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Extension of IMPMC code toward time evolution simulation

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Abstract A self-consistent modelling of divertor plasma and impurity transport has been developed. The key feature of this integrated code, SONIC, is to incorporate the elaborate impurity Monte Carlo code, IMPMC. Monte-Carlo (MC) approach is suitable for modelling of interactions between impurities and walls, including kinetic effects, and the complicated dissociation process of hydrocarbons. The MC modelling, however, has the disadvantage for long computational time, large MC noise, and assumption of steady state. The first and second difficulties were solved by developing a new diffusion model and optimizing with a Message Passing Interface (MPI) on the massive parallel computer. The third subject is solved by extension of IMPMC code toward time evolution simulation. A time-dependent simulation with impurity MC code involves a problem to increase number of test particles. The particle reduction method to resolve this problem is newly developed and validated.

Keywords: Monte Carlo Modelling, Impurity transport, Divertor modelling, JT-60U

1 Introduction

The high heat load onto divertor plates is one of the most crucial issues for future fusion reactors. The remote radiation cooling is considered to be a most effective method for reduction of the heat load onto the divertor plates. To achieve enhanced radiation, it is necessary to establish the control method for impurity retention in the divertor region. Investigating the impurity and plasma transports, 2D multi-fluid divertor codes have been developed, e.g. B2 [1], EDGE2D [2], UEDGE [3], where the impurity transport is solved as fluid species. We have proceeded to another approach for impurity modelling [4]. Monte-Carlo (MC) approach is adaptable for complex divertor geometry and some physical processes in modelling [5]: interactions between impurities and walls/divertor, and kinetic effects can be easily included into the modelling. Furthermore, only MC model can practically deal with the complicated dissociation process of hydrocarbons [6]. Therefore, some elaborate Monte-Carlo impurity transport codes, e.g. DIVIMP [7], IMPMC [4], MCI [8], DORIS [9], have been developed to investigate impurity transport in more detail. In such a MC code, the impurity transport has been solved under fixed parameter of background plasma. For a consistent analysis, we develop a coupling of IMPMC code into a 2D divertor code (SOLDOR/NEUT2D) [10]. The unified code is called SONIC. This task is very difficult due to long computational time and MC noise. These difficulties were solved by developing a new diffusion model [11] and optimizing with a Message Passing Interface (MPI) on the massive parallel computer.

The SONIC code package consists of the SOLDOR code which solves the 2-dimensional fluid equations for plasma ion and electron (D^+, e), the NEUT2D code which solves the kinetic equations for deuterium neutral (D^0, $D_2{}^0$) with MC method, and the IMPMC code which solves the kinetic equations for impurity neutral and ions with MC method. The transports of plasma, neutral and impurity are solved iteratively. As initial simulations with this code, the dynamic evolution of X-point MARFE in JT-60U was investigated [11]. An IMPMC calculation was carried out every 0.1 msec, which corresponds to 100 steps of SOLDOR. In each IMPMC calculation, the impurities are traced till the carbon distribution reaches a nearly steady state. To reduce the MC noise, 50,000 test particles were employed for each of three carbon sources, i.e. physical and chemical sputtering at divertor plates, and chemical sputtering at the dome in the private region. Simulation results basically reproduced the dynamic evolution of X-point MARFE observed in JT-60U. It was found that the radiation near the X-point during MARFE originates in neutral carbons chemically sputtered from the private region.

In these simulations, we treated the impurity transport assuming a quasi steady state. Strictly speaking, this assumption is inadequate because impurity generation and transport are strongly affected by plasma parameter, and vice versa. Hence, we extend the IMPMC code so as to treat transient impurity behavior. In time-dependent simulation with MC code, a serious problem to increase number of test particles arises. It strongly depends on the impurity retention and the duration of simulation. The array size of variables to storage the information of test particles (charge state, position, velocity and statistical weight) cannot be determined in advance. Thus, an out-of-bounds reference may occur during running program and it leads to break execution of program. In other cases, simulations require unexpectedly long computational time. Therefore, it is necessary for the efficient simulation to suppress the number of test particles in MC calculation. The purpose of this paper is to propose a new particle reduction method and validate it.

2 Monte Carlo scheme

We solve the kinetic equations with the Coulomb collision operator for the distribution functions of impurity ions $f_z(\mathbf{r},\mathbf{v},t)$ using the orbit following Monte Carlo technique. The IMPMC code includes the following processes: (1) impurity generation, (2) ionization of sputtered neutrals, (3) parallel motion along the field line, (4) Coulomb scattering, (5) anomalous diffusion across flux surfaces, (6) atomic processes and (7) scoring for impurity density. Here we explain the two processes introduced for a time-dependent simulation.

