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An Implicit Monte Carlo Method for Simulation of Impurity Transport in Divertor Plasma

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A new ''implicit'' Monte Carlo (IMC) method has been developed to simulate ionization and recombination processes of impurity ions in divertor plasmas. The IMC method takes into account many ionization and recombination processes during a time step Δt. The time step is not limited by a condition, $\Delta t \ll \tau_{\min}$ ($\tau_{\min}$; the minimum characteristic time of atomic processes), which is forced to be adopted in conventional Monte Carlo methods. We incorporate this method into a one-dimensional impurity transport model. In this transport calculation, impurity ions are followed with the time step about 10 times larger than that used in conventional methods. The average charge state of impurities, $\langle Z \rangle$, and the radiative cooling rate, $L(T_e)$, are calculated at the electron temperature T_e in divertor plasmas. These results are compared with thosed obtained from the simple noncoronal model. © 1997 Academic Press

1. INTRODUCTION

Impurity behavior in divertor plasmas, as well as in core plasmas, is one of the important issues to be clarified for the fusion research. In order to study the impurity behavior numerically and analytically, various physics phenomena, such as (a) impurity generation on the vessel wall, (b) ionization of sputtered neutrals, (c) impurity ion transport, (d) Coulomb scattering, and (e) atomic processes, have to be included in the model. Various kinds of simulation models have been developed up to now. Basically they are classified in two categories. One is the fluid approach [1–3] and the other is the Monte Carlo approach [4, 5]. The Monte Carlo approach is suitable for modelling of atomic processes combined with the impurity transport calculation.

If ionization and recombination processes are simulated by a conventional simple hit-or-miss Monte Carlo method, the time step is required to satisfy a condition, $\Delta t \ll \tau^{i/r}$, where $\tau^{i/r}$ is the characteristic time of ionization/recombination. We have to choose the sufficiently small time step in which the ion cannot suffer multiple ionizations/recombinations. Ionization time and recombination time strongly depend on the charge state of an impurity ion and plasma parameters. The minimum time among those is generally smaller than the other characteristic times of impurity behavior. Thus the characteristic times of ionization and recombination are the dominant factors to choose the time step in a conventional Monte Carlo calculation. As a result, long computation time is required for the impurity transport simulation with the simple hit-or-miss method.

In order to reduce the computation time, a new Monte Carlo method that is free from the condition of $\Delta t \ll \tau^{i/r}$ is required to be developed. Previously, an implicit Monte Carlo method was developed by Fleck and Cummings [6] and by Fleck and Canfield [7] for the nonlinear radiation transport. The radiation field and the material energy density are calculated in a self-consistent manner analogous to the implicit finite difference solution of coupled matter and radiation equations. Against the arbitrary value of the time step Δt, this method provides accurate and unconditionally stable solutions to nonlinear radiation transport problems.

In the present paper, we propose a new ''implicit'' Monte Carlo (IMC) method for the impurity transport in a divertor plasma. A set of rate equations for impurities are solved implicitly and the solutions are applied to a Monte Carlo method. The limit of the time interval disappears in the present implicit Monte Carlo method just the same as in the previous one. As an example of the application, we incorporate the IMC method into an impurity transport code. Although the transport code is spatially one-dimensional (1D), it includes all the physical processes of (a)–(d) mentioned above. The calculation models of these processes are the simplified version of the IMPMC code [5]. Using this 1D transport code, we study the carbon impurity behavior in divertor plasmas. The average charge state of impurities, $\langle Z \rangle$, and the radiative cooling rate, L (T_e), are estimated for the typical divertor parameters. We compare these results with those obtained from a simple noncoronal model proposed by Shimada *et al.* [8].

The new implicit Monte Carlo method is described in Section 2. Test calculations to check the validity of the

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IMC method are also given. In Section 3, calculation results of 1D transport simulation using the IMC method are presented, and estimations of $\langle Z \rangle$ and L (T_e) are discussed. The summary is given in Section 4.

