EFFECT OF RECOMBINATION PROCESSES ON PLASMA PROPERTIES IN THE SCRAPE OFF LAYER OF TOKAMAK DEVICES

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EFFECT OF RECOMBINATION IN THE SCRAPE OFF LAYER OF TOKAMAK PLASMA

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Abstract:

The effect of particle recombination in the scrape-off-layer is investigated performing particle in cell (PIC) simulation of tokamak plasma. For this purpose special routines for Monte Carlo simulation of radiative and collisional recombination are developed using theoretical predictions for the rate coefficients validated up to $100eV$. Simulations with plausible assumptions for the density profile of neutral particles provides to some ambiguity. It can be avoided performing self-consistent simulation of all particles in which neutral content is determined by the rivaling recombination and ionization processes. It has practical implications in the search of conditions to prolong plasma confinement with acceptable divertor loads.

1 Introduction

In many simulations of plasma discharges in tokamak experiments particle recombination in the scrape-off-layer is often neglected due to the small rate coefficients in hot plasma. Calculations are performed neglecting any changes in temperature and density profiles of neutral particles in the simulated volume. Such approach can be unreliable in particular for simulations of phase transitions with drastic change of plasma and neutral gas characteristics (as plasma detachment from the divertor plates [1]). Local treatment of such events is facilitated by making allowing recombination onset with a drop of temperature. For a better understanding of such phenomena it is reasonable to consider the role of charged particle recombination in the whole SOL during plasma discharges.

Here we show results for plasma gross features from simulations with arbitrary assumptions for the density distribution of neutral particles in SOL. Keeping time invariant distribution of neutral particles we find strong dependence of plasma characteristics on the initial assumptions for the neutral component. Such ambiguity hampers the search of conditions with gas or pellet injection to prolong the confinement time of tokamak plasma with acceptable loads on divertor target. This ambiguity could be avoided providing self-consistent simulations of neutral particles.

We have developed a special code version with self-consistent simulation of neutral particles in the SOL and inserted appropriate tools for simulation of recombination processes. They are verified performing appropriate computer experiments. Simulated processes are presented in section 2, description of the routines for three -body and two-body (radiative) recombination is in section 3, results from statistical test of recombination procedures and global verification of the simulations are presented in section 4. In the last section there are compared simulation results obtained with two different assumptions for the neutral particle distributions and the corresponding results obtained with self-consistent simulation of the neutral component.

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).

Present calculations are performed with a new version code (BIT1-S) based on an appropriate method for Monte Carlo simulation of particle collisions. 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 we use the coefficients calculated within the general theory [2] and verifying them with the compilation of recent data. [3] In the BIT1-S there are implemented also the procedure for effective ionization developed in an earlier paper [6] and new procedures for recombination processes presented in another paper. [7]

3 Procedures and method for Monte Carlo simulation

The procedures for charged particle recombination are developed in a similar way to that for effective ionization. [6] In analogy in the present work we have used the rate coefficients calculated by Bates et al. [2] for the recombination processes and approximated them by a polynomial function on electron temperature for fixed plasma densities ($< \sigma_r v > (T, n_e)$, see Fig.1). Using these approximation functions a set of discrete values of $< \sigma_r v >$ with small step on T (0.1 eV for $T_e < 10$ eV and 1 eV for the interval from 10 to 100 eV) and n_e in the interval from 10^{18} to $10^{23}\, m^{-3}$ is prepared in an input file to be used in the simulation of SOL plasma. A special procedure is developed for linear (Lagrange) interpolation calculating the recombination rate for any arbitrary plasma density n_e in the limits 10^{18} and $10^{23} m^{-3}$ and temperature from $0.1\, eV$ till $100\, eV$. By means of this procedure the rate coefficients for recombination are calculated during the code run for the current electron temperature and density in particular grid cell.

