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ScienceDirect
Journal of Nuclear Materials 363–365 (2007) 1061–1065
journal of nuclear materials
www.elsevier.com/locate/jnucmat

Numerical simulations of plasma wall interactions for ITER

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Abstract

At the ELMy H-mode of ITER repetitive transient processes may cause wall material vaporization and subsequent contamination of the confinement region. The magnetic configuration relaxing to the stationary confinement may significantly change the load distribution over the vessel surface. The plasma flux to the wall causes back fluxes of atoms into the confined plasma. The work is concerned with recent progress in the implementation of plasma wall interactions for the new tokamak equilibrium code TOKES that aims at the transient regime, taking ITER as most challenging target for future applications of the code. The modelling for a carbon surface and coupling of wall emitted fluxes with the confinement plasma are explained. The surface obeys the toroidal symmetry, being of arbitrary poloidal cross-section shape. Heat transport in the wall, surface evaporation, propagation of vaporized atoms in the vessel volume and ionization of wall atoms are implemented. Preliminary results are obtained.

PACS: 28.52.−s; 52.55.−s; 52.55.Fa; 52.40.Hf

Keywords: Plasma–material interaction; Divertor; First wall

1. Introduction

In the tokamak ITER, high heat depositions up to 3 MJ/m^2 [1] on the time scale ~0.3 ms may cause wall material vaporization and subsequent contamination of plasma. The magnetic field varies, changing the separatrix strike position on the divertor surface. The most damaging wall scenarios have been simulated with the code FOREV [2]. However, FOREV allows only the simulation of rather short processes (a few ms) in a fixed magnetic field configuration. It cannot handle the propagation in the vessel of neutral atoms. Therefore for elaborated modelling a new code TOKES (Tokamak Equilibrium and Surface processes code) is being developed. Earlier activities concerned the implementation of the confined plasma [3]. In this work wall-relevant issues are reported.

The vessel's wall obeys toroidal symmetry. The wall material graphite is implemented so far. In the poloidal cross-section, the surface is approximated with cone segments. Due to the same algorithm for each wall segment, uniform calculations for the whole surface are achieved including the

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doi:10.1016/j.jnucmat.2007.01.140

divertor, the dome and the main wall. For modelling the neutral particles (atoms, photons and neutrons) the Monte-Carlo method is applied. They are spread over the volume as random beams localized in specified solid angles, for instance the wall emitted atoms in 2π steradians (half-isotropic).

Section 2 explains the implementation of sputtering, scattering and sticking of plasma particles and wall heat transport including surface evaporation. Sections 3 and 4 are dealing with the propagation of neutrals through the vessel by means of special triangle meshes over the poloidal plane. The magnetic surfaces are constructed as chains of line segments situated in the triangles, which provides optimal coordination of the neutrals and the plasma. Section 5 presents first simulation results.

2. Implementation of wall processes

2.1. Particle fluxes between the plasma and the wall

All ions arriving at the wall during one time step are assumed to recombine at the surface. They and other arriving atoms are collected as computer data with regard to their numbers and the energy they brought with, separately for each kind of atom and wall segment. The recombination energy is added to some data item Q_w that accumulates the heat absorbed in a wall segment; the incoming electromagnetic radiation is also added to Q_w.

The neutrons released in the fusion reaction are assumed to penetrate through the surface. They are counted as a separate data item for each wall segment. Originally intended for future estimations of material damage and heating, the neutron statistics already became useful in particle conservation checks to ensure correct calculations, for which the code sums the counted neutrons with the nucleus neutrons of collected atoms and plasma ions, and subtracts the ones of fuelling beam atoms and the atoms emitted by the wall.

The atoms of some kind accumulated during a time step τ either stick in the wall or elastically scatter from it. However, at first their energy collector value is divided by the collected number in order to obtain the averaged impact energy E_a, which is used for the calculation of the sputtering yield Y taken from Ref. [4, p. 166]. The sticking atoms remain in their classes, to allow for re-deposition. Their summed-up impact energy is added to the wall heat Q_w, along with the sublimation energy.

