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Monté Carlo Simulation for Particle Behavior of Recycling Neutrals in a Tokamak Divertor Region

Deok Kyu Kim and Sang Hee Hong
Seoul National University
San 56-1, Shinlim-dong, Kwanak-gu, Seoul 151-742, Korea
Kihak Im
Korea Basic Science Institute
52 Yeoeun-dong, Yusung-gu, Taejeon 305-333, Korea
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Abstract

The steady-state behavior of recycling neutral atoms in a tokamak edge region has been analyzed through a two-dimensional Monté Carlo simulation. A particle tracking algorithm used in earlier research on the neutral particle transport is applied to this Monté Carlo simulation in order to perform more accurate calculations with the EDGETRAN code which was previously developed for a two-dimensional edge plasma transport in the authors' laboratory. The physical model of neutral recycling includes charge-exchange and ionization interactions between plasmas and neutral atoms. The reflection processes of incident particles on the device wall are described by empirical formulas. Calculations for density, energy, and velocity distributions of neutral deuterium-tritium atoms have been carried out for a medium-sized tokamak with a double-null configuration based on the KT-2 conceptual design. The input plasma parameters such as plasma density, ion and electron temperatures, and ion fluid velocity are provided from the EDGETRAN calculations. As a result of the present numerical analysis, it is noticed that a significant drop of the neutral atom density appears in the region of high plasma density and that the similar distribution of neutral energy to that of plasma ions is present as frequently reported in other studies. Relations between edge plasma conditions and the neutral recycling behavior are discussed from the numerical results obtained herein.

1. Introduction

It has been known that recycling processes of fusion fuel elements by neutralizing target plates affect the plasma properties in the edge region of the tokamak device owing to the significant wall recombination and moreover bring about global effects on the core plasma [1-3]. The transport phenomena of recycling neutrals are associated with the particle and energy fluxes to device walls as well as the power and particle balances by transferring mass, momentum, and energy between neutral and plasma particles. Especially, in the plasma detachment phenomena observed in recent tokamak experiments, neutral transport is supposed to be playing a key role and need more investigations [4-6].

Since mid 1970s, a variety of numerical schemes have been applied to the transport analyses of edge neutral atoms and molecules moving unaffected by magnetic fields in tokamak fusion reactors. In the early stage, inspired by the fact that the neutral particle transport is similar to neutron transport in fission reactors, some researchers used neutronics codes, such as the ANISN code [7], for tokamak studies. Later on, several neutral transport codes using the same computational techniques as used in neutronics codes were developed only for fusion research. For instance, the SPUDNUT [8] and ANTIC [9] codes were made for calculations of the neutral transport in the slab or the cylindrical geometry using the integral form of Boltzmann' s equation. Also Monté Carlo method has been serving as a very useful tool for developing neutral transport codes from the early period [10] in spite of some computational defects, and many important calculations have been carried out to date by various advanced codes [3]. Monté Carlo method has advantages especially in multi-dimensional computations and now is widely spread in this research area with the rapid improvement of computer processors. Recently there has been a great effort to carry out the numerical analysis on neutral particle transport by means of fluid approach, but the calculated results of fluid schemes are less satisfactory than those of Monté Carlo method due to the device-geometrical dependence and various atomic processes of neutral particles. For more accurate analyses on the tokamak edge plasma physics it is essential to carry out optimally coupled calculations of the neutral and plasma transport codes. The algorithm to be used in the present work is based on the common Monté Carlo particle-tracking method [1,3,10,11] and the coupled calculations with an existing plasma code are to be presented.

The fuel elements of the tokamak in this study are assumed to be a mixture of deuterium (D) and tritium (T) atoms with a number fraction of 50:50. Two major interactions between charged and neutral particles included in this transport model are charge-exchange and ionization processes in the tokamak edge region. Charge-exchanging neutrals can freely migrate into the central region of the tokamak, and the ionization processes of neutral atoms result in the effect of increasing the population and energy of plasma ions. Consequently, refueling in the steady-state tokamak operation can be achieved by the perfect recycling processes. Particles reflected on the wall or solid target plates are simulated by empirical formulas [12].

This physical model is applied to example calculations of edge neutral properties in a virtual tokamak device, which is based on the KT-2 conceptual design [13]. The input plasma parameters are provided from the EDGETRAN code [14], which is a two-dimensional edge plasma transport code previously developed in the authors' laboratory, and the spatial resolution in the Monté Carlo code has been established to validate the variation of plasma properties.