2-1. Scoring for impurity density in transient state:

Test particles are emitted from the divertor plates every typical transient time ΔT= 0.1 msec. The number of emitted particle (n_{emit}) is typically 500 in each processor. The number of processor used in calculations is N_{PE} = 30. The total particle number is N_{emit} = 500 × 30 PE = 15000. When some of them return to the plates by the friction force, their tracks are terminated, as they are absorbed at the plates or walls. At present, the self-sputtering process is not treated. Using track-length estimator method, the impurity density is calculated during ΔT, as expressed by

$$n_j = \frac{\Gamma_0}{N_{emit}} \cdot \frac{1}{V_j} \sum_k \omega_k \cdot \tau_k^j , \qquad (1)$$

where τ_k^j is the time for particle k to pass through cell j, V_j the volume of cell j, $\omega_k = \Gamma(t)/\Gamma_0$ the statistical weight, $\Gamma(t)$ the amount of sputtered impurity at t and Γ_0 the reference value.

2-2. Reduction of test particles:

As simulation proceeds, most of test particles exist in the main plasma (see broken lines in Fig.2 (a)), and the density of impurity ion there is uniform in poloidal direction. Excessive test particles in the main plasma are unnecessary. Particle reduction is, therefore, performed for C^{6+} particles in the core region (r/a < 0.95). The process consists of 3 steps as shown in Table 1; sorting of weight, pairing and Russian roulette. We illustrate this scheme concretely. The main plasma is divided into 31 zones (Fig.1). The number of test particles of C^{6+} in the zone i is assumed to $n_{i\text{-zone}}$ = 203. It exceeds a maximum number of n_{max}=200, which is specified as input parameter.

Table 1 Monte Carlo scheme to reduce test particle number in core plasma. It illustrates the procedure when 3 particles are terminated. Symbol of w95 represents the weight of the 95th particle.

sorting particle by weight												$n_{i\text{-zone}}$ = 203,	n_{max} = 200		
	1	2	3	4	5	6	7	8	9		199	200	201	202	203
	w95	w21	w52	w203	w115	w160	w145	w176	w146	.....	w36	w60	w68	w23	w5
pairing															
Russian roulette			X		X	X		(X : terminated)							
w95 => w95+w160, w160 => 0, w21 => w21+w115, w115=>0, w52 => 0, w203 => w203 + w52															
	$w95^N$	$w21^N$	0.0	$w203^N$	0.0	0.0	w145	w176	w146	.....	w36	w60	w68	w23	w5

Then, 3 particles should be terminated. Sorting by weight and pairing are necessary to level weight. Russian roulette decides which particle to be terminated. The weight of the terminated particle is added to that of survival particle. To avoid the communication between processors, the particle reduction is applied independently for each processor. The plasma parameter and the impurity density have a poloidal asymmetry in the edge (0.95 < r/a < 1.0). Therefore, the particle reduction cannot be applied in this region.

3 Simulation results

The initial simulations were carried out for the typical discharge of the JT-60U (I_p=1.5MA, B_T=3T, P_{NB}=5MW) with the SONIC code package [11]. The computational mesh is shown in Fig.1. In these simulations, an attached plasma was obtained in a steady state before a strong gas puffing. After a gas puffing, the plasma was changed from the attached to detached plasma, and finally an X-point MARFE occurred. Such evolution of the radiation profile was similar to that observed in JT-60U experiment.

