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Modeling of neutral transport for self-consistent transport simulations in tokamaks

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A model of the neutral transport in tokamaks has been developed suitable for a one-dimensional transport code, TASK/TX. The model consists of the one-dimensional diffusion equations for slow, thermal and halo neutrals, which are simultaneously solved together with two-fluid equations and Maxwell's equation. The behavior of the slow neutrals is easily modelled by a one-dimensional diffusion equation owing to short mean free path, while that of the thermal neutrals with long mean free path is not straightforwardly. The development of the way to evaluate an effective mean free path reflecting their two-dimensional motion and velocity realized the reasonable estimation of the thermal neutral diffusivity for a one-dimensional diffusion modeling. The validity of the model has been confirmed by a Monte Carlo code in the cases with various plasma parameters.

Keywords: neutral transport, mean free path, diffusion modeling, transport simulation, tokamak

1. Introduction

A prediction of density profiles in coming burning plasmas is one of the most important issues because the fusion output increases with the peakedness of the density profile. The density profile is determined by the particle transport and the particle source. While the particle transport is usually governed by the turbulence-induced diffusion and inward pinch [1], the source for charged particles in a plasma has strong ties with the behavior of neutral hydrogen atoms and plays an important role especially in the formation of the density profile in the edge region. Since the neutrals cannot be confined by the magnetic field, for a transport modeling they should be treated in a manner different from charged particles. In this paper, we model the behavior of the neutrals as a set of equations suitable for a one-dimensional multi-fluid transport code, TASK/TX [2]. TASK/TX has been used to study the ripple-induced toroidal rotation [3, 4] and to analyze the characteristic of the $\vec{j} \times \vec{B}$ torque induced by charge separation of fast particles generated by a neutral beam (NB) injection [5]. The detail of the code will be described in the next section.

In an actual plasma, there are countless energy groups of neutrals: they gradually penetrate into the core plasma, suffering from multi-step charge exchange. Actually from the aspect of fluid modeling for neutrals, however, only finite energy groups can be handled. In our modeling, we consider three groups of neutrals and a first-step charge exchange. We need to confirm the validity of the assumptions made in our modeling by using a Monte Carlo calculation.

Several kinds of atomic processes and molecular dynamics occur near the wall, as a surface-plasma interaction. For instance, the dissociation process of hydrocarbons has been included in detail in a more sophisticated SOL-divertor integrated code [6]. However, we now develop a neutral transport model so as to precisely study the behavior of the neutrals as a particle source, and in that sense a detailed consideration of the surface-plasma interaction is outside of the scope of our study. We just assume that cold neutral atoms with $3 \sim 5\,\mathrm{eV}$ are born from the wall after the dissociation processes of molecules.

A Monte Carlo approach provides a flexible and convenient framework for developing numerous physics calculations in terms of neutrals [7]. It can easily include the countless energy groups of neutrals and the geometrical effect and accurately evaluate a neutral density profile within a statistical error. Monte Carlo codes have been widely used to analyze the neutral population in experiments and to predict the neutral transport in simulations, over the entire plasma including the core region [6, 7, 8, 9, 10, 11]. The Monte Carlo approach is, however, not always suitable for a coupling with a time-dependent transport code because it requires much computation cost and its solution inevitably includes a statistical error. From the aspect of the compatibility of a fluid-type transport code and the long-time simulation, a fluid modeling of the neutral transport is still considered to be important.

There have been many neutral transport modelings except a Monte Carlo approach: analytic models for the estimation of the neutral density profile [12, 13, 14] and computational diffusion models in a two-dimensional geometry [15, 16, 17]. These modelings are essentially based on the assumption of short

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mean free path of neutrals, i.e. frequent charge exchange. In the region inside the edge region in present-day tokamak discharges, however, thermal neutrals could have long mean free path. It is then difficult to directly apply these modelings to a wide range of plasma parameters, with which transport codes must deal. We therefore would like to develop a one-dimensional neutral transport model, compatible with TASK/TX and applicable to a wide range of plasma parameters.

In this paper, a one-dimensional neutral diffusion model in cylindrical coordinates is proposed for the three-group neutrals, on the basis of the diffusion approximation idea [15]. The rest of this paper is as follows. The next section describes a brief summary of TASK/TX, and a neutral transport model consistent with TASK/TX is shown in section 3. Simulation results for the validation of our model are given in section 4. Finally we summarize our results in section 5.