2. IMPLICIT MONTE CARLO METHOD

2.1. *Conventional Simple Hit-or-Miss Method for Ionization and Recombination Processes*

In this subsection, a conventional simple hit-or-miss method and its demerits are briefly reviewed.

In order to obtain the change in the impurity population of the kth charge state, first, the probability of transfer to the neighboring $(k \pm 1)$th states by ionization or recombination during a time step Δt is given. The total probability of transfer is approximately given by $\nu^{\text{total}}\Delta t$, where $\nu^{\text{total}} = \nu_k^{\text{i}} + \nu_k^{\text{r}}$ is the sum of the transfer rates by ionization and recombination. Next, a uniform random number ξ_1 $(0 \le \xi_1 < 1)$ is generated. If $\xi_1 \le \nu^{\text{total}}\Delta t$, an ionization or recombination event is assumed to occur. Finally, the type of event (ionization or recombination) is decided by another uniform random number ξ_2 $(0 \le \xi_2 < 1)$. If $\xi_2 \le \nu_k^{\text{i}}/\nu^{\text{total}}$, then an ionization event has occurred. Otherwise a recombination event has occurred. Above procedures are repeated for each impurity ion and in each time step.

In this method, we cannot treat multiple ionization/recombination processes during one time step, because the transfer probability $\nu^{\text{total}}\Delta t$ represents only the transfer to the neighboring states. As a result, if we take a large time step during which ions can experience many ionization/recombination events, these processes cannot be described correctly.

Thus, in the simple hit-or-miss method, we have to carefully choose the time step enough small so as to satisfy the condition, $\Delta t \ll \tau_{\min}$, where $\tau_{\min}$ is the minimum characteristic time of ionization and recombination processes. In each time step, $\tau_{\min}$ is recalculated for each test particle. Therefore, a large amount of computation time is generally required for the impurity transport simulation with the simple hit-or-miss method.

2.2. *New "Implicit" Monte Carlo Method*

To reduce the computation time, we develop a new "implicit" Monte Carlo (IMC) method. The IMC method is based on the feature that the ionization and recombination rates of impurity ions depend mainly on the local plasma parameters and do not depend on the impurity population itself. This feature of rate coefficients makes it possible to calculate all the possible transfer probabilities after a time step Δt beforehand. Once all of the probabilities are found, a uniform random number can determine what charge state a test particle is in after Δt. As mentioned above, in the conventional simple hit-or-miss method, the transfer probability only to the neighboring charge states is used. This is the intrinsic difference between the IMC method and the conventional hit-or-miss method.

Taking into account all the possible charge states, the probability of transfer $P_{k' \to k}(\Delta t)$ from k'th to kth charge state after a time step Δt can be obtained from the solution of a set of the following rate equations,

$$\begin{aligned} \frac{dn_k}{dt} &= \nu_{k-1}^{\text{i}} n_{k-1} - (\nu_k^{\text{i}} + \nu_k^{\text{r}}) n_k + \nu_{k+1}^{\text{r}} n_{k+1}, \\ \Sigma_k n_k &= n \quad (k = 0, 1, ..., K), \end{aligned} \tag{1}$$

where n_k is the density of impurities in the kth ionization state and K is the maximum ionization state of the impurity ion. We solve Eq. (1) by using a full-implicit time difference scheme,

$$\begin{aligned} n_k(t + \Delta t) - n_k(t) &= \nu_{k-1}^{\text{i}} \Delta t n_{k-1}(t + \Delta t) \\ &\quad - (\nu_k^{\text{i}} + \nu_k^{\text{r}}) \Delta t n_k(t + \Delta t) + \nu_{k+1}^{\text{r}} \Delta t n_{k+1}(t + \Delta t). \end{aligned} \tag{2}$$