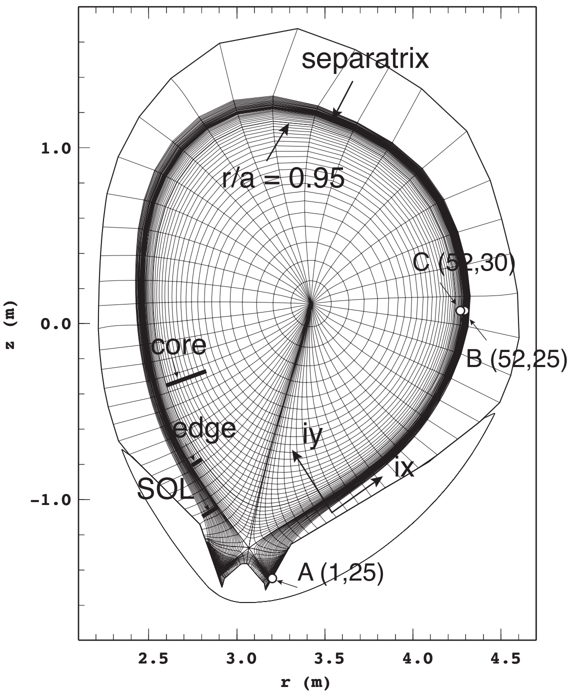


Fig. 1 Computational mesh. The edge (0.95 < r/a < 1) and the core region (r/a < 0.95) is divided into 10 and 21 zones, respectively. The carbon density at the cells denoted by A, B and C are shown in Fig. 3 and 4. Each zone consists of 60 cells.

Using the plasma parameter in this attached plasma, the simulations for physical sputtering of carbon impurity are carried out with the extended IMPMC code. Since the purpose of this paper is to validate the particle reduction method, the back ground plasma parameter is fixed throughout the simulations. For simplicity, the impurity neutrals and ions are assumed to be absorbed at the plates and walls. The total amount of carbon impurity sputtered is 1.7×10^{21} 1/s. 500 test particles are emitted from divertor plates every $\Delta T = 0.1$ msec in each processor and the particle number of C^{6+} ions which exist in a zone (r/a < 0.95) is limited to $n_{max} = 200$. Figure 2 (a) shows the total number of test particles among the processors in the divertor, SOL, edge (r/a > 0.95) and core region (r/a<0.95). The number in the divertor is multiplied by 20 because it is too small. Solid lines represent for the case with the reduction method turned on, and broken lines represent for the case turned off. Without the particle reduction, total particle number increases with time and reaches 1.1×10^{6} after 70 msec. On the other hand, the reduction method reduces the total particle number to 0.36×10^{6} and keeps it in time.

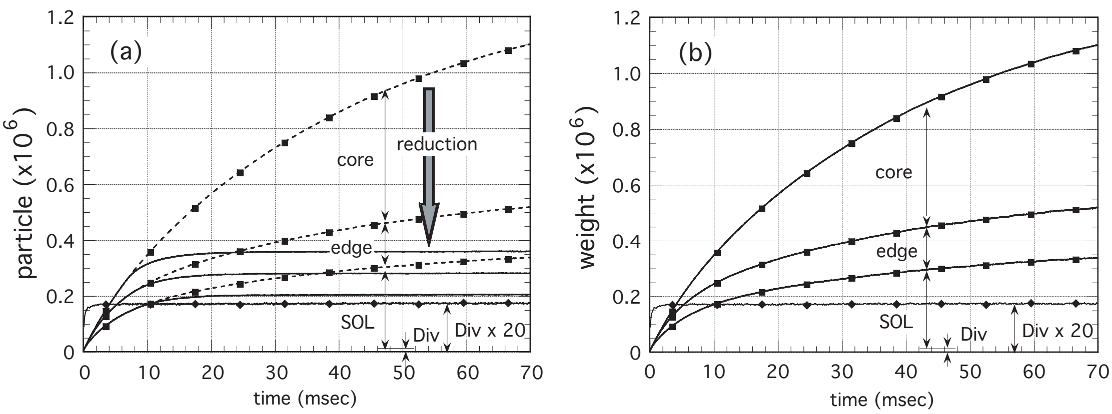


Fig. 2 (a) Time evolution of particle with (solid lines) and without (broken lines with symbols) particle reduction. (b) Time evolution of total weight with (solid lines) and without (symbols) particle reduction.

Thereby, the computational time to require the trace during $\Delta T= 0.1$ msec is reduced from 9.4 sec to 3.1 sec. The total weight in each region is unchanged as shown in Fig. 2 (b). It means that the reduction method has no influence on the global quantities. The steady state in the divertor region is obtained within 1 msec, but the impurity density in the main plasma arrives at a steady state after 200 msec, which is confirmed in another simulation with $n_{emit} = 200$.

We also verify the local value of radiation and impurity density in 3 cells, which are located in different regions, i.e. outer divertor, SOL and the edge. The radial index of iy=25 indicates the flux tube nearest to the separatrix surface in the SOL. Figure 3 shows that the local value is unchanged whether the reduction method is turned on (solid lines) or off (symbols), because the recombination process has little effect on the C^{4+} density in the SOL of the attached plasma. The total particle number of C^{4+} in SOL region is reduced by only 0.5%. The MC noise in the radiation and the impurity density at the strike point is not so high to prevent from getting the converged solution in SOLDOR. The particle reduction is applied for C^{6+} particles inside the zone with iy=35.