In Section 2, a simple physical model for a case of complete recycling by poloidal divertor plates is suggested and Section 3 describes a Monté Carlo scheme for neutral particle transport in the proposed model. Section 4 shows calculational results for a medium-sized tokamak with double-null poloidal divertors and its physical meanings are discussed.

2. Physical Modeling

2.1. Neutralization of Plasma Ions

In the core region of a toroidal plasma column with nested magnetic flux surfaces, plasma particles are transported to the peripheral region mainly by radial diffusion processes perpendicular to the magnetic field lines. Consequently they enter the scrape-off-layer(SOL) where magnetic flux lines intersect with neutralizing target plates such as poloidal divertors. Thus the fuel D-T ions flow toward the divertor plate along the magnetic field lines and when they get close enough to the plate surface, they are accelerated by the narrow sheath potential and collide with the plate. Eventually plasma ions are neutralized through recombination processes in the target plate. The number of plasma ions incident to the target plate equals the number of ions entering the sheath layer. Usually the thickness of a sheath region in front of the target surface is in order of a few Debye lengths, and the target surface and the sheath edge are assumed to be coincident with each other in the computational grids [14].

Assuming the sonic-flow($\overrightarrow{c_s}$) boundary condition at the sheath entrance, the total number Q of incoming ions per unit second is calculated as the product of the ion influx $n_i\overrightarrow{c_s}$ and the surface area $\overrightarrow{A_s}$ of the target plate :

$$Q=\int_A(n_i\,\overrightarrow{c_s})\cdot d\vec{A}\ . \tag{1}$$

The fraction of neutralized fuels returning to the edge plasma is almost unity in the steady-state operation of tokamak. Some of neutral particles are directly reflected as atoms, and the others which have been captured in the lattice atoms of the target surface are released in a molecular form with the energy of the plate temperature. These molecules are almost immediately dissociated into Franck-Condon atoms with about 4 eV energy [3].

2.2. Particle Interactions in Plasma

The neutral particles, atoms or molecules, suffer various kinds of interactions with plasma ions or electrons while migrating through the SOL area [2]. D or T molecules are almost instantly separated into Franck-Condon atoms after the desorption from the target plate under typical edge plasma conditions. Thus the main concern in the neutral particle transport becomes the transport of neutral atoms. Neutral atoms are considered to experience two major interactions with plasmas particles. One is charge-exchange reaction between neutral atoms and plasma ions, and the other is ionization of neutral atoms by colliding electrons, of which mechanisms are shown below :

Charge exchange : $D(T)^0+D(T)^+\rightarrow D(T)^++D(T)^0$

Electron impact ionization : $e+D(T)^0\rightarrow D(T)^+\ 2e$

2.3. Wall Reflection Model

It is known that, when a light particle such as deuterium or tritium collides onto a solid surface, the probability of direct reflection, which is called the particle reflection coefficient, is a function of the atomic masses of the incident and target materials and the incident angle and energy. An assumption of normal incidence of plasma ions onto the plate surface seems proper in this study due to the sheath acceleration near the surface. The particle(R_N) and energy(R_E) reflection coefficients are defined as, respectively,

$$R_N=\frac{N_{out}}{N_{in}}\ , \tag{2}$$

$$R_E=R_N\frac{\overline{E}}{E_0}\ , \tag{3}$$

where N_{in} and N_{out} are the numbers of incident and backscattered particles, respectively, E_0 is the incident particle energy, and $\overline{E}$ is the mean energy of reflected particles. They are usually obtained by empirical formulations from numerical simulations and measurements [12].

The direction of a reflected particle from the target surface depends mainly on its incident angle and energy. For normal incidence, the reflection angle has a cosine distribution around the normal direction if the incident energy is not too high.

However, the incident angle has little effect due to the roughness of surface material and is not taken into account in this simulation.

3. Monté Carlo Algorithm

3.1. Calculation of Non-Collisional Robability

In a plasma, the non-collisional probability, $\xi(x+dx)$, for a neutral particle moving a distance of $x+dx$ without interactions with other particles is expressed as

$$\xi(x+dx)=\xi(x)-\xi(x)\frac{dx}{\lambda(x)}, \tag{4}$$

where $\lambda(x)$ is the mean-free-path of a neutral particle for all kinds of collisions. The solution of this equation is given by

$$\xi(x)=\exp\left[-\int_0^x\frac{dx'}{\lambda(x')}\right]. \tag{5}$$

For a small distance of x, i.e., $\Delta\lambda$, Eq.(5) can be rewritten as

$$\xi_{\Delta\lambda}=\exp\left[-\frac{\Delta\lambda}{\lambda}\right] \tag{6}$$

by assuming that λ is kept constant during a short flight of $\Delta\lambda$.