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 ($< \sigma_r v >^{rad} = 0$) three-body recombination subroutine is called. In the present calculations the released energy for ionization ($13.6 eV$) 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 ($< \sigma_r v >^{col} = 0$ 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. If the temperature is between the two thresholds, T_c and T_r, the type of collision is chosen with Monte Carlo procedure over the linear approximations of the rate distributions of the both reactions. Approximation parameters are defined from the rates for the boundary temperature values in correspondence with the local plasma density.

Particle-In-Cell (PIC) method for plasma simulation is used in which particles of a given spice are incorporated in clusters and considered as computer particles. The simulation volume is presented as 1D grid with a constant step. Diffusion equations of plasma particles and their collisions are performed in time intervals with constant step adopted to the initial conditions.

An appropriate method for fast Monte Carlo simulations of computer particle collisions was implied in our code version BIT1-S accounting for the wide variations of the rate coefficients of the main processes [8].

A special variant of the original XPDP1 code was developed for self-consistent simulation of plasma and neutral particles in each grid cell. This version is adopted to account for the local dynamics in the SOL during plasma discharge. We estimate the number of collisions in particular grid cells using the local values of plasma characteristics (electron temperature, plasma and neutral gas densities) while in the original XPDP1 scheme the total probability for electron, also ion collisions is calculated for the whole volume:

$$P_{tot.,e} = 1 - exp\{-[\bar{n}_0 < \sigma v >_e^* + \bar{n}_i < \sigma_r v >]\Delta t\} \quad (10)$$

and for ion collisions

$$P_{tot,e} = 1 - exp\{-[\bar{n}_0 < \sigma v >_i]\Delta t\} \quad (11)$$

where

$$< \sigma v >_e^* = (\sigma^e_{el.coll.} + \sigma_{excit.} + \sigma_{ioniz.})\bar{v} \quad (12)$$

and for the ion collisions

and

$$< \sigma v >_i^* = (sigma_{elas} + \sigma_{ch.ex.})\bar{v} \quad (13)$$

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

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

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

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

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

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

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.

4 Verification of simulation results

The rate of plasma decay due to the recombination processes was checked analytically using a method described in 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 method for simulation of particle collisions.

In order to perform strict statistical test of recombination procedures we run BIT1-S code in conditions of hot plasma allowing construction of histograms in the wide range of temperature variations. We have assumed a constant temperature and density profiles of neutral particles computed with Monte Carlo Codes (Nimbus, Eirene) [9] (Fig.2a presents this density profile). The dimensions of the simulated volume were scaled for the SOL in TCV, [10] with a length of the simulated volume $0.264\,m$ (about 10 times reduction). An outward flow from the crossing point of the separatix (placed in the middle of the volume) is assumed with a constant intensity $7.3\,10^{24}\,part./m^3/s$. The thermal energy of plasma in the source is $42\,eV$ for the both components assuming dynamic equilibrium in the pedestal region (magnetic field intensity is 0). In this condition 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. Electron density is about $n_e = 6\,10^{17}m^{-3}$ almost in the entire SOL. It is below the lower limit of plasma density in the input data (see Sec. 3). Bellow this limit effective ionization processes are entirely excluded. In this way we have gathered enough statistics from the calls of recombination processes during $2\mu\,s$ of plasma with constant density and temperature profiles. The constructed histogram is shown on Fig.3. It is in satisfactory agreement with the distribution of the recombination rates inserted in the input data file for plasma density $10^{18}\,m^{-3}$.

A method for global verification of the simulated results has been used [8] in the analysis of the simulation results shown on Fig.4a. They were obtained assuming the neutral density distribution in Fig 2a. Our test is made within one time step $\Delta\,t = 7\,10^{-13}\,s$. Due to the strong variation of the neutral density profile we estimate the contribution from particular collisions splitting the whole volume in three parts: 'source volume' ($V_{source} = 1.7\,10^{-6} m^3$), 'divertor volume' ($V_{DIV} = 10^{-7}\, m^3$) and the biggest remainder part we name 'SOL volume' ($V_{SOL} = 3.7\,10^{-6}\, m^3$). The total number of electron-ion pairs in the whole volume is about 10^{14} taking for the average density $2\,10^{19}/m^3$.

