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Modelling of SOL transport and radiation losses for ITER with the integrated tokamak code TOKES

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ABSTRACT

For integrated simulations of tokamak plasma equilibrium and surface processes the code TOKES was recently designed. The new radiation database and SOL model are described. The work highlights development details and reveals the effects of the incorporated models. The erosion of Be-, C- and W-atoms and their ionization in SOL and the multi-fluid transport in the confinement region are calculated for the whole ITER deuterium discharge with neutral beam heating.

1. Introduction

In ITER, carbon- and tungsten based materials are assumed for the divertor and beryllium for the main chamber wall [1]. Tungsten will make the plasma wall interaction especially complex. The presence of not fully ionized W-ions in the confinement region can cause enhanced radiation flux over the whole vessel surface. The distribution of plasma impact on the divertor surface is strongly determined by the structure of the scrape-off layer (SOL).

Recently, the integrated code TOKES was developed [2]. It obeys the toroidal symmetry in terms of functions of cylindrical coordinates (r,z). The code contains models for the magnetic field, plasma diffusion, thermal conductivity, fuelling, impact on the walls and influx of eroded neutrals into the confinement region. The models use poloidal magnetic flux coordinates $w(r,z)$, and the plasma is numerically organized as some layers along the contours of constant w. Triangular meshes coupled with the plasma layers allow simulation of neutral rays in the entire vessel.

In this work the next steps of TOKES design are described. Section 2 explains the new TOKES radiation database, which comprises bremsstrahlung, recombination- and resonance radiation information. Section 3 describes the new SOL model, which – although preliminary – allows estimations of the recycling of eroded atoms. Section 4 demonstrates the new TOKES features.

2. Radiation database and data approximation

TOKES model for radiation transport was described elsewhere [3]. The ion population densities N_{mzk} have the isotope index m (from H, D, T to W), the charge state $z = 0, 1, \ldots$ and the bound electron index $k = 0,1,2,\ldots$ The ionization dynamics and radiation transport are calculated along with the electron temperature T_e and density N_e and the rates of ionization/recombination and excitation/deexcitation transitions among energy levels E_{mzk}. For each m and z, g_k are the level's statistical weights and $\Delta E_{kk'} = E_{k'} - E_k > 0$ the resonance transition energies. The photon absorptions and emissions are described in terms of opacities, which are emission coefficients β and absorption coefficients κ that include spontaneous and induced radiation.

The database of TOKES contains constants E_{mzk}, g_{mzk}, the oscillator strengths $f_{mzkk'}$ and the transition frequencies $\nu_{mzkk'}$ for resonance excitations and ν_{mzk} for the ionizations of atoms and ions by electron and photon collisions, which was collected using diverse sources and approximations. The ground state ionization potentials $I_{nz} = E_{m,z+1,0} - E_{m,z,0}$ (with n the chemical number of isotope m) are available for all m and z [4]. Usually, only the frequencies of the transitions from ground state to excited states of neutral atoms ($z = 0$) are known. Therefore for ions ($z > 0$) the scaling laws described in [5] for $\nu_{mzkk'}$ and ν_{mzk} on the ratios $I_{n+z,z}/I_{n0}$ are applied along the isoelectronic sequences $n - z$ = constant.

The atomic data on resonance transitions (E_{mzk}, g_{mzk}, $E_{mzkk'}$ and $f_{mzkk'}$) are taken from a free access database [6], but many are missing there even at $z = 0$. E.g. those of Ca to Ta are hardly present but 74 (W), despite that [6] seems most abundant and adequate source. Therefore, the lacking data of chemical numbers n' are obtained by extrapolations from available numbers n, at first assuming the same transition structure within a periodic group and applying the ionization potential scaling for all z along the isoelectronic sequences.

The complexity of atomic data (see Fig. 1) with characteristic level maximum index $K > 10^2$ prevents in reality direct multi-species self-consistent radiation transport simulations. In TOKES the data are reduced. For each m and z, near energy levels k are grouped

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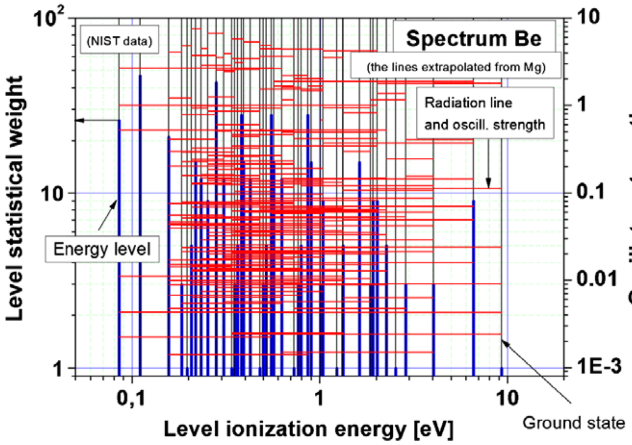