Thus we call the present method an "implicit" Monte Carlo method. Equation (2) is a set of linear equation system for $n_k(t + \Delta t)$ and is rewritten as

$$A_k n_{k-1}(t + \Delta t) - C_k n_k(t + \Delta t) + B_k n_{k+1}(t + \Delta t) = -D_k, \tag{3}$$

$$\begin{aligned} A_k &= \nu_{k-1}^{\text{i}} \Delta t, \\ B_k &= \nu_{k+1}^{\text{r}} \Delta t, \\ C_k &= 1 + (\nu_k^{\text{i}} + \nu_k^{\text{r}}) \Delta t, \\ D_k &= n_k(t). \end{aligned}$$

Equation (3) is solved algebraically by the tridiagonal matrix algorithm under the initial conditions, $n_{k'}(t) = n$ and $n_{k \ne k'}(t) = 0$. Using the solution for kth charge state, $n_k(t + \Delta t)$, we define the probabilities of charge state transfer from k'th to kth ionization state after a time step Δt as $P_{k' \to k}(\Delta t) = n_k(t + \Delta t)/n(t + \Delta t)$.

These probabilities are tabulated prior to the Monte Carlo calculation. In the Monte Carlo calculation, the transfer of ion charge-state is determined from a uniform random number, ξ $(0 \le \xi < 1)$. If

$$\sum_{i=0}^{k-1} P_{k' \to i}(\Delta t) \le \xi < \sum_{i=0}^{k} P_{k' \to i}(\Delta t), \tag{4}$$

then a test impurity changes its charge state from k' to k.

In this method, many ionization and recombination processes during one time step are described correctly. As a result, the time step in the IMC method is not restricted by the condition, $\Delta t \ll \tau_{\min}$. Therefore, if this method is applied to the impurity transport simulation, the time step should be determined from the characteristic time of the

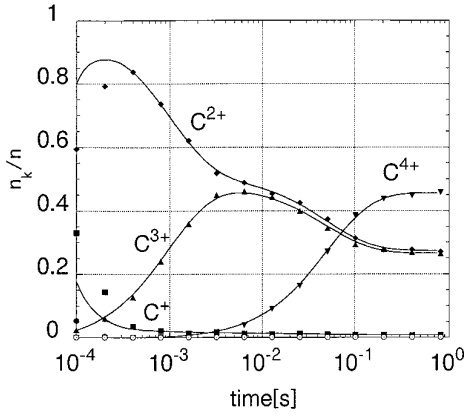

FIG. 1. Time evolution of density fraction of each ionization stage, n_k/n. Symbols are calculated by the IMC method with $\Delta t = 1 \times 10^{-4}$ s, and solid lines are analytic solutions. Plasma parameters are $T_e = 10$ eV and $n_e = 10^{19}$ m^{-3}.

transport process not of the atomic processes. Generally, the characteristic time of the transport process is larger than the minimum characteristic time of ionization and recombination processes. As a result, the IMC method is effective to reduce the total computation time compared with the simple hit-or-miss method.

2.3. *Test Calculations*

In this subsection, we check the validity and the effectiveness of the IMC method for the simple case. We consider only atomic processes of carbon impurities in a uniform plasma with electron temperature of $T_e = 10$ eV and density of $n_e = 10^{19}$ m^{-3}.

Figure 1 shows the time evolution of impurity charge state population, $N_k \equiv n_k(t)/n_0$, calculated by the IMC method. The accurate solution to Eq. (1) is shown by solid line to be compared with the solution from the IMC method (symbols). The initial condition is $n_0(0) = n_0$ and $n_{k\neq 0}(0) = 0$. The time step is chosen to be $\Delta t = 1 \times 10^{-4}$ s. In this calculation, 5000 test particles are used. Statistical error is less than 2% for this case, and the use of a larger number of particles changes little the result. When the characteristic time of evolution, $\tau \equiv n_k(\mathrm{d}n_k/\mathrm{d}t)^{-1}$, is comparable to Δt; i.e., in the initial stage of $t < 10^{-3}$ s, the error evaluated as

$$\left|N_k^{\mathrm{IMC}} - N_k\right| \approx (1 + \Delta t/\tau)^{-1} - \exp(-\Delta t/\tau) \qquad (5)$$

becomes about 0.2. If one needs more accurate results than those of the IMC method, one should use the analytic solution to differential equation Eq. (1), instead of the solution to difference equation Eq. (2), to calculate the transfer probability.

