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Validation of a Model for Recombination in Tokamak Scrape-Off-Layer Plasma

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Abstract. A phenomenological model for recombination in the scrape-off-layer of tokamak plasma is proposed. Software tools for examination of the model are tested with 1D Particle-in Cell (PIC) simulation of stable plasma in tokamak. The model is validated using global parameters for a 2MW L mode density shot performing 2D calculations of plasma discharge evolution. The role of recombination in different plasma states is discussed

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1 Introduction

The charged particle recombination in the scrape-off-layer (SOL) is often ignored in many computer simulations due to the small rate coefficients in hot plasma. Evidence for the important role of volume recombination is found in detached divertor plasma in conditions causing drastic change of plasma state and disruption [1]. Understanding the contribution of recombination has practical sense in finding favorable conditions to maintain plasma confinement. The lack of direct measurements of the neutral gas in the SOL and data for the cross section of charge particle recombination lead to the necessity to use some model descriptions in the kinetic simulations.

We propose a model based on the rate coefficients of volume recombination in tin plasma predicted theoretically [2] (up to 10 eV) and verified them with the recent compilation of data for the rate coefficients up to 100 eV [3]. Our goal is to check whether these rate coefficients could be used in an appropriate phenomenological model. The coefficients are approximated with parametric functions adjusting them to higher temperatures and various plasma densities. Corresponding procedure functions have been developed and verified in 1D simulations of SOL plasma [4]. It became clear the necessity of self-consistent simulation of neutral particles and improved scheme for particle collisions in grid cells. Different code versions were developed to get consistent results. For validation of the model we have performed 2D calculations of the gross features during plasma discharge.

The model and the calculation tools are described in the next paragraph. An analysis of the simulation results is presented in the third and the forth paragraphs. In the fifth paragraph we present results from 2D calculations validating the model with the global parameters for the 2MW L mode shot 39588 in JET [1].

2 Model Assumptions and Calculation Tools

The model uses data approximations of the effective ionization and recombination rate coefficients (shown in Figures 1 and 2, respectively). They are presented in [4] and [6] as functions of electron temperature at arbitrary plasma densities between 10^{18} and 10^{23} m^{-3}.

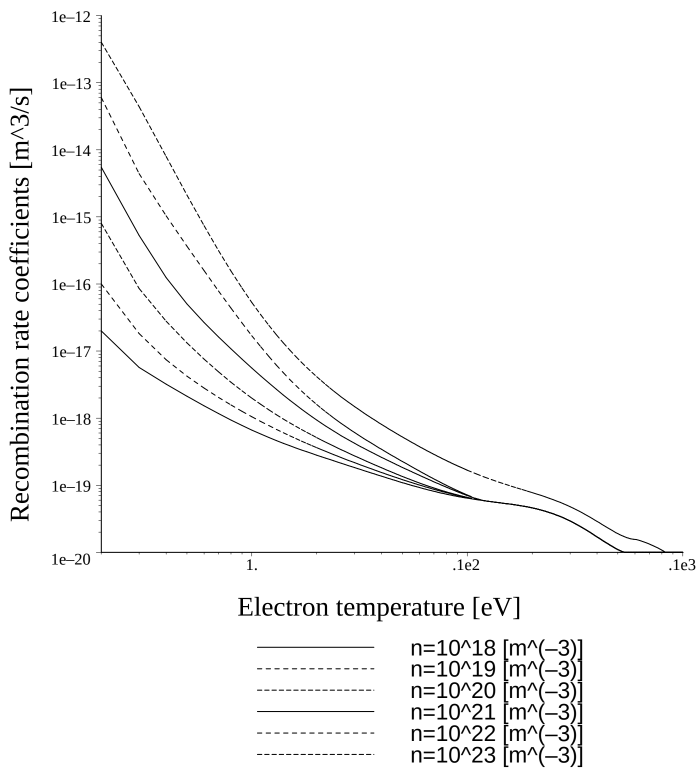

Figure 1. Data approximation of the recombination rate coefficients.