2.2. Heat transport in the wall

The striking particles may produce significant wall heating up to the vaporization threshold thus also producing atoms emission. The temperature $T(t,x)$ is described with one-dimensional heat conduction equation as a function of time t and the local depth x:

$$c\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + W. \tag{1}$$

The boundary conditions are $k(\partial T/\partial x)|_{x=0} = -q_0$ and $T(x_c) = T_c$. A temperature T_c of a cooling equipment in the bulk at some depth $x = x_c$ is assumed. The heat capacity c and the thermal conductivity k are some given functions of T taken from the heat conduction code MEMOS [5]. W is a volumetric heating term due to eddy currents and stopping of the neutrons, and the surface heat flux $q_0 = (Q_w - N_{vap}E_{subl})/\tau S$, where N_{vap} is the number of wall material atoms vaporized during the time step and S the area of the surface segment. Eq. (1) is numerically solved by approximation with an implicit conservative finite-difference scheme.

The vaporized number N_{vap} of carbon atoms is calculated using MEMOS data on saturated vapour pressure $p_{sat}(T_s)$ as a function of surface temperature T_s. The vapour amount is obtained by $N_{vap} = (1/4)n_{vap}v_T S\tau$, with the surface vapour density $n_{vap} = p_{sat}/T_s$, and the averaged velocity of vaporized atoms $v_T = (8T/\pi m)^{1/2}$. The energy $N_{vap}E_{subl}$ taken off at a time moment t_0 cools pre-surface meshes, which can cause a significant drop of q_0 and thus T_s at a large τ. As p_{sat} depends strongly on T_s, at the moment $t_0 + \tau$ the drop of T_s would drastically decrease N_{vap}, which at $t_0 + 2\tau$ can cause N_{vap} getting much larger than that at t_0. To overcome this numerical instability, a simplified energy balance equation for only the first few meshes is solved before each time step in order to adjust T_s and N_{vap} to each other, assuming the same temperature T_s of these meshes, and only afterwards Eq. (1) is processed. The vaporized atoms are emitted with the energy $(5/2)T_s$.

3. Neutral beams and magnetic surfaces modelling

The toroidal symmetry of the distribution of atoms emitted from the wall surface allows the reduction of calculations to one starting toroidal angle ζ. Simulation for one straight trajectory that starts at $\zeta = 0$ and stretches into the vessel

(representative ray) describes the whole symmetric set of the trajectories parameterized by ζ. A ray either stretches until full absorption in the plasma or penetrates the vessel striking the opposite wall. TOKES simulates a real fuelling beam injected through a window in the surface also as if the beam would be symmetrically spread over ζ. For the plasma absorption this assumption is adequate, because due to the high thermal velocity of plasma particles the real beam produces negligible non-homogeneity of plasma along each magnetic surface, thus interacting with the plasma like the spread beam (the typical electron temperature non-homogeneity is estimated as $\Delta T_e/T_e \sim 10^{-9}$). However, the damage the real beam may cause to the opposite wall is localized on the toroidal angle thus destroying the symmetry, but in ITER full absorption of the beam in the plasma will be achieved.

The numbers N_a and energies E_a of the atoms to be emitted from each wall segment are in advance accumulated as data pairs $(N_a, N_a E_a)$, separately for the scattered, sputtered and vaporized atoms. When N_a exceeds some given minimum value, or the accumulation period exceeds some given maximum time, the next ray of N_a atoms in the ground state of their bound electrons and with kinetic energy E_a per atom is produced. The corresponding data pair is then zeroed, and a new accumulation cycle starts. After many emissions the half-isotropic ray's distribution is achieved at each wall segment. The values of N_a and $N_a E_a$ should be as small as