Fig. 1. Spectrum scheme of Be ($z = 0$, 42 levels, 186 lines).

and a level group q ($q = 0\ldots Q$) is considered as one level of k in some range $k_{1q} \leqslant k \leqslant k_{2q}$. In the iterations the groups are built with the rule 'near levels are attracted and far levels are repulsed' is used. Initially each level is one group, so that $Q = K$ and $k_{1q} = k_{2q} = k$. Then, the minimum 'distance' $\Delta E_k = |E_{k+1} - E_k|(g_{k+1} + g_k)$ between neighbour levels is determined and the two nearest levels (k and $k + 1$) are joined in one group, thus $k_{1q} = k$, $k_{2q} = k + 1$ (for this group) and $Q = K - 1$. This procedure is repeated for neighbouring groups, and the two next nearest groups merge until the needed reduction of Q. The 'distance' is defined as the product of the energy difference between the closest levels of neighbour groups, and the sum of the total weight of the levels of the neighbour groups, which prevents too large $k_{2q} - k_{1q}$.

The numerous transitions among the levels are then reduced to a moderate number of most strong transitions among different groups. Finally, the radiation transport equations are similarly reduced. Fig. 2 demonstrates the group approximation spectrum of Be obtained in TOKES from the spectrum in Fig. 1. For a preliminary validation of the group level data of TOKES the exemplary radiation loss calculations [7] are used comparing them with those produced by TOKES. Varying some dielectronic recombination constants, a good fitting was achieved.

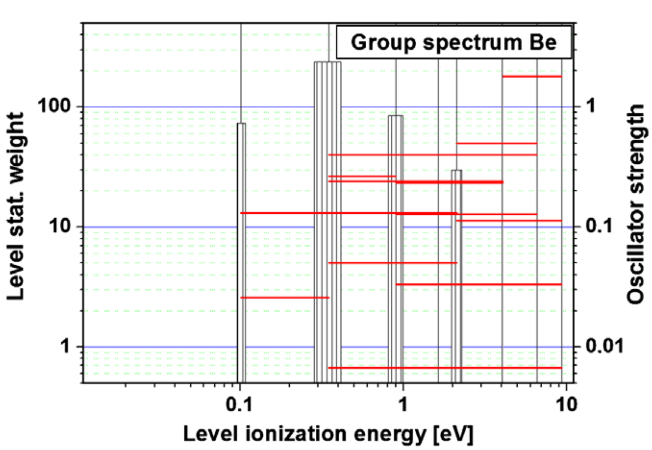

Fig. 2. Reduced spectrum scheme of Be ($z = 0$, 6 group levels, 13 group lines) from TOKES.

3. Modelling of the scrape-off layer

In TOKES, the plasma and its energy dumped into SOL across the separatrix are represented by fully ionized ions and their energies. To the latter, the electron thermal energy proportionally to the ion charge state and the internal energy of plasma ions are added. In this way, an ion m impacting on the wall brings kinetic energy that contains already (a) the contribution of electrons, which the ion gains in reality when crossing the electric sheath in front of the wall, and (b) the recombination contribution (because the ion internal energy would be released at the wall surface).

The ions emerging in the SOL are grouped in bunches, and a bunch carrying ΔN_i ions is simulated as one 'gyro-particle' in the guiding centre approximation [8]. The code calculates the trajectory of the gyro-particle and in particular it calculates also the passing times τ_i of the gyro-particle through each triangle. After each simulation step Δt averaged ion densities $\bar{n}_i$ in each triangle passed by many gyro-particles are calculated as follows. To get $\bar{n}_i$, the product $\tau_i \Delta N_i$ is accumulated per each triangle. the accumulated product is divided by $V\Delta t$, with volume $V = 2\pi rs$, r the centre radius and s the area of the triangle. The result is the triangle's ion density: $\bar{n}_i = (\tau_i \Delta N_i)/V\Delta t$. Similarly averaged, the ion temperature $\bar{T}_i$, the local (in the triangle) leading centre poloidal flux $\bar{w}$ and the SOL width $\bar{\delta}$ are calculated. For instance, $\bar{w}$ and $\bar{\delta}$ allow an approximate drawing of SOL with rectangular fragments (see Fig. 3).