2. Multi-fluid transport code, TASK/TX

We briefly summarize the main characteristics of the one-dimensional multi-fluid transport code TASK/TX with an emphasis on the difference from conventional transport codes. More details about the code and actual expression of the equations are found in [2].

- The code solves the continuity equations, the thermal transport equations and the two-fluid equations of motion for electrons and ions coupled with Maxwell's equations as well as the equations for neutrals and fast beam ions in the cylindrical coordinates (r, θ, ϕ), where r, θ and ϕ denote the radial, poloidal and toroidal directions respectively.
- Since the multiple continuity equations for all charged particle species are solved as well as Poisson's equation, an explicit quasi-neutrality condition need not be imposed.
- Neoclassical effects such as the bootstrap current and the Ware pinch appear through the neoclassical viscous force term in the poloidal equation of motion. The neoclassical viscosities are evaluated by the NCLASS module [18].
- The calculation domain is extended to the scrape off layer across the plasma surface (separatrix) and is bounded by the wall: It enables us not to impose boundary conditions on the plasma surface.
- The formation of the radial electric field is accurately evaluated through Poisson's equation and the radial force balance in a manner consistent with the flows and background plasma profiles.

There are several kinds of particle sources in the TASK/TX system. Thermalization of fast beam ions is the major particle source of the bulk ions. Furthermore, ionization of neutrals is also the major source, usually localized near the edge region. Neutrals in a tokamak plasma have many different origins, such as recycling, gas puffing, NB injection and so on. An accurate estimation of the particle source is required to study the behavior of the particle transport and the resultant density profiles; hence these processes should be carefully taken into account in the code.

To that end, TASK/TX solves the slowing down equations for fast ions and the neutral diffusion equations together with the two-fluid equations and Maxwell's equations. We should deal with the neutral transport equations in a manner different from other equations. This is because the motion of neutrals is not restricted by the magnetic field unlike charged particles. The usual diffusive transport equations are then not directly applied for the neutral transport analysis.

3. Modeling of neutral transport

In order to develop a one-dimensional neutral diffusive transport model, we should reduce an essentially three-dimensional effect to a one-dimensional one. As with most of the neutral transport modelings, we assume that neutrals move around in a two-dimensional plasma cross-section, without considering their movement in the toroidal direction.

In tokamak plasmas, there are many kinds of neutrals from the aspect of their energy and their origin. Neutral atoms with cold temperature of typically 3 to 5 eV, after dissociation of hydrogen molecules, are mainly provided by the wall through recycling and/or gas puffing. We call them slow neutrals hereafter. They are randomly moving around, and subsequently some of them are ionized and the other turn into thermal neutrals with temperature equivalent to that of the thermal ions with which the neutrals collide, due to charge exchange. The so-called first-generation thermal neutrals have long mean free paths and are able to reach the core region, leading to the possible particle source there. In a NB-heated plasma, the situation surrounding the neutrals is somewhat different. For example, a positive-ion based NB unit in JT-60U provides high energetic neutrals with around 80 keV, much higher than the temperature of thermal ions. Due to charge exchange between these neutrals and the thermal ions, the neutrals turn into the fast ions while the thermal ions become the thermal neutrals, which are called halo neutrals. The halo neutrals are similar to the above-mentioned first-generation thermal neutrals in that they have thermal velocities comparable to the background ion temperature. On the other hand, they definitively differ in where they are born. The former can be born anywhere in the path of NB, even in the core region, while the latter can be generated only in the edge region where the cold neutrals can exist. In order to develop a neutral transport model suitable for TASK/TX, we separately treat the behavior of these three groups of neutrals.

A time-dependent basic diffusion equation for neutrals is expressed by

$$\frac{\partial n_{0j}}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD_{0j}\frac{\partial n_{0j}}{\partial r}\right) - \frac{1}{Z_i}n_\mathrm{e}\left\langle\sigma_\mathrm{iz}v\right\rangle n_{0j} + S_{0i}, \quad (1)$$

where the subscript $0j$ denotes the neutral species j: $j = 1$ for the slow neutrals, $j = 2$ for the thermal neutrals and $j = 3$ for the halo neutrals. n denotes the density, Z_i the charge number of bulk ions, $\langle\sigma_\mathrm{iz}v\rangle$ the Maxwellian averaged ionization cross-section and S_{0j} the source and sink. The diffusivity D_{0j} for neutrals is defined by [16]

$$D_{0j} \equiv \frac{\lambda_{0j}v_{0j}}{3} = \frac{v_{0j}^2}{3n_\mathrm{i}(\langle\sigma_\mathrm{iz}v\rangle + \langle\sigma_\mathrm{cx}v\rangle)}, \quad (2)$$

where λ_{0j} denotes the mean free path, v_{0j} the Maxwellian averaged thermal velocity and σ_cx the charge exchange cross-section.