Following the scheme in the original code the total probability $P_{tot} = 4\,10^{-6}$ for all electron collisions was calculated in the beginning of the code run. Thus, the total number of colliding pairs is respectively $1.2\,10^8$ in the 'source', $2.7\,10^8$ in 'SOL volume' and in 'divertor volume' it is about 10^7.

Making calculations for the balance between different types of collisions we share collision number between recombination, effective ionization, excitation (with de-exitation) and elastic scattering (the last three processes have similar frequency). Due to the shape of the neutral density profile recombination process dominates in the 'source volume', become less frequent than the effective ionization in the biggest part of SOL and negligibly small in 'divertor volume'.

During the code run plasma flux with intensity $4\,10^{25} pairs/m^3 s$ is 'injected' in the 'source volume'. Respectively, for time Δt are added $4.8\,10^7$ electron-ion pairs.

The ratio between recombination and ionization processes in the 'source' is about 3.6. This ratio is calculated assuming rate coefficients $3\,10^{-20} m^3/s$ and $3\,10^{-14} m^3/s$, respectively for recombination and effective ionization. For the neutral density we take $5.5\,10^{12} m^{-3}$ (see Fig.2a). Thus, about $6.5\,10^7$ pairs recombine and $1.8\,10^7$ are created in the 'source volume'. Since the number of injected pairs is $4.8\,10^7$ about 10^6 pairs pass in the 'SOL region'.

In the 'SOL volume' we use the same rate coefficients. Due to the strong variations of the neutral density (n_0) we split the SOL volume to 8 parts and take for each of them the average value of n_0. Thus, for the whole volume $\sum n_{0,i}\,\Delta\, V_i = 1.4\,10^9$. The ratio between ionization and recombination processes is about 19. Accounting that the total number of colliding particles is $2.7\,10^8$ we obtain about $4.7\,10^6$ recombined pairs and $8.9\,10^7$ electron-ion pairs. Thus, about $8.4\,10^7$ pairs could 'appear' not changing neutral particle density according to the original XPDP1 scheme.

In the divertor region the neutral particle density is about $10^{19} m^{-3}$ and plasma density tends to $1.7\,10^{19}$. The ratio between recombination and ionization collisions is $1.7\,10^6$ and the total number of colliding pair is 10^7. Thus only 6 pairs recombine and $3.3\,10^6$ pairs are created without changing the number of neutral atoms in the original scheme.

Making balance between created and recombined pairs in 'SOL'and 'divertor' regions and taking into account that 10^6 from injected pairs are also propagating from the 'source' to the divertor plates we obtain that $9.6\,10^7$ particles escape from the volume during $\Delta\, t$. Thus, we estimate approximately that $4.8\,10^7$ pairs are absorbed in the divertor plates. It is in good agreement with the simulation results: the outward electron flux from divertor target is registered during the run (it is about $6.5\,10^{23}\, part/m^2\, s$). Having in mind that the cross section of the flux is $10^{-4}\, m^2$ and the time of flight is $\Delta\, t = 7.10^{-13}$ we obtain $4.6\,10^7$ electron-ion pairs are crossing divertor target. This is a global confirmation of the simulation results. Local violation of particle number conservation is allowed by the original XPDP1 scheme in the frame of which the neutral density distribution remains time invariant. It has been avoided in self-consistent simulations of neutral particles.

5 Results and discussion on the effect of recombination

For the results in Fig.4a we have used the first version of BIT1-S assuming neutral density distribution presented in Fig.2a and the scheme for time invariant neutral component from the original code XPDP1. According to this scheme neutral density distribution is not changed during simulated collisions. A similar run but without recombination leads to unstable plasma with increasing density [7]. Progressive violation of particle conservation is seen due to the original scheme for time invariant neutral density distribution. This effect diminishes assuming neutral particle profile with higher densities (shown with the tick line on Fig.2b). As a result we obtain stable plasma with the same density profiles in the both cases, with and without recombination (see Fig. 4b). One could conclude that the effect of recombination processes is negligibly small at high density of the neutral component. Both distributions on Fig.4a and Fig.4b are obtained at the same moment ($14\,mks$). They differ apparently. In order to avoid this ambiguity we developed a code version with self-consistent simulation of neutral particles. In Fig. 5a,b is shown the time variation of the total number of charged and neutral computer particles obtained in a run with the same initial conditions as in Fig. 4a: the run is started assuming neutral density profile shown on Fig.2b. As one can see on Fig. 6a during the time of code run the density profile of neutral component becomes essentially changed.