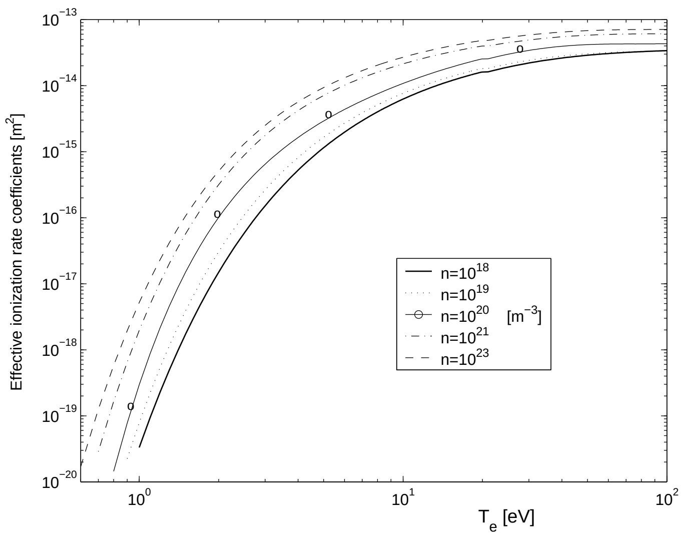

Figure 2. Data approximation of the effective ionization rate coefficients.

In order to examine the model it was developed a special method for Monte Carlo simulations. Procedure functions were developed and implemented in BIT1-S code simulating Deuterium (D) plasma in SOL [4]. It is based on the BIT1 version [5] of the original code XPDP1 [6] (available in internet). All these codes do not provide self-consistent simulation of neutral particles and use assumptions for time invariant neutral density and temperature profiles shown on Figure 3a,b. Neutral density profiles are characterized with sharp peaks near the targets and low density in the 'source'.

In BIT1-S code interacting particles are chosen over entire simulation volume as in the original XPDP1 code. According to that scheme both the density and the temperature profiles of D atoms remain unchanged during the simulation. Such assumption was made expecting the frequency of plasma particle collisions with D atoms to be small enough to affect the characteristics of the neutral gas in SOL. It could also fit conditions maintaining invariant density of neutral particles with special gas puffing.

A new method for Monte Carlo simulations of particle collisions is used in BIT1-S code instead of the 'Null Collision Method' [7] in the original XPDP1 code. Correspondingly, a new module was implemented in BIT1-S code allowing fast simulations in wide range of collision probabilities during plasma discharges in tokamak experiments.

In the BIT1-S code are implemented original procedures for simulation of 2-body (radiative) and three-body (collisional) recombination described in details in [4]. A special procedure combines collisional excitation, effective ionization, de-excitation and spontaneous transition like in [8]. Elastic collisions of electrons and Deuterium ions with D atoms, charge exchange between D ions and atoms are simulated as in the original XPDP1 code. Procedures for Coulomb collisions and electron recycling from the walls are taken from the BIT1 code [5].

The scrape-off-layer is considered as a tube volume spread alongside magnetic field lines 'strengthen' between divertor targets in the middle of which is the "source" of plasma [8]. The connection length and the cross section are 0.054 m and 10^{-4} m^{-2}, correspondingly; the "source" length is 6.7×10^{-3} m. In this simplified linear geometry the "source" corresponds to the separatrix area in which the outward plasma flow escapes from the core and enter in the SOL. The code is simulating 1D poloidal propagation of plasma in the "source" and in the remainder part of the SOL including divertor region at the ends of the tube.

3 Results from Non-Consistent Simulations of Neutral Particles

Here we discuss results obtained with the early version of BIT1-S code with non consistent simulation of neutral particles.

Injected plasma in the "source" has a constant intensity, 4×10^{25} part/m$^3/s$ and thermal energy 113 eV for the both electron and D^+ ions assuming dynamic equilibrium in the pedestal region. Figure 4 shows plasma density profile obtained with neutral density distribution vanishing in the source region [8] (the upper curve in Figure 4) and a lower curve obtained with the flatter neutral density profile in Figure 3. In the both cases the total probability for particle collisions (3×10^{-6}) was determined for the entire simulated volume using maximum densities. In the first case a code run [4] without recombination leads