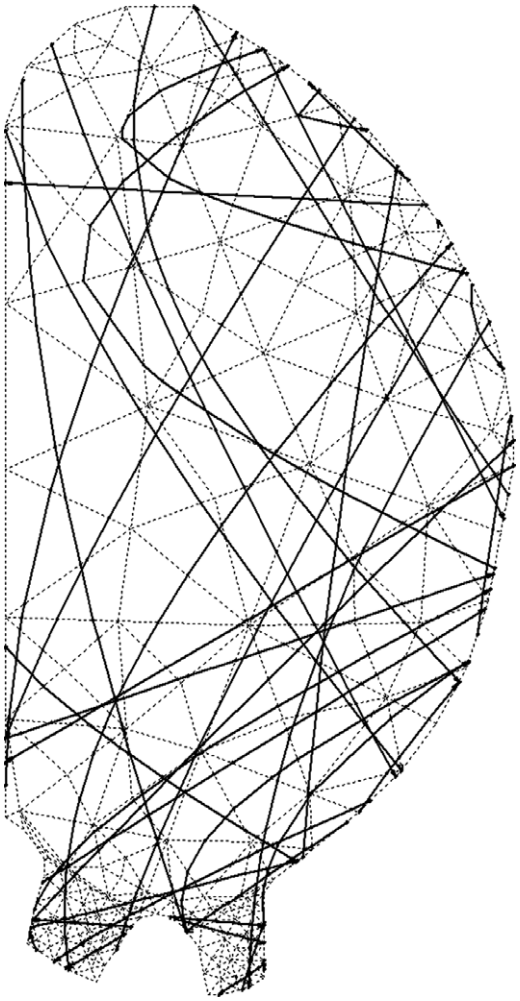

Fig. 1. ITER poloidal plane with typical rays (solid curves) representing neutrals (atoms and neutrons) or photons on the triangle mesh (dashed lines). The mesh sizes follow the local density of given wall segments.

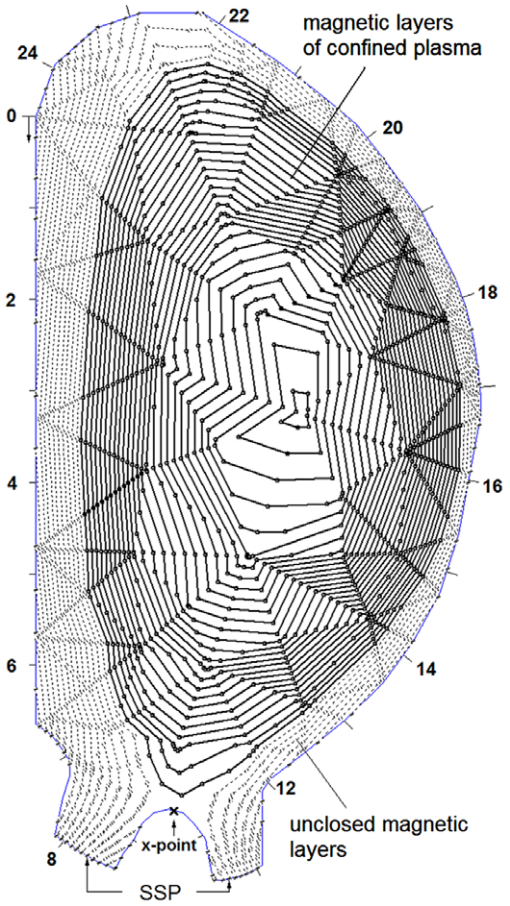

Fig. 2. The poloidal cross-section of magnetic layers. The solid closed curves indicate the layers filled with confined plasma. The thin unclosed curves indicate the layers containing SOL plasma of a small density. The lost plasma strikes the surface mainly at the separatrix strike points (SSP). The numbers around the boundary mark (in metres) the wall coordinates.

available computer speed allows (presently $N_a = 10^{17}$ and $N_a E_a = 1$ J are chosen).