Thus, the collisional probability after the flight of length $\Delta\lambda$ is $1\text{-}\exp(-\Delta\lambda/\lambda)$. For a *uniform random variate* ξ sampled radomly between 0 and 1, if $\xi<1\text{-}\exp(-\Delta\lambda/\lambda)$, it is believed that there has occurred a collision during the flight.

3.2. Particle Tracking

The Monté Carlo algorithm adopted in this numerical work is based on the SEURAT code [11], which is the earlier version of the DEGAS code. Fig. 1 depicts the algorithm of the particle tracking for one test flight particle. Initially a test particle is generated with a weighting ω represented as a ratio of the total number Q of ions incident on the plate to the total number N of test flights. The position where a test particle starts to fly is sampled according to the distribution of the ion influx onto the target plate, which is provided by a two-dimensional plasma transport code, EDGETRAN. Once a test particle is generated, it is moved by a small step length ($\Delta\lambda$) in a sampled direction and then it is checked if there occurs a collision using the collisional probability function, $1\text{-}\exp(-\Delta\lambda/\lambda)$, where λ is the total mean free path of the particle in a new position. The reaction cross-sections of charge-exchange and electron impact ionization are obtained from the thoretical formulas in other numerical studies [9,10] and used for calculations of local λ values. All the plasma properties such as density, ion temperature, and electron temperature are obtained by the EDGETRAN calculations. If a collision happens, it is supposed that the number of particles corresponding to the ionization fraction, ρ, of the test flight weight are ionized and the rest of the test particles undergo charge-exchange processes. This tracking method is called the *supressed absorption* technique and can reduce the standard deviations in a calculation significantly. Next continue the test flight with a new energy and a new direction assigned. Here, the ionization fractionrh ρ is defined by

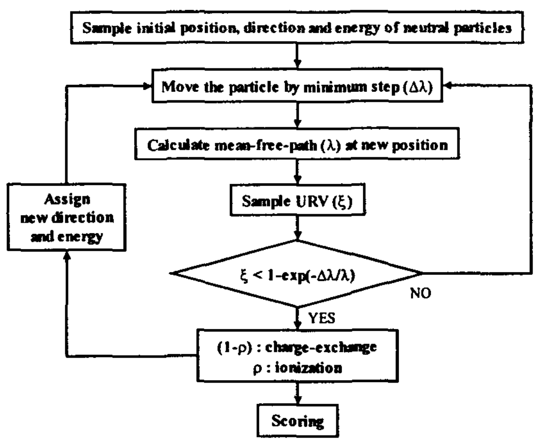

Fig. 1. Particle Tracking Algorithm for Recycling Neutrals in Monté Carlo Method.

$$\rho = \frac{\langle \sigma v \rangle_i}{\langle \sigma v \rangle_i + \langle \sigma v \rangle_{cx}}, \tag{7}$$

where $<\sigma v>_i$ and $<\sigma v>_{cx}$ are the ionization and charge-exchange rate coefficients respectively.

3.3. Scoring of Variables

The physical properties in the divertor region calculated from the Monté Carlo simulation are density, energy, and velocity of neutral atoms together with energy loss rate of the plasma ions by charge-exchange interactions, energy contribution of the ionizing neutrals, and reaction rates. Those variables are obtained in each grid cell as averaged values.

In the following, some example calculations are described. The total number of ionized particles in the j th cell is calculated from the reaction rate equation :

$$\sum_{k=1}^{N} \omega_i^{k,j} = n_0^j n_e^j \langle \sigma v \rangle_{ej} V_j \ , \tag{8}$$

where j, k, $\omega_i^{k,j}$, n_0^j, n_e^j, V_j, and $<\sigma v>_{ej}$, are grid cell index, test flight index, number of ionized particles, neutral density, electron density, cell volume, and ionization reaction rate coefficient, respectively. Among them, the only unknown is the neutral density. The neutral energy $\bar{E}_0^j$ is the average of ionized neutrals' energies E_0^{kj} :

$$\bar{E}_0{}^j = \frac{\sum_k^N E_0^{kj} \omega_i^{kj}}{\sum_k^N \omega_i^{kj}} \ . \tag{9}$$