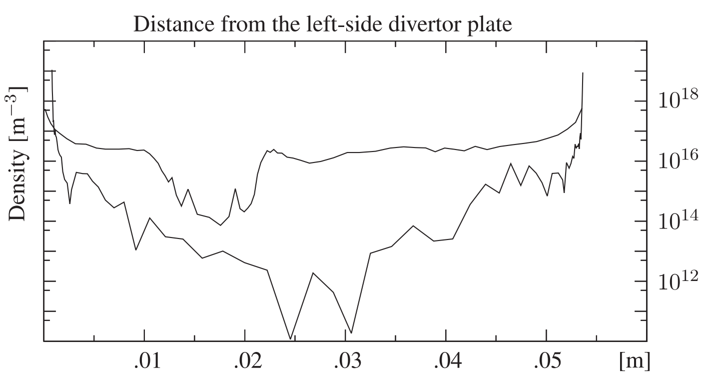

Figure 3. Neutral particle profiles in divertor plasma: **(a)** according to [9]; **(b)** private communication.

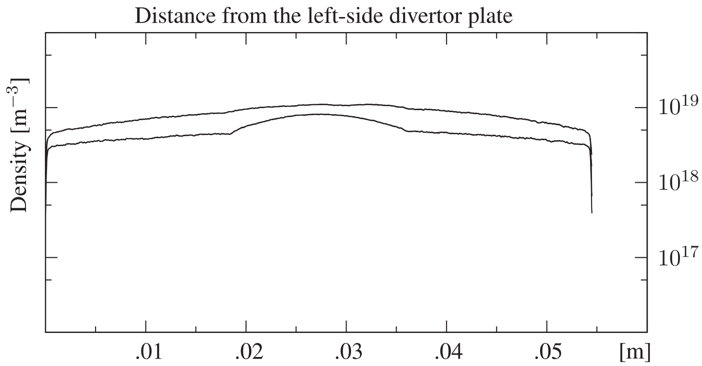

Figure 4. Plasma density profile assuming a neutral density distribution shown in Figure 3a.

to unstable plasma with increasing density. The difference with stable plasma densities increases with time and provides to a wrong conclusion that the effect of recombination is overestimated (in the case of higher neutral gas density the effect from recombination is negligible). To avoid some misunderstandings we perform global verification of the results shown with the upper curve in Figure 4, within one time step $\Delta t = 7 \times 10^{-13}$ s, splitting the simulated volume to 'source', 'main SOL' and 'divertor region'. In Table 1 are shown: the calculated number of recombined pairs (R Number), that of ionized atoms (I Number), the average density of atoms and electron-ion pairs. The average plasma density is 8×10^{18} m^{-3}.

Table 1. Global verification of simulated results in Figure 4.

region	V, m^3	$\langle n_0 \rangle$, m^{-3}	$e - i$ pairs	R Number	I Number
source	1.7×10^{-6}	2.2×10^{12}	1.4×10^{13}	4.15×10^{7}	1.15×10^{7}
SOL	3.7×10^{-6}	3.8×10^{14}	3.0×10^{13}	2.0×10^{6}	3.8×10^{7}
divertor	10^{-7}	1.0×10^{19}	5.0×10^{11}	6.0×10^{0}	1.0×10^{6}

Following the scheme in the original code the total probability for all types of electron (also ion) collisions was calculated to define the number of colliding particles. Simple calculations for the main electron collisions (recombination, effective ionization, excitation with de-excitation and elastic scattering) show that in the conditions leading to the results in Figure 4 the recombination processes dominate in the 'source volume', becomes less frequent than the effective ionization in the 'main SOL' and negligibly small in 'divertor region'. The ratio between the number of ionization and recombination processes in the 'source' is about 0.3, in the 'main SOL' is about 19 and 1.7×10^{6} in 'divertor region'. About 3.8×10^{7} ('extra') ions appear in the 'main SOL' and 10^{6} in 'divertor region' not changing neutral particle density. It is possible in the original code scheme allowing time invariance of the neutral particle number. Making balance between created and recombined pairs in the 'main SOL' and 'divertor region', and taking into account that 10^6 from the injected pairs pass in the 'source' and propagate to the divertor plates, we obtain that 8.6×10^7 particles escape from the volume during Δt. Thus, 4.3×10^7 pairs are absorbed in each divertor plate in good agreement with the simulation results: the outward electron flux from divertor target is registered during the run (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 $\Delta t = 7 \times 10^{-13}$ we obtain 4.6×10^7 electron-ion pairs are crossing divertor targets.