The large scale in Fig.5a illustrates clearly the regulation role of recombination to reach appropriate ratio between neutral and plasma density in a stable state. When the channel for recombination is switched off neutral particle density vanishes to 0.

In Fig.6 we present the density (a) and temperature (b) profiles of electrons(e), ions (i) and neutral particles (0) obtained at the $18\,mks$ of the same run presented on Fig5. One can see rather smooth density profile, quit different from the initial one in Fif2a. The smooth spatial distribution of neutral density is reached in stable state as a result of the rivaling processes of charged particle recombination and atom ionisation.

Despite that in non-consistent simulations are in general uncertain it is possible to find appropriate initial conditions to reconcile the computational results with some data for during a period of stationary state of tokamak plasma [7]. In all cases there are needed however self-consistent simulations to validate the model. It could help plasma control and searches for operation with acceptable loads on divertor plates.

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Figure captions

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

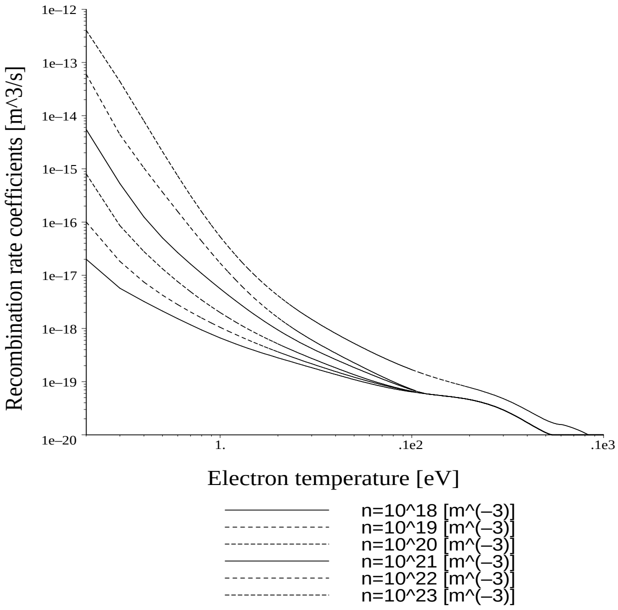
Fig.2: Neutral particle profile: (a) according [9], (b) private information.

Fig.3: Comparison of simulation rates for recombination with the experimental data from Fig.1.

Fig.4: Plasma density profiles obtained with BIT1-S code at $14\,mks$: (a) assuming neutral profile in Fig.2 a ; (b) assuming neutral density profile in Fig.2 b .

Fig.5: Time variation of charged (e) and neutral (0) computer particles in self-consistent simulation: (a) in a large time scale;(b) in a smaller time scale.

Fig.6: Density (a) and temperature (b) profiles of charged (e) and neutral (O) particles in steady state plasma obtained at ($18\,mks$) from the same run as in Fig. 5.



1e–12
1e–13
1e–14
1e–15
1e–16
1e–17
1e–18
1e–19
1e–20
Recombination rate coefficients [m^3/s]
1.
.1e2
.1e3
Electron temperature [eV]
n=10^18 [m^(–3)]
n=10^19 [m^(–3)]
n=10^20 [m^(–3)]
n=10^21 [m^(–3)]
n=10^22 [m^(–3)]
n=10^23 [m^(–3)]