The mean free path of the slow neutrals is much smaller than those of other kinds of neutrals because of their slow thermal velocity. In the edge region with low electron temperature, they quickly suffer from ionization, not long after their birth at the wall. Therefore the population of the slow neutrals is highly localized in the edge region. Their density significantly decreases with distance from the wall and almost vanishes around typically $\rho \equiv r/a \approx 0.9$, although the boundary varies depending on the background electron temperature and other conditions. Here r is the local minor radius and a the minor radius. Owing to the short mean free path, i.e. frequent collisions, the behavior of the slow neutrals can be properly modelled by a one-dimensional diffusion equation. For the slow neutrals, the source and sink term consists of the charge exchange loss, recycling and gas puffing as follows:

$$S_{01} = -n_\mathrm{i}\left\langle\sigma_\mathrm{cx}v\right\rangle n_{01} + S_{01}^\mathrm{rcyl} + S_{01}^\mathrm{Puff}.$$

On the contrary, the mean free path of the first-generation thermal neutrals is rather long because of their high temperature due to charge exchange with thermal ions. It could be half of the minor radius a. The thermal neutrals are born in the region where the slow neutrals exist, and they can penetrate deep into the core due to their long mean free path. We would fail to reasonably estimate the density profile

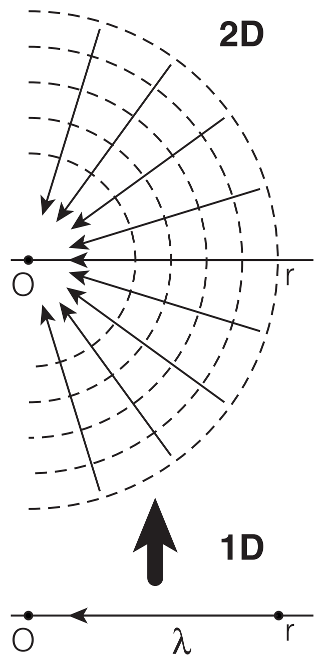

Fig. 1 Illustration of a wrong modeling of first-generation neutral trajectories, denoted by slim arrows, born at the magnetic surface r. The magnetic surface is denoted by the broken line and the magnetic axis by O.

of the thermal neutrals if we directly utilized eqs. (1) and (2) without any special treatment in terms of the long mean free path. Since the source of the thermal neutrals are localized in the edge region as explained above, the thermal neutral density decreases with distance from there. In a diffusive manner, the neutrals tend to move towards region of the lower density, that is, the magnetic axis from the high density region. If we model their movement in a two-dimensional space as a one-dimensional diffusion equation (1) without careful consideration, the movement towards the magnetic axis in the radial direction is regarded as if the neutrals intentionally funneled towards the magnetic axis in two-dimensional space, as seen in fig. 1. In this case eq. (2) yields the excess estimation of D_{02}, predicting the excess neutral density in the core. Of course this cannot happen in an actual plasma. In fact the neutrals born at a certain flux surface overall move inwards as mentioned above, while they can move any direction. This effect should be appropriately included in the one-dimensional modeling.