The energy loss rate of ion by charge-exchange process is given by

$$\frac{\sum_k^N \omega_{cx}^{kj} (E^+ - E_0)^{kj}}{V_j} \ , \tag{10}$$

where E^+ is the energy of charge-exchanging ion, and the contribution of the ionized neutral energy produced by electron impact ionization is found from

$$\frac{\sum_k^N \omega_i^{kj} E_0^{kj}}{V_j} \ . \tag{11}$$

For these varables, it has not been yet quantitatively examined how the standard deviations from the true values are affected by computational factors. But it is known that generally the bigger flight number and the larger grid size reduce the standard deviations and ensure the improved reliability of calculations.

4. Results of Calculations

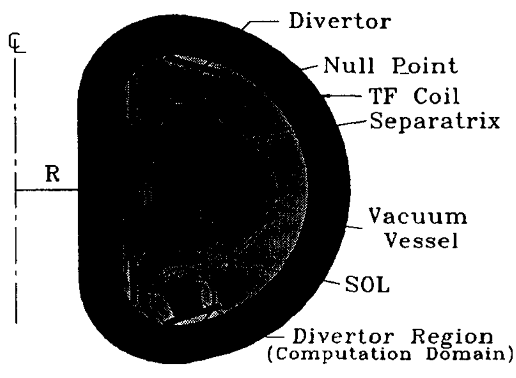

Fig. 2. A Schematic Diagram of the Poloidal Cross-section of a Double Null Tokamak.

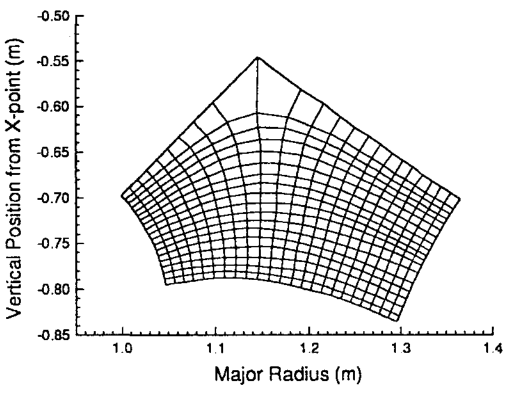

Fig. 3. A Mesh Configuration of a Typical Divertor Region Used in the EDGETRAN Calculations.

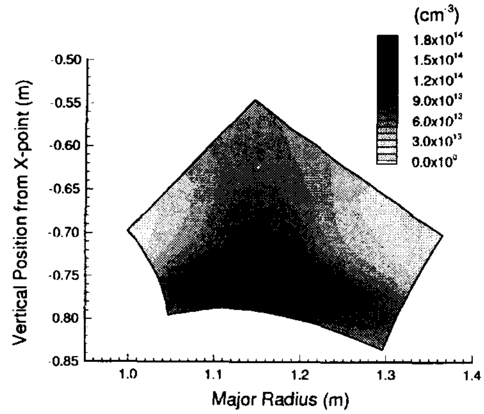

Fig. 4. Plasma Density Distribution in the Divertor Region.

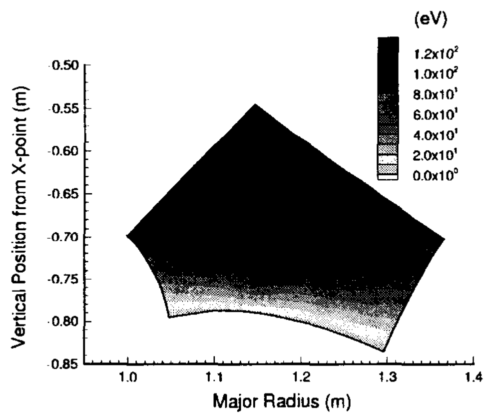

Fig. 5. Energy Distribution of Plasma Ions in the Divertor Region.