For an appropriate description of the rays and their crossing with the confined plasma, TOKES produces two overlapping meshes in the vessel, one for the rays, and the other for the plasma. For the rays, adjoining toroidal cells with triangular poloidal plane cross-sections are generated covering the whole vessel volume (see Fig. 1, dashed lines). The straight rays seen in the figure as the solid curves approximated with the chains of lines cross those cells.

The plasma in TOKES is assumed to be distributed over another set of line chains ('magnetic layers') that follow the magnetic surfaces. An example configuration obtained with TOKES is shown in Fig. 2. Like the ray lines, the lines of magnetic chains are also ending at the triangle sides. Thus the magnetic layers are also constructed of cone segments. This structure provides optimal coordination of the rays and the plasma. The poloidal magnetic flux w is calculated only at the triangle nodes, and linear interpolation is employed for getting $w(r,z)$ at either r and z, providing a unique set $\{k\}$ of magnetic layers with different constant magnetic flux values w_k.

4. Realization of interaction of neutrals with plasma

The interaction of atoms of mass m_a with the plasma is calculated sequentially along the ray, triangle by triangle. The interaction algorithm is as follows. The lines of the contours k crossing the triangle are prescribed with the fractions s_k of triangle's area s proportionally to the line length, so that the triangle is distributed over the contours: $s = \sum_k s_k$. Initially the path l across the torus of this triangular cross-section is calculated, then the traversing time $t = l/v_a$, with $v_a = (2E_a/m_a)^{1/2}$ the atom's velocity, and also the poloidal fluxes w_1 and w_2 at the ray's enter and the exit of the triangle. The ray is assumed to penetrate the whole triangle's torus, interacting with the whole contours k that contain plasma, in the sequence of w_k on the interval (w_1, w_2) (if this sequence is empty, the triangle gets skipped). The layer-ray interaction time τ is obtained distributing the time interval t over the relevant contours: $\tau = ts_k/s$. Thus the ray interacts with all its plasma, however proportionally to the area involved.

The atoms entering the plasma layer are assumed to occupy for the period τ the whole layer's volume V homogeneously. This approximation is adequate because the ray represents the mentioned trajectories of toroidal symmetry. The ionization and charge-exchange are implemented in TOKES, including the impact of energetic beams on plasma ions, but to the date only preliminary simulations are achieved. The current state we describe exemplifying the neutral ionization by electrons.

The TOKES code allows incomplete sets of ions charge states in the plasma, for instance C^{6+} ions may be present but C^+ to C^{5+} species not. However, this means a deterioration of the modelling, because the ionization energy E_i and the ionization cross-section σ_i for C^{6+} are very different from those for C^+. As yet, TOKES is not able to calculate the real multi-stage ionization, which would demand the complete ions sets. Instead, a compromise solution is implemented. For instance, the C neutral is ionized in the simulation as if the C^+ species would be available, thus using the cross-section of the process $e + C \rightarrow 2e + C^+$, but C^{6+} is immediately produced (not C^+) together with 6 ionized electrons (not 1) implying that the following ionization stages up to C^{6+} occur with a very fast rate, which is not justified so far.

In the model the ionization rate $k_i = \langle \sigma_i v_e \rangle$ (v_e is electron thermal velocity) means simultaneous ionization of $Z \geqslant 1$ electrons after the impact of a single electron onto one neutral atom. Due to the ionizations the number N of entering atoms in the volume V decreases and the number N_e of plasma electrons increases: $N = N_0 - (N_e - N_{e0})/Z$, with given initial numbers N_0 and N_{e0}. The electrons spend certain energy E_i per ionization of Z new electrons and cool down. The equations describing the electrons read:

$$\frac{dN_e}{dt} = Z\frac{k_i}{V}N_e N, \tag{2}$$

$$\frac{d}{dt}\left(\frac{3}{2}N_e T_e\right) = -\frac{E_i}{Z}\frac{dN_e}{dt}. \tag{3}$$

