Test particle modelling of impurity collisional transport in tokamaks

Zh.S. Kononenko[1], Ye.O. Kazakov[2]

[1] *Independent Scholar; E-mail: kononenko.zhanna@gmail.com*

[2] *Department of Applied Physics, Chalmers University of Technology, Euratom-VR Association, Göteborg, Sweden*

Introduction The test particle modelling is widely used in fusion research to study the transport processes. With this method one can evaluate the radial diffusion coefficients [1], estimate the heat loads on different plasma-facing components, determine the poloidal and toroidal distributions of fast ion and runaway electron losses, study the toroidal field ripple induced transport, etc. In contrast to any analytical theory (such as the neoclassical theory or the drift kinetic equation [2]), the test particle modelling is a direct numerical method, which does not rely on any approximations for the Larmor radius of the particle, the aspect ratio of the machine or the poloidal magnetic field. The price paid for such an intrinsic simplicity is that the test particle modelling commonly involves very intensive CPU calculations.

In this work we describe a numerical code which evaluates the diffusion coefficient of monoenergetic test particles (impurities) in the tokamak geometry. The full orbit integration of particle motion is accompanied by the Monte Carlo collision operator, which scatters both the pitch and the gyro angles of the particle. As an application of this method, we discuss how the magnetic islands produced by the resonant magnetic perturbations (RMP) affect the collisional transport of impurities [3].

Numerical method Test particle codes used for transport studies usually consist of two basic modules. The first module describes the deterministic motion of particles in the given magnetic configuration. Usually the particle trajectory integration module involves the use of the guiding center equations. The effect of particle gyrorotation can often be neglected, which results in a substantial reduction of the CPU time needed to trace a particle. Unfortunately, for some problems of interest this approximation cannot be applied; then, one has to solve the full orbit equations of motion. Such an approach should be used, for example, for studying the dynamics of alpha particles and fast ions with large Larmor radius. Recently, this approach has been actively used for calculations of particle transport in spherical tokamaks. For spherical torii the inverse aspect ratio and the poloidal magnetic field are no longer small parameters, thus the fundamental approximations of the neoclassical theory cannot be applied.

The full orbit equation of motion for a particle under the influence of the Lorentz force is solved in the quasitoroidal system of coordinates (r,θ,φ), where r is the radial coordinate, and θ and φ are the poloidal and toroidal angles, respectively. We consider a simplified tokamak magnetic configuration with circular magnetic surfaces

$$\vec{B} = \frac{B_0 R_0}{R}\left[\vec{e}_\varphi + \frac{r/R_0}{q(r)\sqrt{1-(r/R_0)^2}}\vec{e}_\theta\right], \quad (1)$$

where $q(r)$ is the safety factor (see, Fig. 1), and $R = R_0 + r\cos\theta$.

The second module of the code describes the stochastic scattering of test particles due to the Coulomb collisions with background plasma species. Usually the Monte Carlo equivalent collision operators are used, which change randomly the velocity of the particle after each time step of the integration procedure. In calculations based on guiding center equations it is sufficient to use a collision operator that changes the pitch angle of the particle only [1]. However, for the full orbit modelling an implementation of the scattering of both of the particle pitch angle and the gyro phase is needed. A Monte Carlo collision operator suitable for the exact trajectory integrators was derived by Boozer in Ref. [4]:

$$\vec{\mathrm{v}}_n = (1-\nu_\mathrm{d}\Delta t)\,\vec{\mathrm{v}}_0 \pm \sqrt{(1-0.5\nu_\mathrm{d}\Delta t)\,\nu_\mathrm{d}\Delta t}\,(\vec{\pi}_0 \pm \vec{\tau}_0)\mathrm{v}_0, \quad (2)$$

where $\vec{b}$ is the unit vector along the magnetic field; $\vec{\mathrm{v}}_0$ and $\vec{\mathrm{v}}_n$ are the velocities of the particle before and after the scattering, respectively; $\vec{\pi}_0 = \vec{b}\times\vec{\mathrm{v}}_0/|\vec{b}\times\vec{\mathrm{v}}_0|$ and $\vec{\tau}_0 = \vec{\pi}_0\times\vec{\mathrm{v}}_0/\mathrm{v}_0$ are two unit vectors perpendicular to $\vec{\mathrm{v}}_0$. Here, ν_d is the collision (deflection) frequency and Δt is the integration time step, which is chosen to satisfy $\nu_d\Delta t \ll 1$. The full orbit Monte Carlo collision operator uses two random numbers for each particle at each time step. The sign plus or minus in Eq. (2) should be chosen randomly, but with equal probabilities. The collision operator given by Eq. (2) ensures that after sufficiently long time particle spends equal time at all values of the pitch and gyro angles. The deflection frequency to be used in the collision operator is given in Refs. [1–3].