4.1. Input Plasma Field Distributions

Fig. 2 is a schematic diagram of the poloidal cross section of a double-null tokamak with poloidal divertors. The shaded area in a circle is the computational domain for a divertor region which is assumed to have an up-down and in-out symmetry. Its mesh configuration used in the EDGETRAN code is shown in Fig. 3. At each node of this mesh, the plasma fields are assigned with the values from EDGETRAN calculations and serve as input data for ambient properties in the present Monté Carlo simulation. Figs. 4-6 exhibit

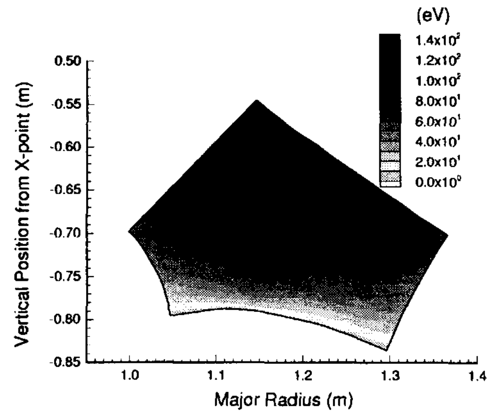

Fig. 6. Energy Distribution of Plasma Electrons in the Divertor Region.

the edge plasma field distributions for density and energies near a divertor plate of the KT-2-like tokamak and they show the characteristics of an attached plasma.

4.2. Calculated Neutral Particle Fields

The simulation has been carried out with 2×10^6 test flights and each test flight represents 1.56×10^{14} neutral particles since the total number of generated particles is 3.12×10^{20} per second and unit toroidal length (cm) in the present plasma condition. In general, the optimal number of test flights varies with the background plasma conditions and the grid cell size, but the test flight number of 2×10^6 taken in this simulation has given satisfactoy results in respect of both computational time and spatial smoothness.

Figs. 7 and 8 show the density and energy distributions of recycling D-T neutral atoms. The neutral density appears rapidly decreasing with the distance from the target surface due to severe ionization processes near the plate. The number of ionizing neutral particles depends on the plasma density and electron temperature in the SOL. In this case, the locally peaked plasma density distribution as seen in Fig. 4 seems to act as a kind of barrier that prevents neutrals from penetrating into the core plasma due to the very high ionization rate. In fact, a considerably large portion of neutral particles are ionized within a few cm from the divertor plate as shown in Fig. 7 and over 99.8 % of neutral particles are ionized within the edge region. The comparison of Fig. 8 with Fig. 5 indicates that the neutral energy distribution becomes similar to that of plasma ions since the charge-exchange neutrals exchange their energies with the ions. These resultant distributions of the neutral density and the energy turn out to be in good agreement with other similar calculations [15,16].

Figs. 9-11 show the distributions of neutral velocity vector, the ion energy loss rates by charge-exchange, and the energy contributions of ionized neutrals in the divertor region. The neutral atom velocity distribution in Fig. 9 indicates the fact that the neutral atoms are headed toward the core plasma in most of the edge region, which enables refueling by recycling neutrals. It is also notable that energy transfer by charge-exchange or ionization of the neutral particle is highly localized near the plate surface as appeared in Figs. 10 and 11, even though it may depend on the plasma conditions. The distribution of enegy transferred through the atomic processes gives information on the consequences of each interaction. It is expected that the energy transfer processes as a whole bring about the ion temperature drop so that a cold edge plasma can be ended up with. The ion energy generation rate of recycling neutrals is higher than the energy transfer rate through charge-exchange reactions over a large area in the vicinity of the divertor surface. In this case, the charge-exchange rate coefficient $<\sigma v>_{cx}$ is slightly higher than the ionization one $<\sigma v>_{ie}$ at the ion and electron temperatures of several tens eV. One possible reason for the low energy tranfer rate by charge-

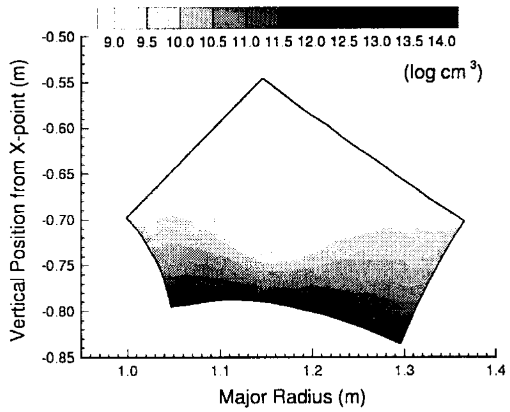

Fig. 7. Density Distribution of D-T Neutral Atoms in the Divertor Region.