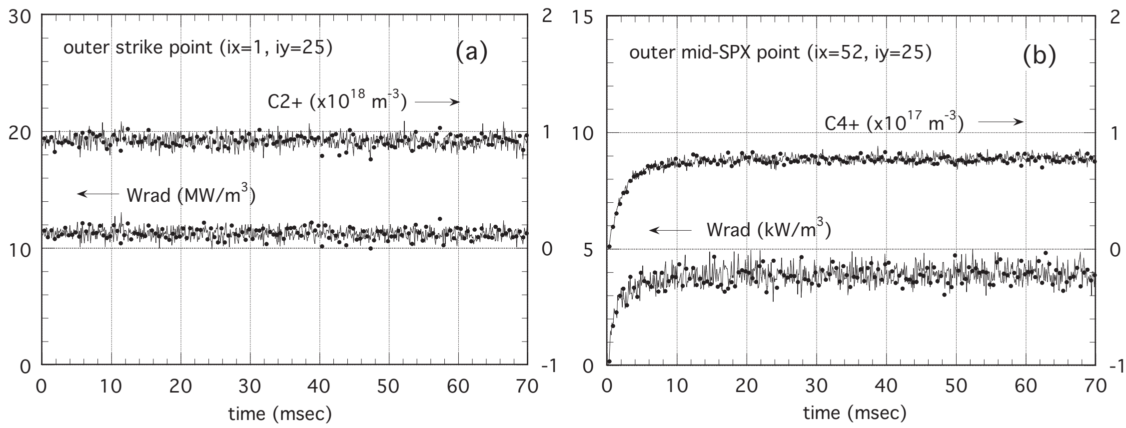
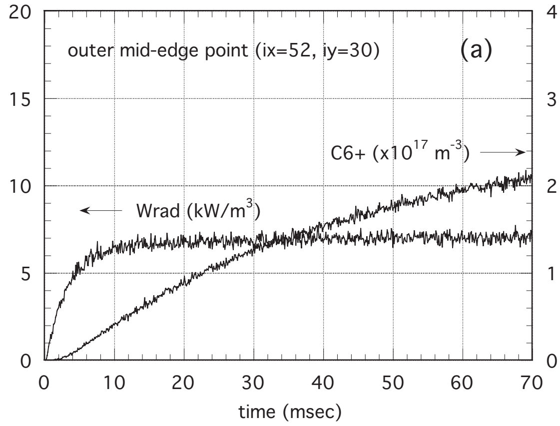


Fig. 3 Time evolution of radiation and impurity density (a) at the outer strike point (indicated by A in Fig.1) and (b) at the outer mid-plane (indicated by B). Solid lines: with particle reduction method, symbols: without.

Figure 4 shows radiation and C^{6+} density in the cell of the edge. By decreasing the particle number, it leads to increase the variance in the impurity density as a nature in MC calculation. However, the MC noise remains in a permissible level. To exhibit the significance of the sorting by weight, the unusual particle reduction method where pairings are chosen randomly are applied. As shown in Fig. 3(c), the noise is very large compared with the normal method (Fig. 3(b)). The normalized standard deviations of C^{6+} density from 60 msec to 70 msec are σ_a=2.0%, σ_b=6.5%, σ_c=16% for the case of (a), (b) and (c), respectively. The factors of σ_b/σ_a=3.2 and σ_b/σ_a=7.8 are not correspondent to the ratio of $1/\sqrt{(N_b/N_a)}$ $=1/\sqrt{(N_c/N_a)}$=2.2, where N is the total particle number in the zone with iy=30. The distribution of the frequencies of particle weight at 70 msec is shown in Fig. 5. The normal reduction method limits the maximum weight to 22, while the random choice of pairing produces a few test particles with very heavy weight which are irregular in size from 50 up to 417. In a cell, there exists at most one or two of such “monster” particles. When a monster particle passes through a cell or enters into a cell, the large noise in the impurity density appears. In order to suppress MC noise associated with particle reduction, the pairing after sorting by weight is essential.