The analytical calculations confirm the simulation results and verify the software tools. However the simulation results were obtained making assumption for the neutral density profile remaining invariant during the code run. Such assumption could be valid only in special cases, not in general, and not in the case presented in Figure 4. A strong signal to not be appropriate is the 'extra' electron-ion pairs created while neutral particle number remains the same.

Computer experiments performed assuming neutral particle profile with higher densities (in Figure 3) lead to stable plasma in the both cases: with and without recombination [10]. In the both cases there are obtained identical temperature and density profiles. Obviously, in the case of higher densities of neutral particles the effect of recombination processes is negligibly small in the entire SOL volume.

These computer experiments were performed with the same initial conditions, only the assumptions for the neutral density distributions are different. They provide to completely different conclusions: the first one for essential role and the second one for negligible contribution of recombination. There is no direct data for the neutral particle density to decide which one is more realistic. Apparently, not consistent simulations give a room for controversial conclusions concerning the role of recombination. One must aware that in such simulations the effect of recombination is related with the choice of the density distribution of the neutral gas, consequently the simulation results could be uncertain.

Nevertheless it is possible performing not consistent simulations to adjust the initial assumptions and to reconcile the computational results with some well known plasma characteristics in steady or turbulent plasma in stationary edge localized modes[11]. Agreement can be achieved however with some uncertainty concerning the arbitrary choice of the lateral distribution of the neutral component.

It is clear that the scheme of the original XPDP1 code keeping neutral particle distributions not affected during interactions is completely not appropriate for unstable plasma. Such simulations are not adequate to study phase transitions as those observed in [1]. For this reason the BIT1-S code was improved involving in it procedures for self-consistent simulation of the neutral component [12] and more precise grid simulations [10].

4 Results from Self-Consistent Simulation of Neutral Particles

There were performed several computer experiments with self-consistent simulations of the neutral component. The first runs [12] with the BIT1-SC code version were performed without external magnetic field: $B = 0$ and with intensity of the magnetic field $B = 1.4$ T. The rest of the initial conditions are similar to those in the experiments presented with Figure 4 but D gas was injected instantly with low temperature (0.1 eV). The cold gas injection was made in the beginning of the run with the same intensity as that of the injection of D plasma in the 'source'. During the code run the neutral gas injection is switched off while that of plasma remained constant (4×10^{25} part/m^3/s, as that in the runs for not consistent simulations described in the previous paragraph). A little lower temperature of the 'source' plasma is assumed (80 eV).

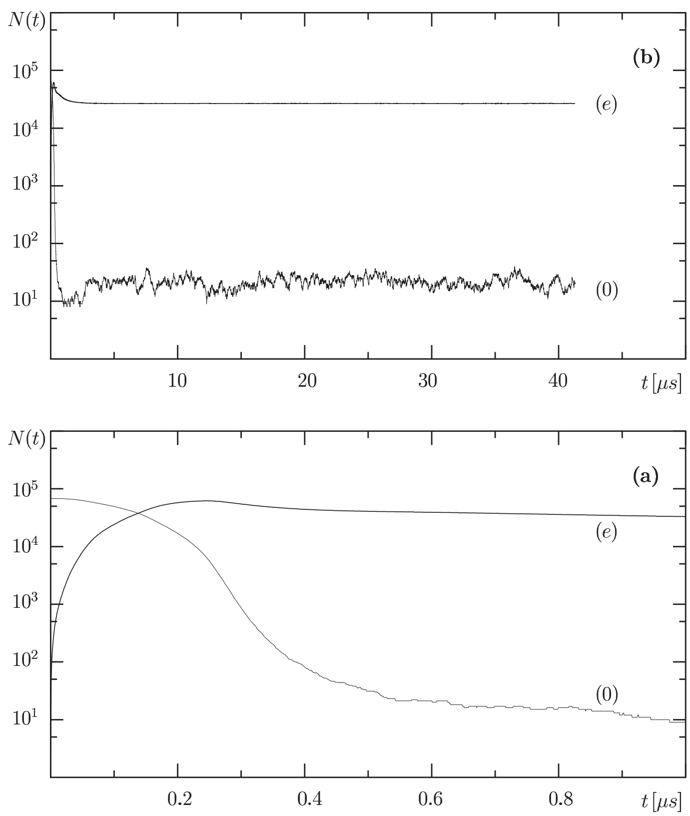

Figure 5. Time variation of charged (*e*) and neutral (*0*) computer particles in **(a)** an early period; **(b)** a steady state plasma. The simulation is performed with the BIT1-SC code version, $\Delta t = 3.5 \times 10^{-12}$ s, and $B = 0$ T.