Here we consider a thermal neutral born at the flux surface n corresponding to r, as shown in fig. 2, in order to estimate the more realistic diffusivity $D_{02}(r)$, which can be applied to eq. (1). We assume that it moves its mean free path length, labelled by λ_n, and then arrives at the surface i. Since in this case we consider only the neutral that moves inside the surface n, a maximum angle is defined as θ_n. The projection

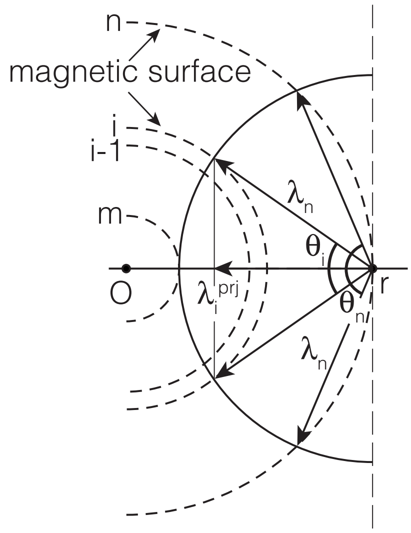

Fig. 2 Illustration of the computation of an effective mean free path of a first-generation neutral at a position r, corresponding to the magnetic surface denoted by n. A mean free path is denoted by λ and an angle between the intersection points of a magnetic surface and a neutral trajectory by θ. The subscripts correspond to the labels of the magnetic surface.

of $\lambda_i(=\lambda_n)$ on the midplane is $\lambda_i^{\rm prj}=\lambda_n\cos\theta_i$. If we regard $\lambda_i^{\rm prj}$ as the mean free path of the neutrals which are born at n and fall into the area between i and $i-1$, the ratio of them to all the neutrals born at n is $(\theta_i-\theta_{i-1})/\theta_n$. Some of these neutrals may arrive at the surface n after moving their mean free path, meaning that they eventually remain at the born surface n. Based on this concept, an effective mean free path used in the one-dimensional modeling must be shorter than $\lambda_n(=\lambda_{02})$. Since this argument can be applied from the surface m to n, where the surface m denotes the farthest surface at a distance of λ_n from the surface n, we finally obtain the effective mean free path $\lambda_{02}^{\rm eff}(r)$ evaluated at r in the form:

$$\begin{aligned}\lambda_{02}^{\rm eff}(r) &= \sum_{i=m+1}^{n}\lambda_i^{\rm prj}\frac{\theta_i-\theta_{i-1}}{\theta_n}\\ &= \sum_{i=m+1}^{n}\lambda_{02}\cos\theta_i\frac{\theta_i-\theta_{i-1}}{\theta_n}. \qquad (3)\end{aligned}$$

We note that we assume no poloidal variation of the neutral density on a flux surface in this estimation.

All the first-generation neutrals are assumed to have mono-energy in our modeling. When we estimate λ_{02} for D_{02}, we must properly determine their thermal velocity v_{02}, i.e. their temperature. The source region of the thermal neutrals exactly coincides with the region where the slow neutrals exist. Even in this narrow edge region, the ion temperature $T_{\rm i}$ significantly varies. Then we assume that the density-weighted volume-averaged temperature is a representative of the various thermal neutral temperatures, as defined below:

$$\bar{T}_{02}\equiv\frac{\int_{r_{01}}^{b}n_{02}(r)T_{\rm i}(r)\,r{\rm d}r}{\int_{r_{01}}^{b}n_{02}(r)\,r{\rm d}r},$$

where r_{01} is the innermost boundary of the region where the slow neutrals exist and b denotes the radius of the wall. By using the Maxwellian averaged velocity $v_{02}=\sqrt{8k\bar{T}_{02}/(\pi m_{\rm i})}$ and the locally evaluated cross-sections, we obtain λ_{02} appearing in eq. (3) and then D_{02} by eq. (2). Here k denotes the Boltzmann constant and $m_{\rm i}$ the ion mass. The source term can be expressed as

$$S_{02}=n_{\rm i}\,\langle\sigma_{\rm cx}v\rangle\,n_{01},$$

which is the particle supply from the slow neutrals due to charge exchange.

Unlike the first-generation thermal neutrals, the halo neutrals are usually produced in the core region near the magnetic axis because a source profile for the halo neutrals coincides with a birth profile due to NB heating, i.e.

$$S_{03}=S_{03}^{\rm NB}.$$

The typical density profile of the halo neutrals is centrally peaked and gradually decreases towards the edge region, although it depends on the birth profile. Then they mainly tend to diffuse from the core to the edge, with the velocity faster than that of the thermal neutrals. It means that their mean free path is longer than that of the thermal neutrals. Owing to the core-localized source profile and the fairly long mean free path, the halo neutrals can be regarded as a simple outward diffusion in cylindrical coordinates, and in addition many of them may be ionized in the core due to the high plasma density. Therefore we can reasonably use eqs. (1) and (2) for them.