Next, we make the comparison of the CPU time between for the IMC method and for the conventional simple hit-or-miss method. Plasma parameters are the same as for the case of Fig. 1. The minimum ionization and recombination time is $\tau_{\min} = 1.1 \times 10^{-6}$ s, which is the ionization time from C^0 to C^+. Figure 2 shows the required CPU time, $\mathrm{CPU}_{\mathrm{IMC}}$, to obtain the steady state solution as a function of the time step selected for the IMC calculation. The CPU time is normalized by that for the simple hit-or-miss method, $\mathrm{CPU}_{\mathrm{HM}}$, with $\Delta t_{\mathrm{HM}} = 1.1 \times 10^{-7}$ s. As seen from Fig. 2, the CPU time for the IMC calculation decreases almost inverse-linearly with Δt. When we incorporate the IMC method into the impurity transport code, the time step of overall calculation is limited by the characteristic time of the transport process. Therefore we cannot choose an arbitrarily large time step. However, the CPU time required for overall calculation can be reduced by using the IMC method, because the characteristic time scale of the transport process is generally larger than the minimum time scale of ionization and recombination processes.

3. IMPURITY TRANSPORT SIMULATION WITH THE IMC METHOD

In this section, we incorporate the IMC method into an impurity transport code. Since the purpose of this paper is to demonstrate the IMC method being effective for the transport simulation, a simple 1D model is used for the following example calculations. The cross field diffusion and the electric force are neglected. The ionization and recombination processes are simulated by the IMC method. The other physical processes, such as (a) impurity generation at divertor plate, (b) ionization of sputtered neutrals, (c) impurity-ion motion along the field line, and

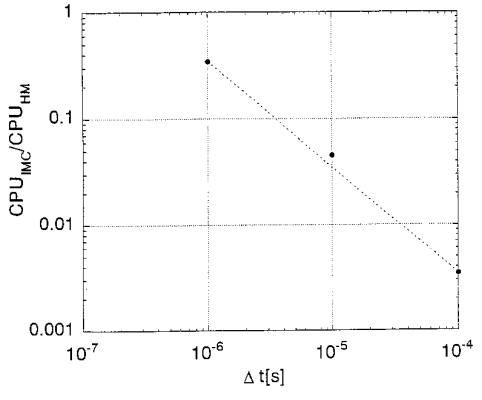

FIG. 2. CPU time required for the IMC calculation, $\mathrm{CPU}_{\mathrm{IMC}}$, normalized by CPU time for a hit-or-miss method, $\mathrm{CPU}_{\mathrm{HM}}$, as a function of time step Δt. The time step in the hit-or-miss method is fixed as $\Delta t_{\mathrm{HM}} = 1.1 \times 10^{-7}$ s. Plasma parameters are the same as in Fig. 1. $\mathrm{CPU}_{\mathrm{IMC}}$ decreases almost inverse-linearly with Δt.

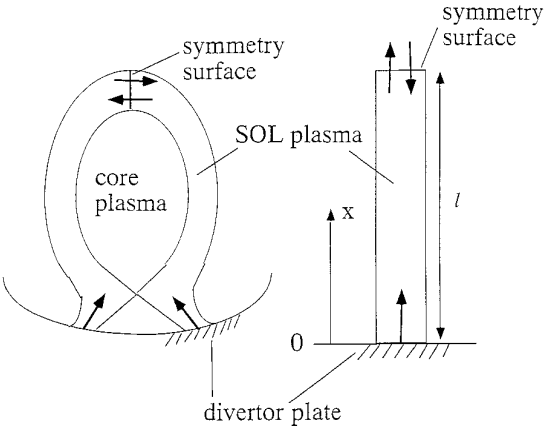

FIG. 3. Model geometry for transport simulation. The SOL length is $\ell = 1$ m and the calculation region is divided into 200 cells. Impurities are sputtered from the divertor plate at $x = 0$ m.