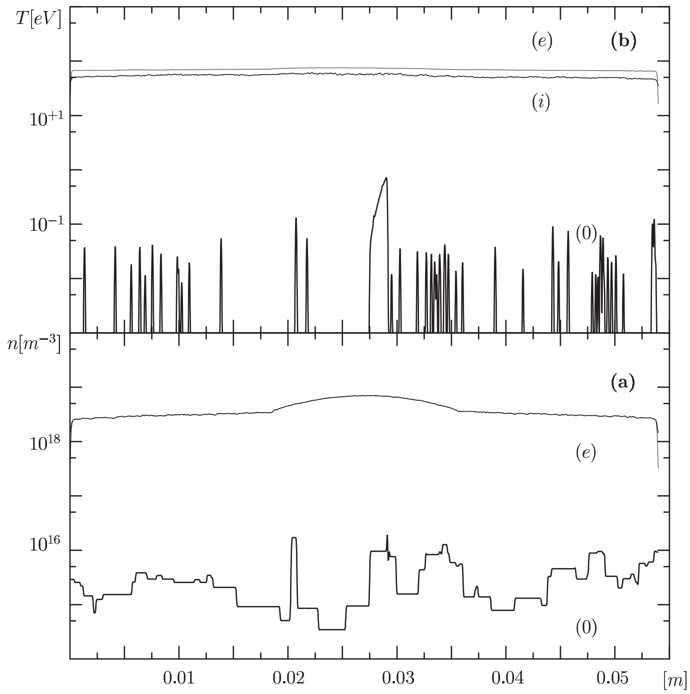

Figure 6. Density **(a)** and temperature **(b)** of charged (*e*) and neutral (*0*) particles in steady state plasma. The simulation is performed with the BIT1-SC code version, $\Delta t = 3.5 \times 10^{-12}$ s, and $B = 0$ T.

Results without magnetic field are shown in Figure 5a,b and Figure 6a,b. The former represents the rise of charged particle number and decrease of atom number in two time scales, the latter represents density and temperature profiles of the both components at a stable stage. It is clearly seen on Figure 5a,b that the total number of neutral particles is changing in self-consistent simulation. Without recombination it is vanishing to 0. With recombination the lowest value is much above 0 due to the established equilibrium. A constant ratio between neutral and charged particle contents is achieved in few mks. It is determined by the ratio between ionization and recombination rates and the speed of plasma propagation in the SOL. The lateral density distribution of neutral particles in the stable state is also automatically established as a result from the rivaling processes of ionization and recombination. It is quite different from the assumed distributions in Figure 3: rather smooth, no peaks are created near the targets in the conditions of plasma injection and equilibrium between the key processes.

In Figure 7 and Figure 8 we show results from BIT1-SC run with external magnetic field ($B = 1.4$ T). One can see that the ratio between plasma and neutral gas contents (about 10^5) is about an order of magnitude bigger than in Figure 6