The atomic rays that cross the triangles are treated similarly, obtaining corresponding averaged parameters $\bar{n}_a$ and $\bar{T}_a$ required for the calculation of atom-ion interactions (the neutral rays are described in [2]). To give an example, the charge-exchange (CX) in each triangle is simulated in the following way. The CX algorithm consists of two parts. First part calculates CX rate in terms of amount of ray atoms N_a and the ion densities $\bar{n}_i$. The atom ray passes through a triangle for a while τ_a, meeting there the SOL ion density. The number of CX events follows as

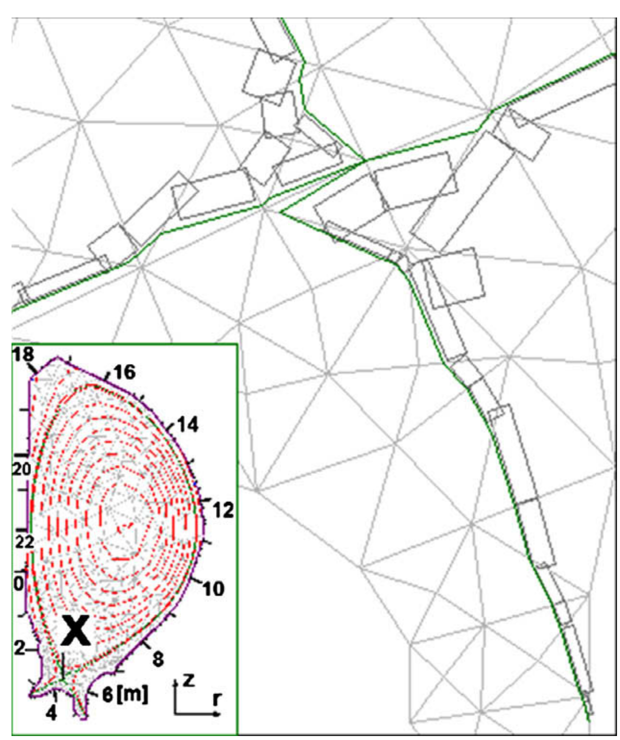

Fig. 3. SOL as collection of fragments on TOKES triangle meshes (vicinity of x-point is magnified).

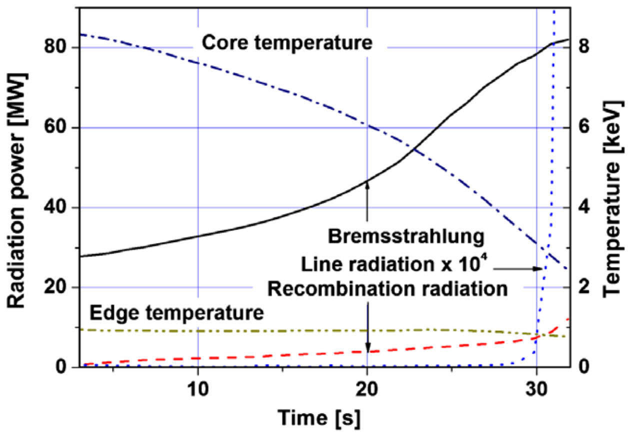

Fig. 4. Radiation losses and plasma temperatures obtained with TOKES, 80 MW heating.

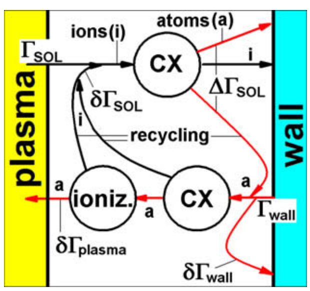

Fig. 5. Scheme of SOL processes in TOKES: influx of lost ions (Γ_{SOL}), atom fluxes after charge-exchange ($\Delta\Gamma_{SOL}$), flux from the wall (Γ_{wall}) and contributions to it ($\delta\Gamma$).

$\Delta N^{(1)}_{CX} = \frac{1}{2} k_{CX}(\bar{T}_i, \bar{T}_a)\tau_a \bar{n}_i N_a$, with k_{CX} the charge-exchange rate of the TOKES database. Second part does similarly in terms of gyro-particles and the atom densities $\bar{n}_a$. $\Delta N^{(2)}_{CX} = \frac{1}{2} k_{CX}(\bar{T}_a, \bar{T}_i)\tau_i \bar{n}_a N_i$. Physically both these contributions describe the same physical process of CX, therefore in each algorithm the factor ½ appears in the CX rate and their results are summed. The new ions and the new atoms appeared after those events are accumulated (alone with their energy and momentum) in special structure of triangle. The ionization in SOL is also similarly modelled. At the end of time step the structures are cleared in each triangle by emitting new atomic rays and ion bunches. The conservation of particle number for each kind m, energy and momentum is observed.

