

Integrated modelling of plasma-wall interactions in tokamaks with B2.5 : mixed materials, layers and coatings, bundled charge states, and hydrogen inventory

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I. Motivation

Plasma-wall interactions (PWI) in tokamaks have traditionally been modelled as a one-sided problem, meaning that models either concentrate on the plasma side, treating the wall as a material boundary condition with constant properties, or inversely, consider the evolution of a material surface exposed to a given incident plasma. Only recently have efforts been undertaken to follow self-consistently the evolution of the target material under plasma exposure, the transport of the eroded particles back into the plasma and the consequent changes to the plasma parameters [1, 2]. With the current advent of “mixed materials” tokamaks, namely the tungsten covering in ASDEX-Upgrade, the JET ITER-like wall project and most importantly the ITER wall itself, new phenomena of preferential erosion, impurity transport and redeposition have to be included if the models are to be of value for assessing wall characteristics such as divertor lifetime and ELM survivability. Moreover, the issue of tritium retention, or more generally of hydrogen isotope inventory within the vessel walls is of critical importance for ITER licensing and operation. Therefore, a work programme has been underway for several years involving the B2.5 edge plasma fluid simulation code [4] (part of the SOLPS5.0 code package) to address these issues. In this paper, we review work on three related topics. First, we present an extension of the mixed materials model for plasma-facing components that can now take into account intentional material coatings and re-deposited material layers. Second, we introduce a bundle charge state model into the code, aimed at treating high-Z ions, and show some sample runs with Ar as a radiating impurity, bundled and unbundled. Third, we discuss the current status of a multi-scale” model of hydrogen diffusion in carbon-based materials for eventual use in a wall particle inventory model.

II. Mixed materials wall model in B2.5: coatings and layers

The mixed materials model for plasma-facing components, introduced in [1,3], has been extended to allow for material coatings and re-deposited layers. At every time step during the simulation, we solve for the time evolution of the size and chemical composition of re-deposited layers onto plasma-facing wall elements, as well as their surface temperature and, optionally, the full 2-D temperature distribution within them. Each wall element can be resolved in depth and is allowed one (optional) change in composition in its bulk, corresponding to intentional coatings, either through manufacture of the wall tile or by wall conditioning processes such as boronization or beryllium evaporation [5]. This is particularly relevant in regard to the new all-tungsten ASDEX-Upgrade and the ITER-like wall project at JET, where most of the tungsten tiles are actually carbon tiles with tungsten coatings, and this should be taken into account when computing the

thermal history of the tile. Currently, we consider only elemental mixtures and neglect any chemistry taking place in this layer. This will be included in a later version of the model. Moreover, we do not take into account the hydrogen content of the layer (but see Section IV below). We compute the thermal and physical properties of the layer as linear combination of the bulk (or coating) and re-deposited elemental materials properties. A fuller model including alloying of the surface layer material is being considered.

A related open issue remains the treatment of preferential sputtering [6,7], within the mixed materials layers. Depending on conditions and local chemistry, sputtering can favour enrichment in the heaviest element, or in the less abundant component. It can also be affected by differences in vapour pressure and surface binding energy. For now, these effects are neglected and the sputtering yield of an incoming projectile is the weighed sum of its yield against each element times its local abundance, as in [1].

To illustrate the use of this new model, we show results for simulations of an ITER plasma with Be main chamber walls and a carbon divertor. Figure 1 gives the fractional contents of the bulk and re-deposited materials while Figure 2 shows the rate at which the surface elements are eroded or grow because of PWI and material migration.

