing point of the separatix is assumed with a constant intensity $7.3 \times 10^{24}$ part./m$^3$/s. The thermal energy of plasma in the source is $42$ eV for both components assuming dynamic equilibrium in the pedestal region (magnetic field intensity is $0$).

A narrow plateau of plasma particle number is reached after $2$ $\mu$s. It lasts about $2$ $\mu$s before the decay of plasma. During this time interval the plasma temperature and density profiles remain approximately constant. The electron density is about $n_e = 6 \times 10^{17}$ m$^{-3}$ almost in the entire SOL. It is below the lower limit of plasma density of the input data. Below this limit effective ionization processes are entirely excluded.

We have gathered statistics from the calls of recombination processes with constant density about $10^{18}$ m$^{-3}$ in a wide temperature range. The constructed histogram is shown in Figure 3. It is in a satisfactory agreement with the distribution of the recombination rates inserted in the input data file for plasma density $10^{18}$ m$^{-3}$.

We simulated poloidal plasma propagation from the sparatrix to the divertor plate assuming radial and toroidal invariance. We assumed outward flow from

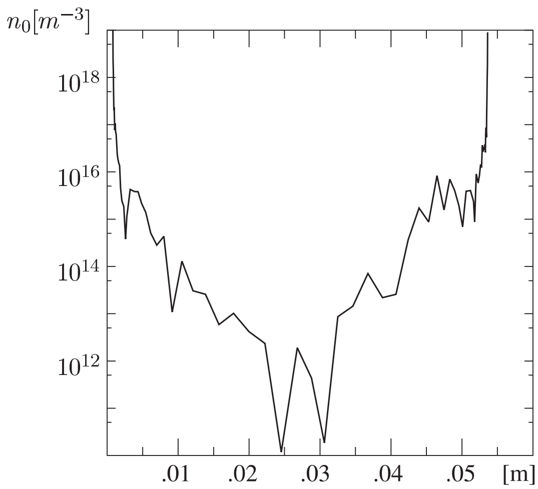


Figure 2. Neutral particle profile in divertor plasma simulation.

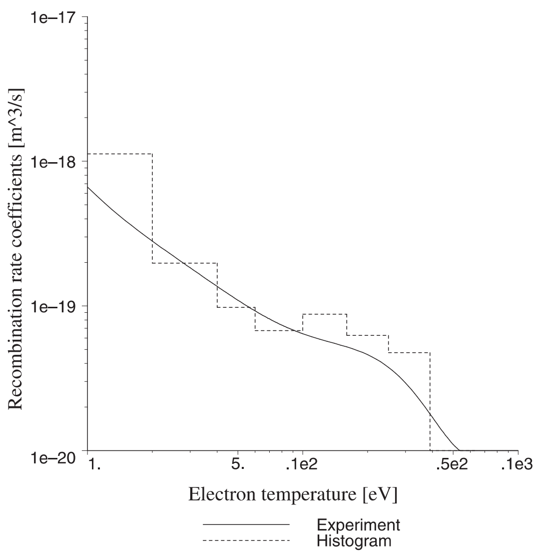


Figure 3. Comparison of the histogram of simulated recombination processes with the experimental data from the input file (see Figure 1).

the crossing point of the separatix with a constant intensity $4 \times 10^{25}$ part./m$^3$/s. The thermal energy of plasma particles in the source is $113$ eV for both components assuming dynamic equilibrium in the pedestal region during ELMs. A constant density profile of deuterium atoms is assumed with sharp peaks in the divertor region (see Figure 2).

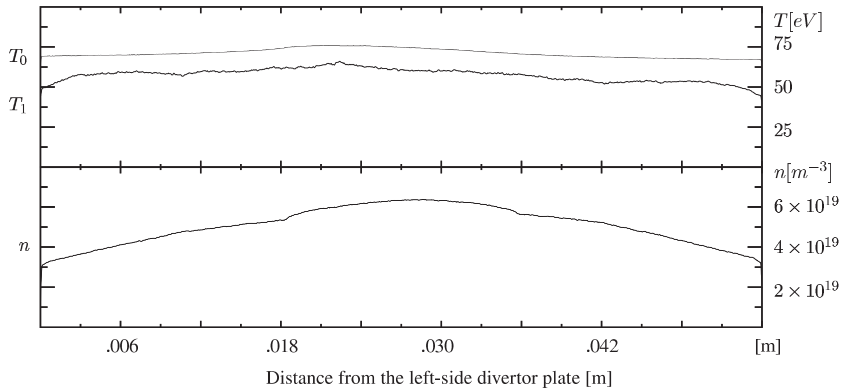


Figure 4. Temperature profiles for electrons – $T_0$ and ions – $T_1$ (upper plot), and profile of plasma density – $n$ (lower plot) without recombination of charged particles.

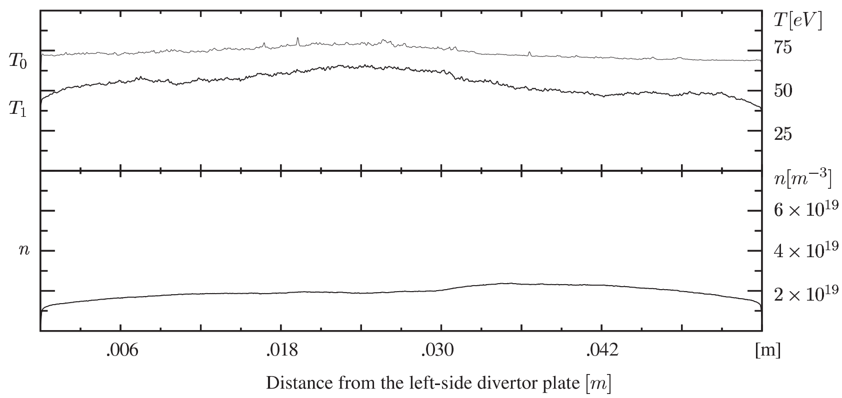


Figure 5. Temperature profiles for electrons – $T_0$ and ions – $T_1$ (upper plot), and profile of plasma density – $n$ (lower plot) with recombination of charged particles.

We compare the temperature and the density profiles from the simulation of SOL plasma without external magnetic field: without and with procedures for recombination processes (Figure 4 and Figure 5 respectively). The former vary with the time, *e.g.* plasma density is rising, the later are obtained for a steady state plasma. The simulation results show decreasing frequency of recombination near the plates of the divertor where the ionization is dominating due to the big concentration of deuterium atoms. More essential effect of the recombination is seen deep in the SOL region where the neutral component is vanishing. The effect of the recombination on plasma temperature is considerably less. In the assumed conditions of constant neutral gas plasma ions are in equilibrium with the atoms via charge exchange. Only small drop of ion temperature is obtained due to decreased concentration of electrons having higher temperature and heating ions via Coulomb collisions. Electron temperature remains almost the same, only radiation recombination is simulated and the released 'ionization' energy is taken by the radiation licking from the thin plasma in the SOL. Considerable cooling is expected with puffing of a cold gas.

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