4. Validation of the neutral transport modeling

In the preceding section, we developed a set of diffusion equations for three-group neutrals based on the physical consideration. We should then confirm the validity of our modeling by comparing a neutral density profile with that by a Monte Carlo code TOPICS/NT [9]. In this section, we focus our attention on the behavior of the slow and thermal neutrals only in an ohmic plasma without NB heating. This is because we devoted our effort to the development of the transport model for the thermal neutrals.

We use JT-60U-like plasma parameters: the major radius $R_0 = 3.2\,$m, $a = 0.8\,$m, the toroidal magnetic field $B_\phi = 2.68\,$T, the plasma current $I_{\rm p} =$

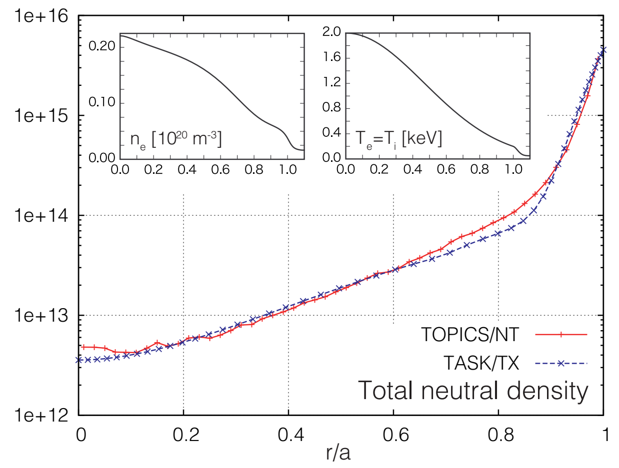

Fig. 3 Comparison of the neutral density profile calculated by a Monte Carlo code TOPICS/NT with that by TASK/TX in a transient phase at $t = 0.1\,\mathrm{s}$, in the lower plasma density case.

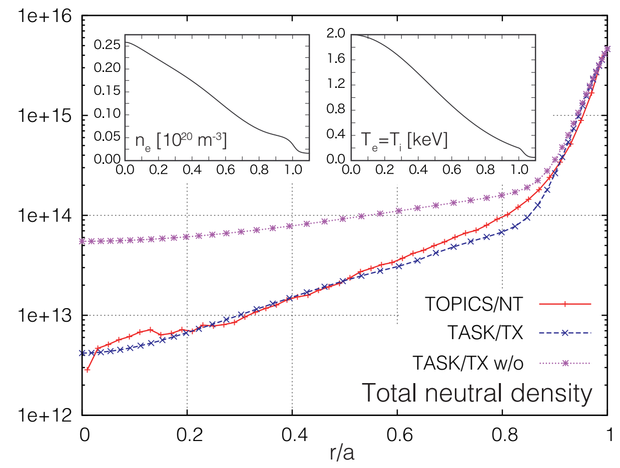

Fig. 4 Comparison of the neutral density profiles calculated by TOPICS/NT, TASK/TX and that without any special treatment for the thermal neutral transport modeling in a quasi-steady state at $t = 0.5\,\mathrm{s}$, in the lower plasma density case.

$1.0\,\mathrm{MA}$, the gas puff rate $\Gamma_0 = 1.0 \times 10^{20}\,\mathrm{m^{-2}s^{-1}}$ and the recycling rate $\gamma_0 = 0.8$. For simplicity, in the following simulations we assume that temperature profiles for electrons and ions are the same and are fixed at initial profiles without loss of generality. TASK/TX calculates the particle confinement time τ_p at every time step, and then for comparison it provides TOPICS/NT with the calculated τ_p as a constraint condition.