III. Bundled charge states

A “bundled charge states” model has also been implemented so as to limit the numerical load of following all the ionisation stages of high-Z ions, a necessary step for simulations with the full ITER material mix (Be/C/W). By “bundling”, we mean that several charges states of the same homonuclear sequence are grouped into a single “species” within the code. Practically, this means that the quantities Z_a , Z_a^2 , E_i and E_t , respectively the species charge, the species square charge, the ionisation energy to that species from the previous species, and the total ionisation energy to that species from the neutral atom of the sequence, become functions of the local electron temperature and density. To compute these new functions, we rely on the collisional-radiative model developed within the ADAS project [8]. Numerically, care was taken to maintain full backward compatibility of the code and transparency for the user. Neutral species are not allowed to be bundled with charged species as their physics is too different.

As a test case to verify the validity of the bundled charge state model implementation and its possible impact on the SOLPS plasma solution, we have run a series of cases with deuterium and argon. One series follows the full set of ionisation stages while the other uses so-called “natural” bundling, i.e. groups together stages whose ionisation energy varies slowly as a function of charge. In the case discussed here, this means that ions Ar^{+2} to Ar^{+6} and Ar^{+9} to Ar^{+14} have been bundled. This results into a reduction of the problem size from a total of 21 to 12 species. The numerical difference between the two models is illustrated in Figure 3.

One aspect in which the bundled charge state method breaks down, at least in its current implementation only dependent on local electron temperature and density, is the treatment of charge-exchange (CX) terms for reactions that do not move the initial ionisation stage of the bundled species outside of its bundle. In our example, this would, for instance, be the reaction: $\text{H}^0 + \text{Ar}^{+4} \rightarrow \text{H}^+ + \text{Ar}^{+3}$. Indeed, the CX rate for the bundle is currently given as the product of the CX rate for the lowest charge state of the bundle times its fractional abundance within the bundle. This means that the data is restricted to “species”-changing rates. In situations where CX processes are important, this changes the ionisation balance of the plasma and the other bundle quantities. The impact of neglecting CX fully is shown in Figure 3 for both models. It is clear that the CX rate difference explains most of the difference between the bundled and unbundled cases.

IV. Status of the hydrogen recycling and inventory model

We have earlier modeled trace hydrogen diffusion in porous graphite using a multi-scale model with molecular dynamics (MD), kinetic Monte Carlo (KMC) and Monte Carlo diffusion (MCD) ([9] and references therein). This multi-scale model has been extended to include additional atomic interactions like dissociation, molecule formation and trapping. Dissociation is included as an energetic process within the KMC ansatz. Molecule formation and trapping are included using the Smoluchowski boundary condition [10], wherein if a diffusing atom comes closer than a certain distance to another atom or trap, they recombine. This distance of closest approach can be deduced from molecular dynamics or from known reaction rates. Therefore we can now model reactive--diffusive processes in a porous geometry.

In Figure 4, we compare our results for hydrogen atomic and molecular recycling as a function of graphite temperature with experimental results [11]. The quantitative mismatch in the cross-over temperature where the H atomic desorption dominates over the H₂ molecule desorption has been shown to depend on the hydrogen fluence, internal void size and void fraction of the graphite [12,13]. Studies of reaction-diffusion of hydrogen from rough surfaces indicate that at graphite temperatures around 300 K most of the molecular desorption is by the Eley-Rideal process wherein an incident atom forms a molecule with an atom adsorbed on the graphite surface. At temperatures equal to and above 600 K, the hydrogen molecular formation and desorption is diffusion limited (Langmuir-Hinshelwood process). This is because at lower temperatures we have a higher hydrogen atom density on the surface and this reduces with an increase in temperature.

Incorporating these effects into a fast, time-dependent analytical model for integration into SOLPS remains to be done. In particular, care must also be taken to properly account for the number of hydrogen being released from the surface in different forms, so that the "return rate" of hydrogen-containing molecules, multiplied by their hydrogen content and added over all species, yield the total recycling coefficient.