Fig.1

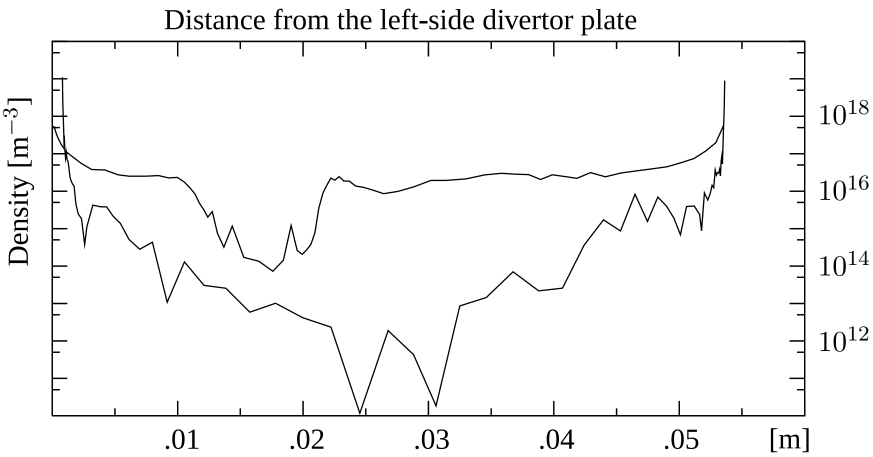
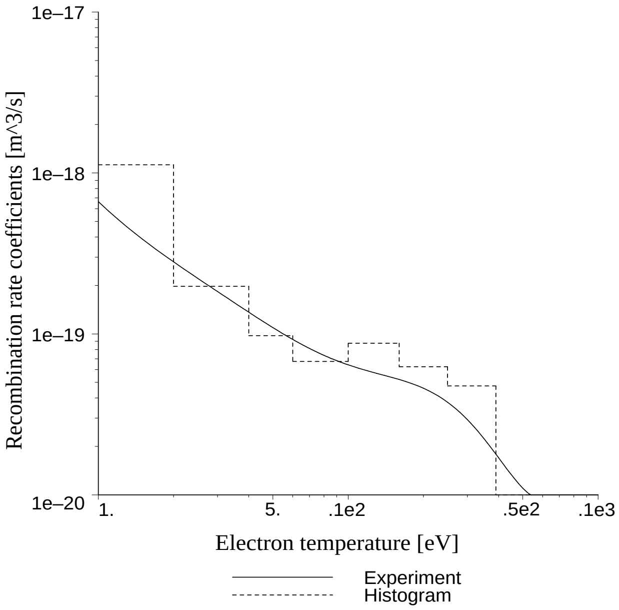

Distance from the left-side divertor plate
Density [m^{-3}]
10^{18}
10^{16}
10^{14}
10^{12}
.01
.02
.03
.04
.05
[m]
Fig. 1.

Fig.2



1e–17
1e–18
1e–19
1e–20
Recombination rate coefficients [m^3/s]
1.
5.
.1e2
.5e2
.1e3
Electron temperature [eV]
Experiment
Histogram