4. Simulation results

As input parameters, TOKES needs only the beam power and the particle inflow by pellet injection. With the new models, three benchmark calculations of full ITER H-mode ELM-free discharge have been performed for auxiliary heating by a 1 MeV D-beam of power 80, 96 or 144 MW and fuelling by pellets simulated homogeneously spreading the inflow 10^{22} s^{-1} of 1 eV D-atoms over the confinement region. In order to avoid some effects not essential for radiation and SOL issues, the plasma shape was fixed, and the fusion reaction was minimized by assigning negligible tritium and helium densities. The MHD stability margin is simulated comparing the parameter $\beta = 8\pi\Sigma_g p_g/B^2$, ($p_g = n_g T_g$) with a given value β_{max}. Thus far β_{max} = 3% is assumed, and B is averaged over the magnetic surface w = const. Meeting $\beta > \beta_{max}$ at some calculation step, p_g are reduced to get $\beta = \beta_{max}$ and the excess plasma is added to the plasma losses across the separatrix.

With 80 MW heating the discharge terminated after 33 s because of increasing radiation losses. Fig. 4 demonstrates the evolution of radiation power and plasma temperature. The main radiation losses are due to bremsstrahlung, the fraction of recombination radiation is rather small, and the line radiation negligible. At the pressure limited by the plasma beta (and thus core plasma pressure $p \approx nT$ is limited by about 5 bar) the radiation losses relate with the core temperature as $(T_{core})^{-3/2}$, which follows from the scaling $T^{1/2}n^2$ of bremsstrahlung power. In the end phase the beam is mainly stopped at the plasma periphery and cannot therefore prevent the radiation collapse.

For 96 and 144 MW heating, after about 20 s a steady state is reached. Fig. 5 shows a schematic representation of the implemented SOL processes. Table 1 summarises general results of the steady state discharges. BP is the beam power. Bremsstrahlung (B) always dominates over recombination (R)- and line (L) radiation. n_D, T_{core} and T_{edge} are averaged over plasma volume. The simulations demonstrate that the plasma edge temperature T_{edge} is above 1 keV. The high energy lost ions bombard the wall. They produce significant sputtering and a significant part of sputtered atoms penetrate into the confinement region. From Table 1 we see also that the role of SOL in stopping of lost ions is small. Only the backscattering of D-atoms is implemented but not the release of D-molecules from the surface. Therefore the influx of D-atoms from the wall is small and the detachment regime in SOL could not be obtained.

Table 2 shows the parameters obtained with TOKES relevant for the impurities in the 96 MW discharge. The radiation losses by the impurities (mainly by W) are small compared to that by deuterium. The C-atoms are sputtered mainly by D-ions that strike the divertor in the vicinity of SSP. W-atoms of the dome and Be-atoms of the main chamber wall are sputtered by neutral D-atoms after

Table 1
Calculated steady state parameters of deuterium species.

BP (MW)	B (MW)	R (MW)	L (W)	n_D (10^{20} m^{-3})	T_{core} (keV)	T_{edge} (keV)	$\Gamma_{SOL/D}$ (10^{20} s^{-1})	$\Delta\Gamma_{SOL/D}$ (10^{20} s^{-1})	$\Gamma_{wall/D}$ (10^{20} s^{-1})
96	21	4.7	11	1.1	10.5	1.07	103	0.12	2.6
144	8.5	0.31	3	0.65	18.5	1.54	103	0.06	1.7

Table 2
Calculated parameters of wall material species for 96 MW heating case.

Impurity species	B (MW)	R (MW)	$n_{impurity}$ (10^{15} m^{-3})	Γ_{wall} (10^{17} s^{-1})	$\Delta\Gamma_{SOL}$ (10^{17} s^{-1})	$\delta\Gamma_{wall}$ (10^{17} s^{-1})	$\delta\Gamma_{plasma}$ (10^{17} s^{-1})
C	1.02	0.12	150	750	20	590	140
W	1.97	4.62	3.1	18.6	1.5	14.7	2.4
Be	5×10^{-3}	2×10^{-4}	1.9	3.00	0.05	0.95	2.00

backscattering that can follow the charge-exchange of D-ions at the divertor surface. Most of the wall emitted C- and W-atoms immediately return to the wall, the others penetrate almost fully into the plasma, and only a small part is ionized in SOL, and wall emitted Be-atoms come mostly into the plasma.

5. Conclusions

The full radiation transport simulations with all kinds of radiation and the SOL model are significant design steps. By this, TOKES acquired major features necessary for two-dimensional integrated tokamak modelling. The considered numerical approach combines hydrodynamic and kinetic descriptions of plasma and neutrals that includes the recycling in SOL.

So far, the modelling stage is only preliminary. The next steps in the improvement of the SOL model are the elaboration of the distribution of lost ions emerging in SOL and the inclusion of other important SOL processes (e.g. implementation of charge-exchange of impurity species and deuterium release from the wall bulk). That would allow comparisons of modelling results with experiments on existing big tokamaks, in which the plasma detachment and significant recycling can be achieved.

With increasing recycling, lower temperature in SOL can be expected, and line radiation losses from SOL can get significant. In that case an expansion of the radiation model for SOL can be necessary.

Acknowledgements

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