In order to evaluate the radial diffusion coefficient, the full orbit equations of motion are solved for the monoenergetic ensemble of $N = 1000$ particles, applying at each time step velocity scattering according to Eq. (2). All particles evolve independently from each other. They start their motion from the flux surface where $q = 2$ $(r_0/a \approx 0.604)$. The initial poloidal and toroidal angles of each particle are distributed randomly, as well as the velocity components. The statistical properties of the ensemble are evaluated by means of calculating the mean-square displacement, $C_2(t) = <(r_i(t) - <r(t)>)^2>$, where the brackets denote the average over the particles in the ensemble.

The diffusion coefficient is defined as the time derivative of the mean-square displacement, $D(t) = (1/2)(\mathrm{d}C_2/\mathrm{d}t)$. The temporal dependence of C_2 defines the type of the diffusion process. For normal diffusion processes the mean-square displacement increases linearly in time. Figure 2 shows a typical dependence of $C_2(t)$ for the ensemble of W^{28+} ions

with the energy E =1 keV. The integration time in our simulations is chosen to be 10 collision times, which equals to 3 ms for the parameters considered. As follows from Fig. 2, for time intervals smaller than the mean time between the collisions there is a ballistic phase when $C_2(t)$ varies quadratically in time. Then, the collisional effects start to dominate and the normal diffusion is observed. The diffusion coefficient is calculated as a slope of the curve for the mean-square displacement. Fitting the curve by the least-squares method, we find that the relative accuracy of the D coefficient estimated in this way is ~ 10%. The accuracy of D evaluation can be improved by increasing the number of particles used in the modelling. The obtained results are in a fair agreement with the results of the neoclassical theory [3].

Effect of RMP on collisional transport of impurities We have used the full orbit test particle code to study the effect of RMP on the collisional transport of impurities. RMP are actively studied in view of the perspective of their use for ELM active control and suppression [5]. The additional coils producing a perturbation to the equilibrium magnetic field are installed on many tokamaks and stellarators. In theoretical studies the magnetic field perturbation can be introduced as $\delta\vec{B} = \vec{\nabla}\times(\alpha\,\vec{B}_0)$, where the scalar function $\alpha = \alpha(r,\theta,\varphi)$ (which has the physical dimension of length) defines the structure of the perturbed magnetic field. For the present study we consider a single harmonic perturbation of the form

$$\alpha(r,\theta,\varphi) = \alpha_{00}\, \mathrm{e}^{-(r-r_{\mathrm{res}})^2/\Delta_{\mathrm{res}}^2} \sin(m\theta - n\varphi)\,. \qquad (3)$$

This perturbation produces a chain of m magnetic islands with a center at the rational magnetic surface $r = r_{\mathrm{res}}$, where $q = m/n$. The magnetic perturbation of the form (3) produces only a single chain of the magnetic islands avoiding the formation of the satellite islands. We focus our attention on the effect of the $m = 2$, $n = 1$ perturbation.

The radial width of the magnetic islands is controlled by the RMP amplitude, α_{00}. The perturbation with the normalized amplitude $\alpha_{00}/a = 10^{-4}$ produces the magnetic islands having a width approximately 10% of the plasma radius.

Figure 3 shows the dependence of $C_2(t)$ calculated for tungsten impurities for different perturbation amplitudes. The lowest curve corresponds to the case of the plasma without magnetic islands. As expected, an increase in RMP amplitude results in greater radial excursions of particle orbits and hence larger diffusion coefficient. The observed diffusion is normal in all cases since the collisions are rather frequent. For the regimes of reduced collisionality the radial particle transport under the presence of the magnetic islands can exhibit sub-diffusive or non-diffusive behavior.

Figure 4 summarizes the obtained results. It shows how the diffusion coefficient for tungsten impurities depends on the RMP amplitude. Under the assumption that the characteristic radial displacement of the particle is simply proportional to the island width, the

curve in Fig. 4 should be linear in α_{00}. However, the observed curve shows a more complex quadratic dependence of the diffusion coefficient on the RMP amplitude. For the case when the island width is 15% of the plasma radius the diffusion coefficient for W^{28+} ions increases by a factor of 8 with respect to the case without perturbation.