Fig.3

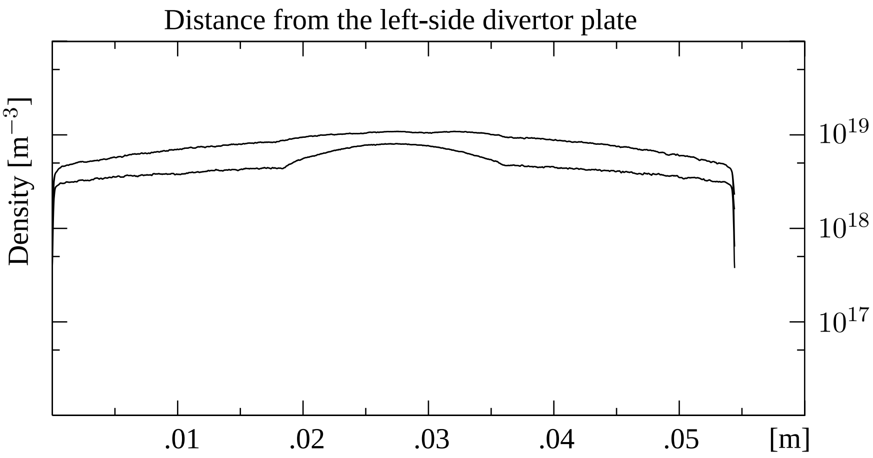
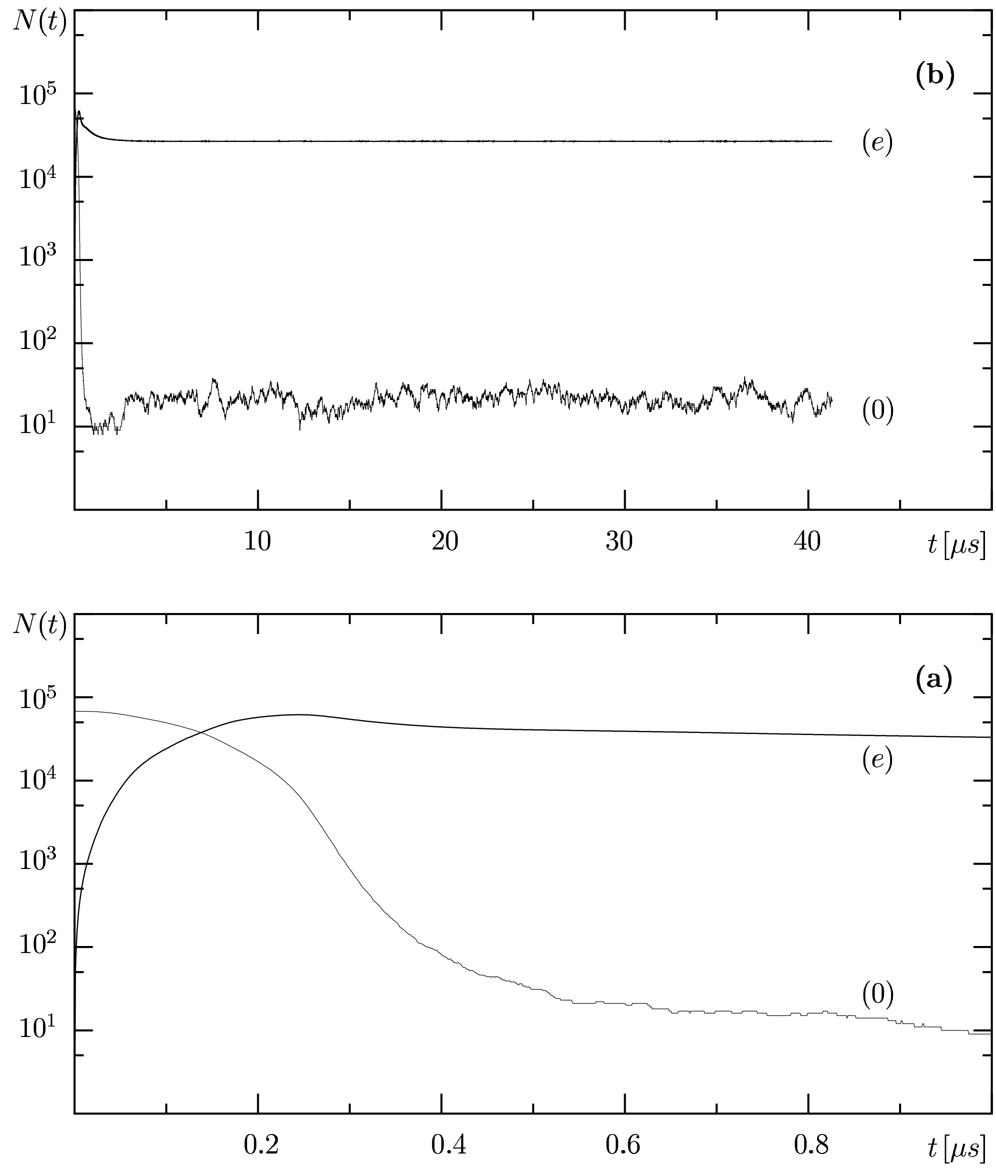

Distance from the left-side divertor plate
Density [m^{-3}]
10^{19}
10^{18}
10^{17}
.01
.02
.03
.04
.05
[m]

Fig. 2.