First of all, we study the case in a lower density plasma, as observed in typical JT-60U ohmic discharges. In a transient phase at $t = 0.1\,\mathrm{s}$, we compare a neutral density profile calculated by TOPICS/NT with that by TASK/TX, as shown in fig. 3. At this time the volume averaged electron density $\bar{n}_\mathrm{e}$ is $9.86 \times 10^{18}\,\mathrm{m^{-3}}$, and the background profiles of the electron density and the temperatures are also seen in the figure. The neutral transport model developed well reproduces the neutral density profile with both the slow and thermal neutrals mixed predicted by TOPICS/NT. Roughly speaking, the slow neutrals dominates the neutral density profile outside $\rho = 0.9$ and the thermal neutrals does inside $\rho = 0.9$. In both regions, the slope of the profile agrees well between two cases. The maximum deviation between both profiles is just by a factor of ~ 1.3. Fig. 4 shows the comparison of the profiles in a quasi-steady state at $t = 0.5\,\mathrm{s}$. We again have a very good agreement between two predictions even in the steady state. The tendency of the profile is almost similar to the transient case. Just for reference, the figure also includes the result by TASK/TX without any special treatment for the thermal neutral transport modeling. More specifically, in this case λ_{02} is adopted instead of $\lambda_{02}^{\mathrm{eff}}$, and the local thermal neutral temperature $T_\mathrm{i}(r)$ is used instead of $\bar{T}_{02}$. This model clearly overestimates the thermal neutral density in the core, indicating that the model developed in this study plays a crucial role in the correct estimation of the neutral density profile. We conclude that the neutral density prediction by TASK/TX agrees well with that by TOPICS/NT, regardless of whether the plasma is in a transient phase or a steady state.

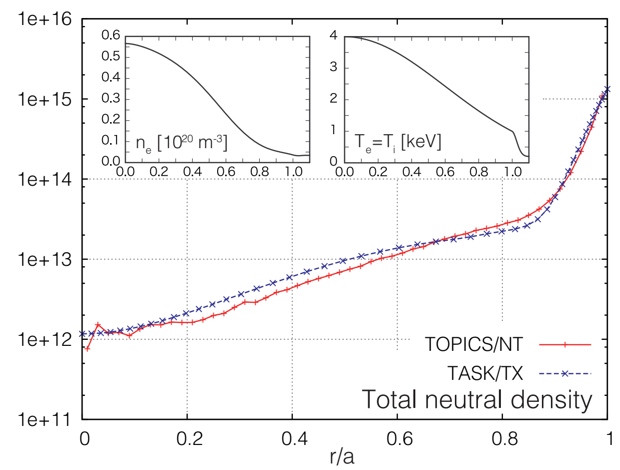

Fig. 5 Comparison of the neutral density profile calculated by TOPICS/NT with that by TASK/TX in a transient phase at $t = 0.5\,\mathrm{s}$, in the higher plasma density case.

It is meaningful to check the model validity in a different operation regime. We then compare neutral density profiles in a higher density plasma with a little high temperature compared with the previous cases. A comparison result with background density and temperature profiles is shown in fig. 5. In this case the ohmic plasma with $\bar{n}_\mathrm{e} \approx 1.73 \times 10^{19}\,\mathrm{m^{-3}}$ is still in a transient phase at $t = 0.5\,\mathrm{s}$. The density profiles are in good agreement with each other again. In comparison with the previous cases, a slight disagreement in the shape of the profiles is found, while the maximum deviation is very small by a factor of ~ 1.4. These results show that the model works well in plasmas with both low and high densities, indicating that it is applicable to the wide range of plasma parameters, which is a very important feature for the model cooperated with a transport code.

5. Summary and discussion

We have developed the one-dimensional fluid-type neutral transport model well compatible with TASK/TX. The main characteristic of the model is to separate all the neutrals into three groups from the aspect of their energy and their origin: the slow, thermal and halo neutrals. The diffusivity for the thermal neutrals with long mean free path, mainly moving from the edge to the core, is carefully modelled considering the neutral motion in a two-dimensional space, as shown in fig. 2. The neutral density profiles predicted by TASK/TX with the model developed were compared with that by a Monte Carlo code TOPICS/NT in the cases with the low or high density in the transient or steady state phase, and the very good agreement has been obtained. It means that the model is useful and suitable for cooperation with a time-dependent transport code, which must cover the wide range of plasma parameters.

There is room for improvement of the model. If it were applied to a plasma with a significantly high density and a low temperature near the edge region, the model prediction would deviate from a Monte Carlo prediction. In such a plasma the mean free path of first-generation thermal neutrals is shorter than that in the above-considered cases. Due to the rather short mean free path, these neutrals may undergo second charge exchange in the outer core region before ionization and then the resultant second-generation thermal neutrals will have higher temperature compared with the first-generation one, leading to longer mean free path. If we introduce the second-step or multi-step charge exchange process into the model, its predictions will agree with Monte Carlo calculations with high accuracy even in such an extreme case.

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