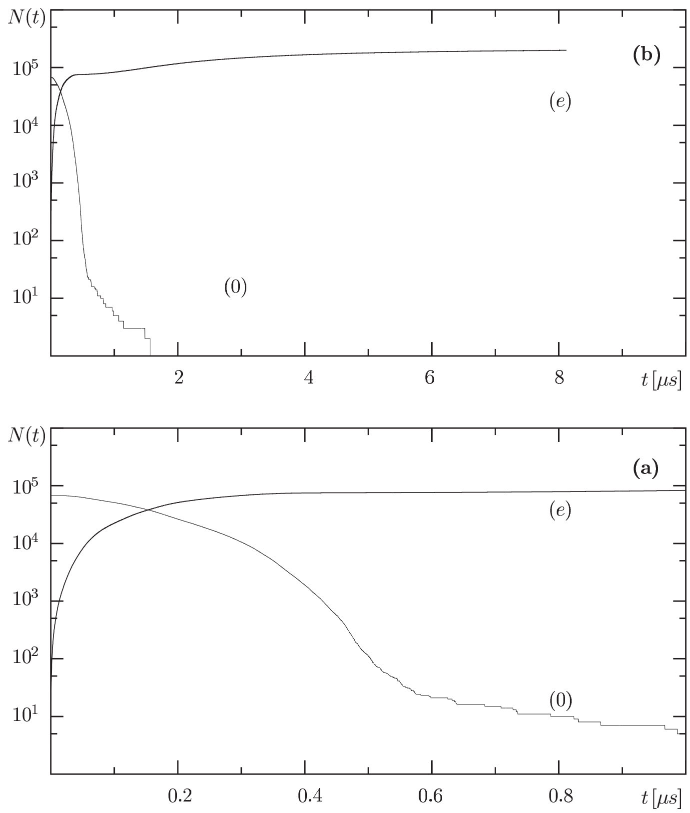

Figure 7. Time variation of charged (*e*) and neutral (*0*) computer particles in **(a)** an early period; **(b)** a steady state plasma. The simulation is performed with the BIT1-SC code version, $\Delta t = 2.8 \times 10^{-12}$ s, and $B = 1.4$ T.

due to the hampering effect of magnetic field on plasma propagation. However it is still less than the expected one within the model and defined by the rates of the key processes and the number density of D atoms in ground level in Saha equilibrium. One could conclude that either the model based on the rates for confined plasma in equilibrium is not completely appropriate for propagating plasma in SOL or there is an effect of the simulated scheme.

To check the above alternative self-consistent simulations in the grid cells were performed with the recent version of the BIT1-SCG code [10]. The expected ratio is achieved.

So one can conclude that the model is appropriate for description of recombination in propagating plasma in tokamak SOL. The new code version could be adapted for simulation of plasma discharge evolution accounting for drastic local changes of plasma characteristics. It is needed however first of all to validate the model with experimental data.

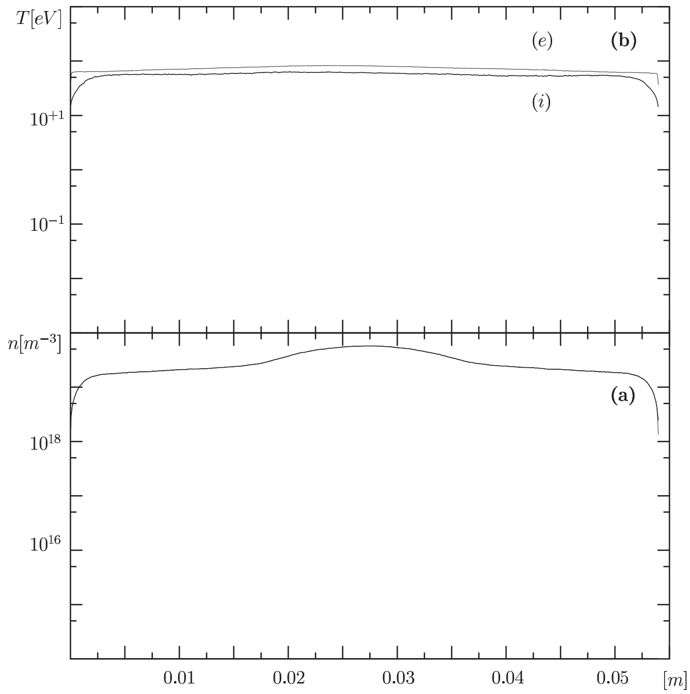

Figure 8. Density **(a)** and temperature **(b)** of charged (*e*) and ions (*i*) particles in steady state plasma. The simulation is performed with the BIT1-SC code version, $\Delta t = 2.8 \times 10^{-12}$ s, and $B = 1.4$ T.

5 Validation of the Recombination Model with Global Plasma Parameters of a JET Shot

We use the global parameters for the 2MW L mode density limit shot 39588 [1] in JET and perform corresponding 2D calculations for the time interval of the shot $17 - 24.3$ s. For these calculations we split the SOL volume to inner and outer parts (above the inner target and above the outer target, respectively) and consider separately divertor volume close to the outer target. The whole SOL volume during this time interval is about 6 m^3 (with effective length 120 m and cross section 0.05 m^2 according a private communication).

Since the ratio between $D\alpha$ and $D\gamma$ radiation manifests detachment of plasma from the inner target at about 17.3 s we assume for initial conditions at 17 s that the temperature of the inner plasma is about 4 eV and that of the outer and divertor plasma $T = 12$ eV; the inner density is about 2.5 times bigger than the density in the outer divertor region, $n_e^{in} = 1.6 \times 10^{19}$ m^{-3}.