Fig.4



N(t)
(b)
10^5
10^4
10^3
10^2
10^1
(e)
(0)
10
20
30
40
t [μs]
N(t)
(a)
10^5
10^4
10^3
10^2
10^1
(e)
(0)
0.2
0.4
0.6
0.8
t [μs]

Fig.5

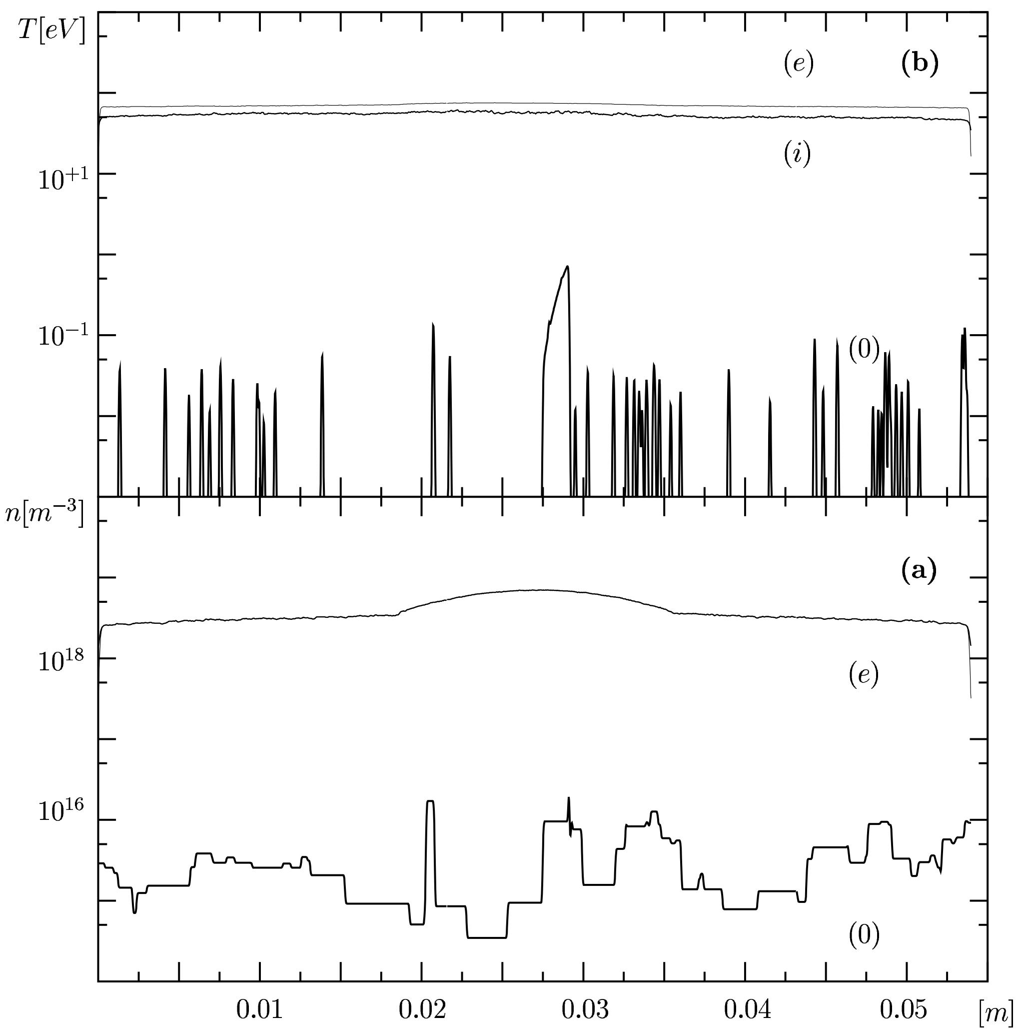


Fig.6