Conclusions A numerical method to evaluate the radial diffusion coefficient of test particles is presented. The Coulomb collisions of test particles with the background plasma are modelled by an equivalent Monte Carlo collision operator, which scatters both the pitch and the gyro angles of the particle. Diffusion coefficients obtained from numerical simulation are in a fair agreement with the results of the neoclassical theory. It is shown that the collisional impurity diffusion can be significantly enhanced by the RMP.

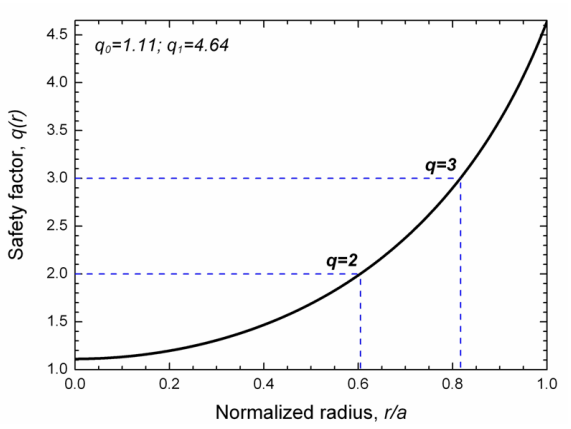

Figure 1. The safety factor profile, *q(r)* used in the simulations ($q_0 = 1.1$, $q_1 = 4.6$).

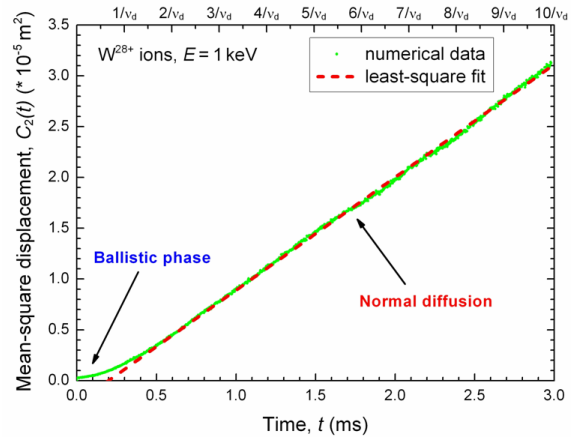

Figure 2: Typical temporal dependence of the mean-square displacement, $C_2(t)$ for the ensemble of $N = 1000$ tungsten ions with the energy $E = 1$ keV.

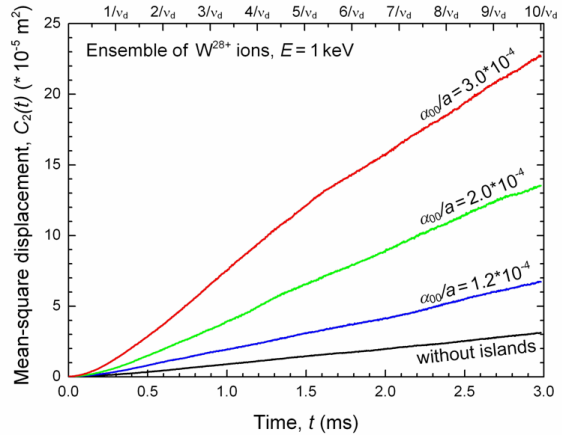

Figure 3: The temporal dependence of the mean-square displacement, $C_2(t)$ for different RMP amplitudes.

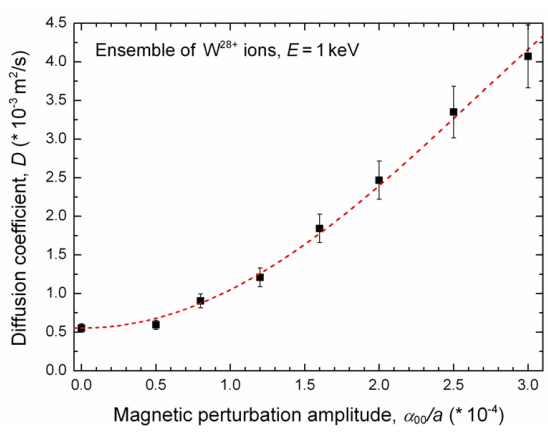

Figure 4: The radial diffusion coefficient for W^{28+} ions as a function of the magnetic perturbation amplitude.

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