The k_i is approximated as a linear function of T_e defined in terms of initial temperature T_{e0} and some final temperature T_{e1} ($T_{e1} < T_{e0}$). At a large τ the cooling can be significant therefore several computing steps with dropping T_e from T_{e0} to T_{e1} are foreseen, and after each step T_{e0} acquires the value of T_{e1} and T_{e1} gets a new lower value. Eventually some final state with $N(\tau)$ atoms at the exit from the

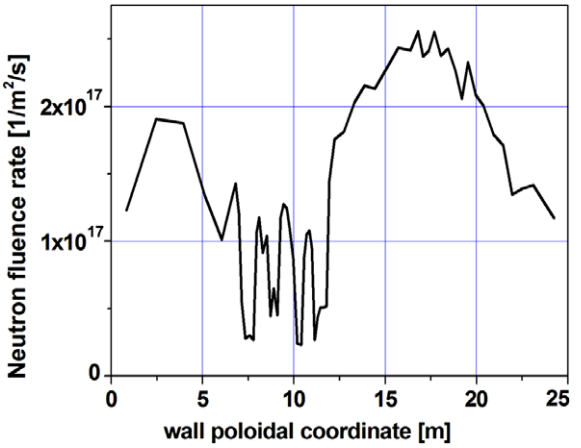

Fig. 3. The distribution of neutron flux through the vessel surface; the wall coordinates are shown in previous figure.

magnetic layer is obtained, and then the interactions with next layers simulated. The ionized atoms are supplied with additional kinetic energy taken from the other ions of the same species, reaching common species temperature.

5. Preliminary benchmark results

This work concerns mainly the implementation technique, and only a few benchmark results on the plasma wall interaction are given. An ITER-like stationary configuration (as is shown by Fig. 2) establishes within about 6 s after starting the discharge simulation for 130 s. By now TOKES is unable to reach the magnetic configuration with the separatrix strike point (SSP) at the side walls of the divertor legs therefore the lost plasma hits the divertor bottom surfaces. In the simulation $N_e = 1.1 \times 10^{20}\,m^{-3}$ and $T_e = 12\,keV$ are maintained at the magnetic axis, and at the last closed layer N_e drops down to $3.6 \times 10^{19}\,m^{-3}$ and T_e to 7 keV. The fuelling D- and T-beams are absorbed in the fusion plasma which diffuses to the SOL.

The SSP heat fluxes are obtained to be 3×10^2 (inner divertor) and $4 \times 10^2\,MW/m^2$ (outer divertor), the large values due to the inappropriate and motionless position of SSP fixed at one wall segment. However, even in this case the surface temperature of the wall of assumed cooling depth $x_c = 5$ cm reaches 1200 K at 130 s, which is much below the vaporization threshold 4100 K. The sputtered atoms propagate until being absorbed either by the walls or ionized at the plasma periphery. Within 60 s the diffusion of C^{6+} establishes rather homogeneous density of $0.8 \times 10^{18}\,m^{-3}$ in the plasma volume. The fusion power of α-particles is equal to 80 MW. The calculated distribution of neutron flux over the vessel surface is shown in Fig. 3. The obtained results need validations.

6. Conclusions

Despite the fact that the 2D code TOKES is still in a preliminary state, the implementation of ITER surface shape and the main wall processes including heat transport, surface evaporation, and sputtering, seems a significant step of development. The random neutral fluxes propagating through the vessel are simulated with representative rays that are naturally coupled with the confined plasma. The coupling is achieved by special meshes built of three-dimensional cells with triangular cross-sections which overlap the magnetic surfaces. By this, TOKES acquired new major features necessary for integrated tokamak modelling.

The next urgent steps for elaborating the plasma wall interactions include accounting for each ionization stage at plasma simulations, implementation of other wall materials (beryllium and tungsten) and improvements of data for different wall processes.

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