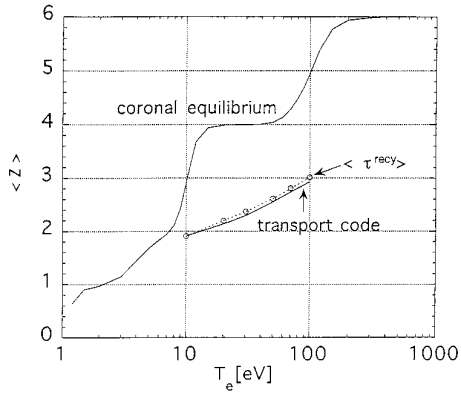

FIG. 5. Average charge state $\langle Z \rangle$ as a function of T_e. Results obtained from the transport simulation (solid line) are compared with those obtained from noncoronal model using $\langle \tau^{recy} \rangle$ (circles). They are also compared with those for the coronal equilibrium.

(d) Coulomb scattering, are modeled as almost the same as in the IMPMC code [5].

In the present simulation, a scrape-off layer (SOL) plasma is simply modeled into a 1D plasma as shown in Fig. 3. The calculation region is divided into 200 cells. The temperature and density of the background deuterium plasma is assumed to be uniform in order to make it easy to compare the results with those from a simple point model calculation later in this section, while the plasma flow velocity is assumed to be $V_f = C_s\,(\ell - x)/\ell$, where C_s is the sound speed of a deuterium plasma, ℓ is the poloidal length of the SOL plasma, and x is the distance from the divertor plate.

Figure 4 shows the density profile of the carbon impurity for the case of $T_e = 50$ eV, $n_e = 10^{19}$ m^{-3}, $\ell = 1$ m, and $\Gamma = 2.3 \times 10^{20}$ m^{-2}/s, where Γ is the sputtered impurity flux. The limitation of maximum time step for the calculation is

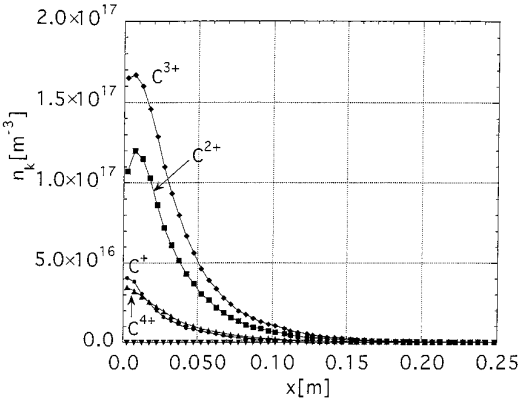

FIG. 4. Spatial profile of carbon density of kth charge state, n_k, at steady state. The horizontal axis is the distance from the divertor plate. Plasma parameters are $T_e = 50$ eV and $n_e = 10^{19}$ m^{-3}.

determined from impurity transport by the condition of $C_s\,(B_p/B)\,\Delta t < \Delta x$, where C_s can be chosen as the typical speed of the impurity ions, B_p/B is the pitch of the magnetic field, and Δx is the size of the cell. The maximum time step is restricted by $\Delta t = 3.9 \times 10^{-6}$ s for $B_p/B = 0.02$, and $\Delta x = 0.5$ cm. If the simple hit-or-miss Monte Carlo method is employed under the same condition, Δt is limited by $\Delta t = 3.3 \times 10^{-7}$ s. Therefore, by employing the IMC method, the impurity ions can be followed with the time step about 10 times larger than that for the simple hit-or-miss method.