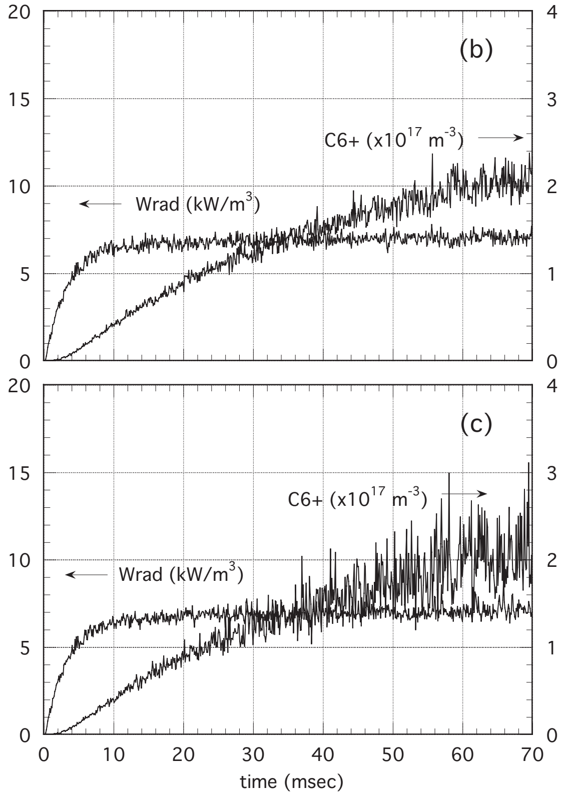


Fig. 4 Time evolution of radiation and impurity density at the edge point. (indicated by C in Fig. 1.) (a): wihtout, (b) with normal particle reduction method, (c): with particle reduction method where paring are chosen randomly.

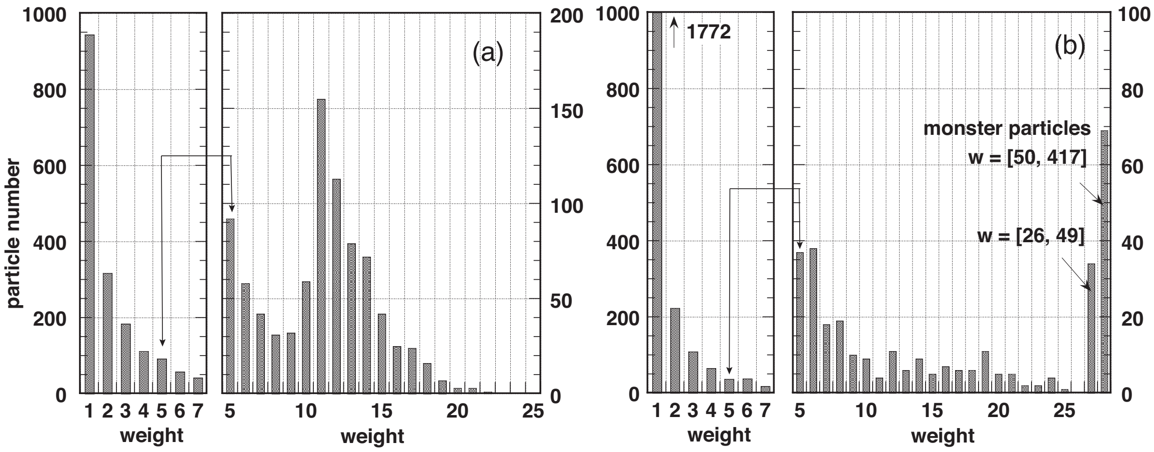


Fig. 5 Distribution of frequencies of particle weight at 70 msec. (a) : with standard particle reduction method, (b) : with particle reduction method where pairing are chosen randomly.

4 Summary

As a self-consistent modelling of divertor plasma and impurity transport, the SONIC code package has been developed. The key feature of this integrated code is to incorporate the impurity Monte Carlo code, IMPMC. In this code, the impurity transport is solved under the assumption of steady state, which is common in MC modelling. However this assumption is questionable due to strong interactions between impurity and plasma. Thus we extend the IMPMC toward time evolution simulation. In time-dependent simulation with MC code, a serious problem to increase number of test particles arises. In this paper, we propose the particle reduction method where the process consists of sorting of weight, paring and Russian roulette. Sorting of weight is indispensable to suppress the MC noise. Our future work is to clarify the kinetic effect on the impurity transport and investigate the impurity retention in the divertor region with the SONIC code coupled with the extended IMPMC. So far, the divertor configuration in JT-60SA has been optimized from a viewpoint of the neutral recycling with SOLDOR/NEUT2D [12]. It will be optimized from a viewpoint of the impurity control with the SONIC code package in the near future.

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