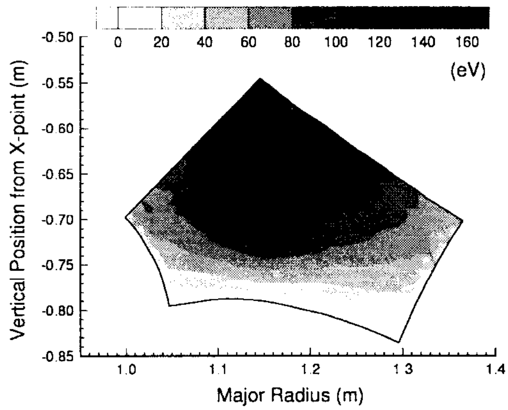

Fig. 8. Energy Distribution of D-T Neutral Atoms in the Divertor Region.

exchange interaction is that the collisional mean-free-path is so short near the target plate that almost every charge-exchange neutral produced after the first collision is supposed to move toward the plate to satisfy the boundary condition of sonic flow at the target and thus the charge-exchange neutrals mostly interact with low temperature ions near the plate surface. It is certain that the results will be changed if the plasma parameters have different values. For example, the charge-exchange region would be broader in a detached plasma condition.

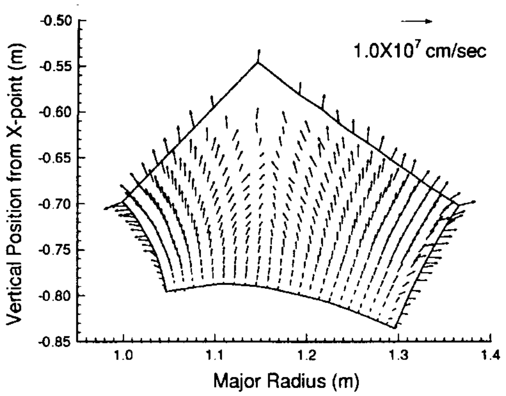

Fig.9. Velocity Vector Distribution of Neutral Atoms in the Divertor Region.

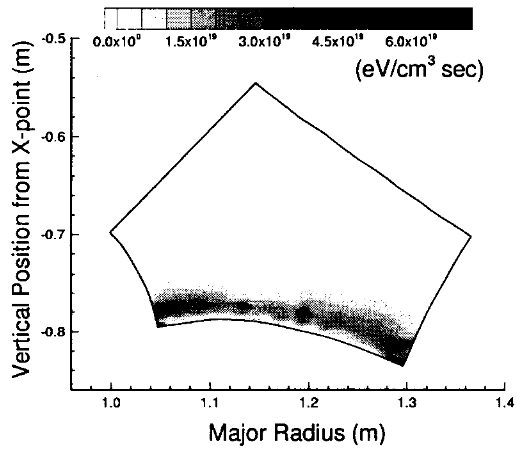

Fig. 10. Ion Energy Loss Rates by Charge-Exchange Processes of Fuel Ions in the Divertor Region.

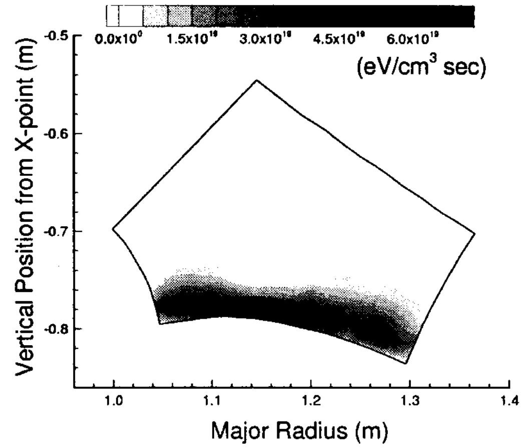

Fig. 11. Ion Energy Generation Rates of Recycling Neutrals by Electron Impact Ionizations in the Divertor Region.

It is also noticeable that two-dimensional computations can give information about the geometrical effects as well as the relationship of the neutral particle behavior with the plasma characteristics. With simple modifications accomplished, the developed Monté Carlo code can be applied to somewhat more complicated cases where, for example, the particle pumping or the whole tokamak area is taken into account. It depends on how the plasma properties can be realized in a Monté Carlo code.

5. Conclusions

A two-dimensional Monté Carlo simulation has been carried out and applied to a transport study of recycling neutrals within the poloidal divertor region of a double-null tokamak. Some physical quantities to explain the neutral atom behavior have been calculated under an edge plasma condition obtained from the EDGETRAN code. From the calculated results, the formation of dense and cold plasmas near the target plate is expected.

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