Now we estimate the average charge state $\langle Z \rangle$ and the radiative cooling rate $L(T_e)$ for carbon impurities, by using the simulation code mentioned above. From the density profiles of the kth charge state $n_k(x)$ in a stationary state, we calculate $\langle Z \rangle$ and $L(T_e)$ as the spatially averaged ones,

$$\langle Z \rangle = \int dx \sum_k k n_k(x) \Big/ \int dx \sum_k n_k(x),$$

$$L(T_e) = \int dx \sum_k L_k(T_e)\, n_k(\xi) \Big/ \int dx \sum_k n_k(x),$$

where $L_k(T_e)$ is the radiative cooling rate of kth charge state ions given in Ref. [9]. For the case of Fig. 4, $\langle Z \rangle$ is obtained to be 2.5 and $L(T_e)$ becomes up to 1.5×10^{-31} Wm^3. If impurities are in the coronal equilibrium, $\langle Z \rangle$ is about 4 and $L(T_e)$ is only about 2×10^{-34} Wm^3.

Figure 5 shows the temperature dependence of $\langle Z \rangle$. All the conditions for the calculation are the same as those for Fig. 4, except the temperature. The value of $\langle Z \rangle$ for $T_e \geq 10$ eV becomes rather small, compared with that for the coronal equilibrium. This is because the ionization process and the transport loss are mainly balanced with each other in divertor plasmas while the ionization/recom-

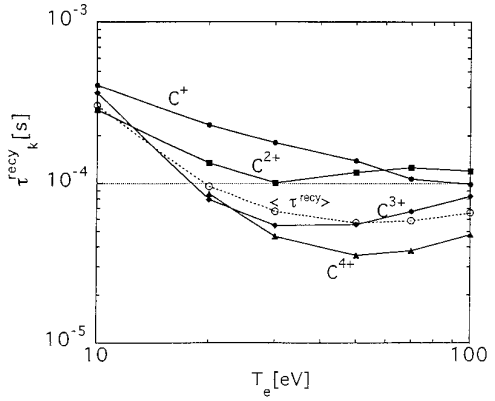

FIG. 6. Recycling time of each charge state $\tau_k^{\rm recy}$ and average recycling time $\langle \tau^{\rm recy} \rangle$ as functions of $T_{\rm e}$.

bination processes determine the population in coronal equilibria.

Here we introduce a simple point model of the form

$$\frac{dn_k}{dt} = \nu_{k-1}^{\rm i} n_{k-1} - (\nu_k^{\rm i} + \nu_k^{\rm r}) n_k + \nu_{k+1}^{\rm r} n_{k+1} - \frac{n_k}{\tau_k^{\rm recy}}. \quad (6)$$

The recycling time, or the loss time, of the kth charge state impurities, $\tau_k^{\rm recy}$, can be defined as $\tau_k^{\rm recy} = \int n_k(x)\, dx/\Gamma_k$, where the loss flux to the divertor plate, Γ_k, is obtained from the transport simulation. This model gives just the same results as those of transport simulations with uniform $\nu_k^{\rm i}$ and $\nu_k^{\rm r}$ values. Previously, Shimada *et al.* [8] already proposed such a simple noncoronal model of the same form as Eq. (6). In Ref. [8], as well as in Ref. [10], $\langle Z \rangle$ and $L(T_{\rm e})$ were calculated by putting $n_{\rm e}\tau_k^{\rm recy}$ as a parameter whose value was assumed the same for all charge states. In order to compare the present results with those of Shimada's model, we introduce an averaged recycling time $\langle \tau^{\rm recy} \rangle$,

$$\frac{1}{\langle \tau^{\rm recy} \rangle} = \sum_k \frac{1}{\tau_k^{\rm recy}} \int n_k(x)\, dx \Big/ \sum_k \int n_k(x)\, dx. \quad (7)$$

Figure 6 shows $\tau_k^{\rm recy}$ and $\langle \tau^{\rm recy} \rangle$ as functions of $T_{\rm e}$, which are obtained from transport simulations for the same parameters as in Fig. 5. The value of $\langle Z \rangle$ from the solution to Eq. (6) fully agrees with $\langle Z \rangle$, obtained from the transport code. Using $\langle \tau^{\rm recy} \rangle$ in place of $\tau_k^{\rm recy}$, we solve Eq. (6) and compare the results with those of transport simulations. As shown in Fig. 5, $\langle Z \rangle$ based on $\langle \tau^{\rm recy} \rangle$ becomes larger a little, because $\langle \tau^{\rm recy} \rangle$ is longer than $\tau_k^{\rm recy}$ for the higher kth charge state.