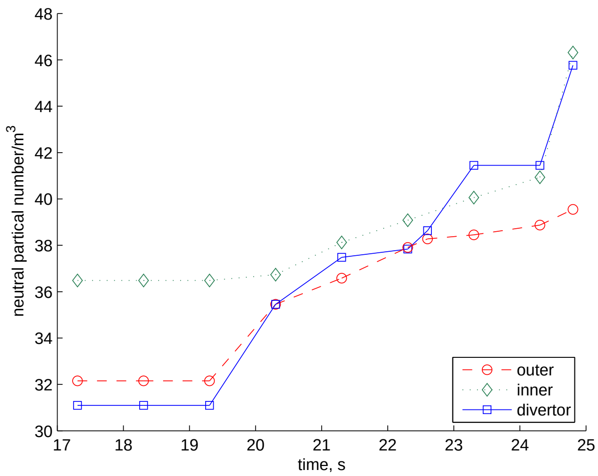

Figure 9. Estimates of the time variation of the neutral particle density.

Assumptions are made also for:

(*) increasing outward flows propagating in the inner and in the outer SOL volumes adjusting them to the variation of the averaged core ($\langle n_e \rangle$) and divertor ($n_{\rm div}$) plasma densities;

(**) different temperatures of the inner, outer and divertor plasma varying them with the time of plasma discharge in accordance to D_{alpha} and D_{gamma} radiation measured above the inner and outer targets.

(***) obeying the conservation laws and adjusting the data for the ion flux in the inner (J_i) and outer (J_o) targets transport of plasma from the inner to the outer target volume is resulting and expansion of divertor plasma preceding disruption. In that way we obtain consistent results for the entire evolution of plasma discharge.

The compiled data are presented in Table 2. They are used for estimation of plasma and neutral particle characteristics in all parts of the SOL volume. The contributions of the key processes, ionization of Deuterium atoms and recombination of charged particles are calculated using the rate coefficients (shown on Figure 1 and Figure 2) in correspondence to the estimated temperature and plasma densities.

In Figure 9 we present our calculated results for the time variation of neutral gas density in the inner SOL volume ($n^{\rm in}$), in the outer SOL volume ($n^{\rm out}$) and in the outer divertor volume ($n^{\rm div}$). The ratio between charged and neutral particle

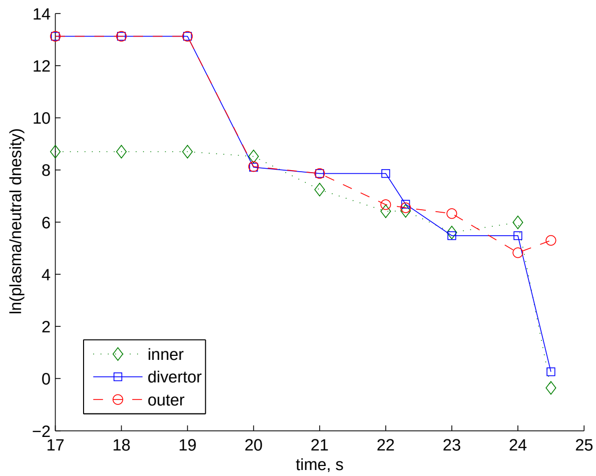

Figure 10. Estimates of the time variation of the ratio: plasma to neutral density.

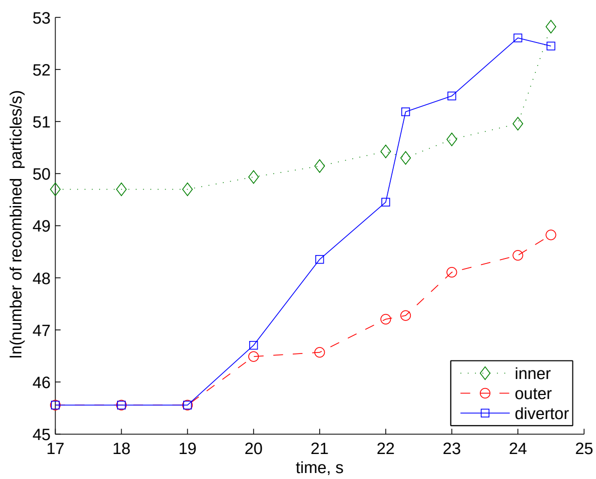

Figure 11. Estimates of the time variation of the number of recombined particles.

densities is presented on Figure 10. The time variation of the average number of recombined pairs per one second (R/sec) in the particular volumes are presented in Figure 11 and the variation of the ratio between ionized atoms and recombined pelectron-ion pairs in Figure 12.