V. Conclusions and outlook

We have reported on three related current axes of development of the SOL plasma simulation suite of codes SOLPS, dedicated to improving our understanding of plasma-wall interactions and their back effects on the plasma. These are: a solution of the surface temperature of the wall elements, but allowing this surface to be a mixture of re-deposited material and bulk and/or coating material; a bundled charge state model, to treat very high Z ion sequences like tungsten; and considerations towards a hydrogen inventory model, to address issues of fuel retention and particle balance. All of these projects are ongoing. Next steps would include, respectively, taking into account the chemistry of surface layers, obtaining and testing bundled atomic data for tungsten, and a solution of the hydrogen content of the wall as a function of time.

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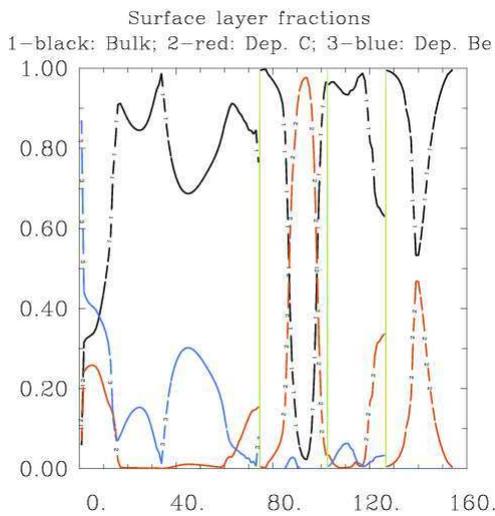


Figure 1. Material fractions in the top layer of ITER wall elements (1-72: Main chamber wall; 73-102: Outer divertor; 103-124: Divertor dome; 125-154: Inner divertor).

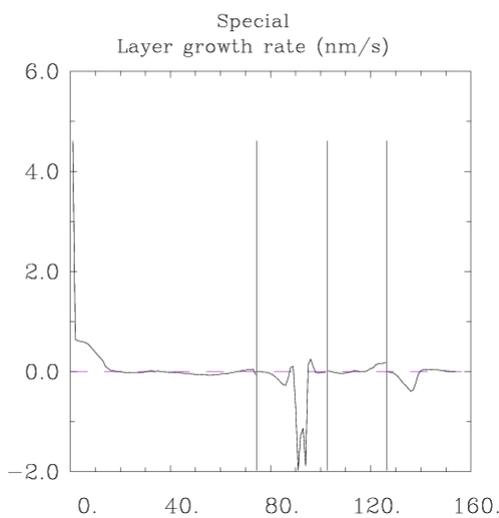


Figure 2. Layer growth rate of the ITER wall elements (same numbering as Figure 1).

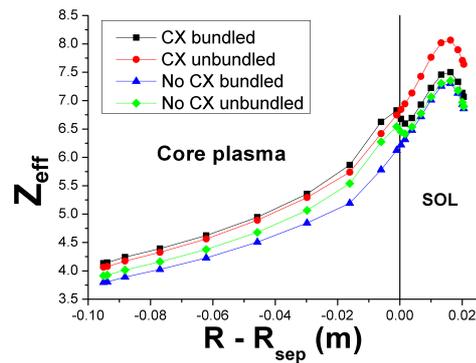


Figure 3. Profiles of Z_{eff} with and without bundling of Ar states and CX processes.

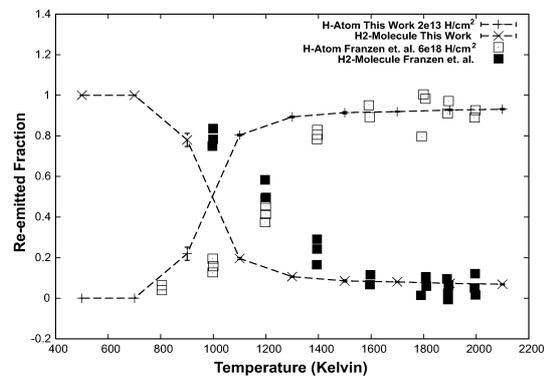


Figure 4. Hydrogen recycling from porous graphite (data in squares from [7]).