Dependence of the radiative cooling rate $L(T_{\rm e})$ on $T_{\rm e}$ is studied as shown in Fig. 7, where plasma parameters are the same as in Figs. 5 and 6. The rate is very large compared with that for a coronal equilibrium with $T_{\rm e} > 10$ eV, and it depends weakly on $T_{\rm e}$. The line radiation from C^{2+} and C^{3+} is strong, but that from C^{4+} is very weak. Therefore carbon impurities with $\langle Z \rangle \approx 4$ in a coronal equilibrium radiate very weakly, while those in a divertor plasma with $2 < \langle Z \rangle < 3$ emit radiation power strongly. The simple model calculation of Eq. (6) with $\langle \tau^{\rm recy} \rangle$ gives $L(T_{\rm e})$, which becomes a little smaller than that of transport simulation. The difference in $\langle Z \rangle$ and $L(T_{\rm e})$ between that for the transport simulation and the simple model calculation is not appreciable under the present condition of divertor plasmas. In nonuniform plasmas, however, the difference may become great. The clarification of such a prediction is a future work using a transport code with the IMC method.

4. SUMMARY

A new "implicit" Monte Carlo method has been developed to simulate ionization and recombination processes of impurity ions in divertor plasmas. The IMC method takes into account many ionization and recombination processes during a time step Δt. The time step is not limited by a condition, $\Delta t \ll \tau_{\rm min}$, which is forced to be adopted in conventional Monte Carlo methods. Major procedures of the IIMC method are as follows:

(1) Probabilities of transfer from k'th charge state to kth state, $P_{k' \to k}(\Delta t)$, are calculated prior to the Monte Carlo calculation. Rate equations are solved by using a full-implicit time difference scheme.

(2) A uniform random number determines the transfer of charge state of a test particle in accordance with the $P_{k' \to k}(\Delta t)$ distribution.

We check the validity and the effectiveness of the IMC method for the simple case in which only atomic processes of carbon impurities are considered. The time evolution of $n_k(t)$ agrees well with the analytical result, except for a few steps at the beginning. The computation time is drastically reduced by the IMC in comparison with the simple hit-or-miss method.

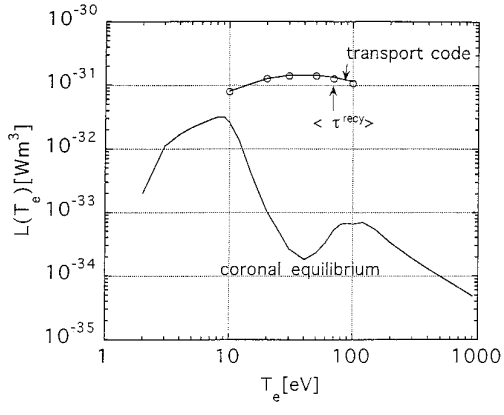

FIG. 7. Radiative cooling rate $L(T_{\rm e})$ as a function of $T_{\rm e}$. Comparison between models are made as the same as in Fig. 5.

Next, we incorporated this method into the 1D impurity transport code. The average charge state of carbon impurities, $\langle Z \rangle$, and the radiative cooling rate, $L(T_e)$, in a divertor plasma are calculated. We compare these results with those of a simple noncoronal model. Once the averaged recycling time is given properly, the difference between them is not appreciable for the present condition. In these transport simulations, impurity ions were followed with the time step about 10 times larger than that used in the conventional simple hit-or-miss method. Thus the IMC method is fairly effective to reduce the computation time.

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