The results presented in Figures 9–12 correspond to the assumptions we have

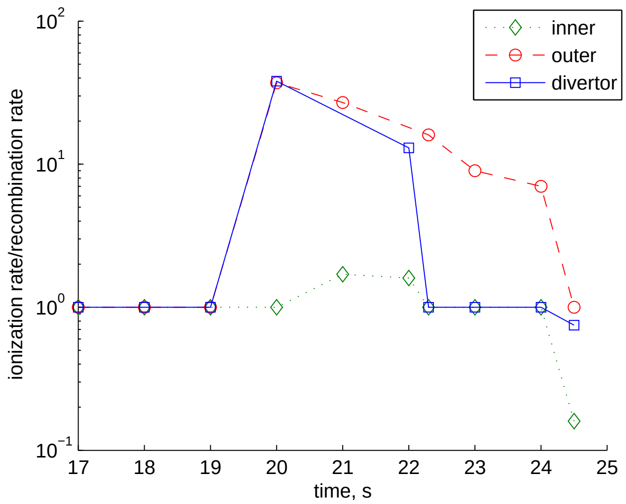

Figure 12. Estimates of the time variation of the ratio: ionized to recombined particles.

Table 2. Compilation of the global parameters for the 2 MW L mode density limit shot 39588[1]

time[s]	17-19	19-20	20-21	21-22	22-22.3	22.3-23.3	23.3-24.3	24.3-24.5
$\langle n_e \rangle$ $[10^{19}\mathrm{m}^{-3}]$	1.6	1.8	2.0	2.3	2.6	2.8	3.0	3.7
n_{div} $[10^{19}\mathrm{m}^{-3}]$	1.6	2.0	5.0	7.0	24.0	24.0	24.0	1.0
$D_{\gamma_i}/D_{\alpha_i}$	0.040	0.040	0.035	0.030	0.035	0.035	0.045	0.020
$D_{\gamma_o}/D_{\alpha_0}$	0.025	0.020	0.018	0.017	0.017	0.035	0.045	0.020
J_i $[10^{22}\mathrm{s}^{-1}]$	1.0	1.0	1.3	1.2	1.2	1.5	1.2	0.7
J_o $[10^{22}\mathrm{s}^{-1}]$	1.0	2.0	3.0	4.0	5.0	3.0	2.8	1.0

presented here concerning the initial conditions. The ambiguity of these assumptions affects on the values of the calculated variables but not the general consistency of model predictions with the compiled data.

6 Conclusions for Validity of the Recombination Model

I. For stable plasma.

We use as a criterion for validity of the assumed model for recombination the ratio between plasma and neutral gas densities. According to this model for confined plasma in equilibrium this ratio is reciprocal to the ratio between the recombination and ionization rates. Is it the same for the steady state of plasma propagation in the scrape off layer from the core to the divertor targets in tokamaks? One can not give a definite answer without direct measurements of the neutral gas density but we make conclusion from the simulations with the available codes.

- (*) Results from non-consistent simulations with BIT1-S code do not give a definite answer for the arbitrary choice of neutral density.
- (**) Self-consistent simulations with BIT1-SC code over the entire SOL volume provide to less value of the n_e/n_o ratio than expected.
- (***) Expected ratio is achieved with BIT1-SCG self-consistent grid simulations making appropriate choice of the grid and computer particles cells. Examination for stability of the simulation results in respect to acceptable variations of the grid and computer cell values was running.

II. For unstable plasma during the evolution of plasma discharge.

- (*) The model predictions are consistent with the global characteristics in a JET plasma discharge.
- (**) The general conclusion is that the effect of recombination should be studied in particular stages of different tokamak operations and this model is an useful tool. The software products developed for this purpose could be used for development of a code for realistic 2D simulations of plasma discharges in tokamak experiments.

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