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# Towards an improved understanding of the relationship between plasma edge and materials issues in a next-step fusion device

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#### Abstract

Long pulse lengths, and high power and particle fluxes ensure that the biggest incremental step in a next-step fusion device will be the understanding and control of the plasma-wall interaction region. High confidence, predictive models are needed to bridge the considerable gap from existing devices. Modelling the strong, non-linear feed-back between the plasma and surface physics in this region will require significant improvements in the range and quality of diagnostic information as well as enhanced data on atomic and molecular processes and material properties. This paper highlights the key data required, discusses the need for improved diagnostics to generate these data and examines the case for future, dedicated experiments for studying plasma-wall interactions. © 2001 UKAEA. Published by Elsevier Science B.V. All rights reserved.

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#### 1. Introduction

The gap between core conditions in existing tokamaks and those required for a next-step device has narrowed significantly in recent years. However, many divertor plasma parameters remain more than two-orders of magnitude below those expected in the next-step devices, principally as a result of the much shorter pulse length and lower stored energy in existing machines. In a long-pulse next-step device, higher particle fluence to material surfaces, and more severe disruption and ELM erosion will limit the lifetime of plasma-facing compo-

nents and produce dust and co-deposited films that retain tritium, with a significant impact to plasma operations [1]. There is an urgent need for better diagnostic coverage and the development of high confidence, predictive models of the wall/edge region.

Modelling of this region is arguably more complex than for the core plasma because of the lack of closed magnetic flux surfaces and the coupled non-linear feedback between a wide variety of plasma physics and materials phenomena [2–4]. Progress is further hampered by the relatively limited diagnostic information and dedicated run-time generally available for plasmawall interaction studies on existing machines, as well as the absence of key fundamental data on specific atomic, molecular and surface physics effects (including mixed material and tokamak-generated surface layer effects). Numerous efforts (e.g. [3,5–14]) have been made to validate the results of existing codes against available

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diagnostic data. Typically, qualitative features can be well modelled but, with a few exceptions (e.g. [5]), quantitative agreement with available experimental data are not generally obtained. The following sections discuss key issues and attempt to provide a focus and direction for future plasma—wall interaction studies.

# 2. Plasma properties

Whilst diagnostics for the efflux of material from surfaces exist (e.g. passive and active spectroscopy see, for example, [5,6,9–11]) and, indeed, are quite common, the same is not true for the efflux of material from the plasma. Little quantitative data is available from experiments for the species composition and energy distribution of the impacting particle flux on surfaces [15], despite the existence of suitable instruments for some time (e.g. [16,17]).

This shortfall in our knowledge probably represents the largest uncertainty in the validation of existing codes. The only detailed information available about the impinging flux is derived from models of the background plasma and impurity transport. Validation of this modelled flux can only be made 'second hand', by examining diagnostic data for the surface efflux, and is far from conclusive.

Another potential source of error arises from the implicit assumption often made in divertor models that all impurity sources lie in the divertor region. However, results from several tokamaks (e.g. [7,18]) clearly indicate that there are significant ion interactions with the first wall. Although these interactions are far weaker than those in the divertor, the area of the first wall is much larger and impurity production from this region may not be ignorable. This effect may be compounded by flows in the scrape-off layer, which have now been observed on several machines (e.g. [19]), and act to draw impurities towards the divertor.

# 3. Surface properties

# 3.1. Hydrocarbon chemistry

Hydrocarbon chemistry, while complex, is central to the chemical sputtering of carbon by hydrogen. Semiempirical models for the sputtering yield differ by more than a factor of two [6,7,11]. This discrepancy arises from the strong dependence of  $\gamma_C$  on surface conditions and has a profound impact on model validation since, in practice,  $\gamma_C$  is often used more as a fitting parameter than an input variable. The situation is further complicated by the mixed material conditions (including codeposited hydrocarbon films) actually present in existing (and next-step) devices (see Section 3.3) [20].

In detached plasma conditions, the production of heavy hydrocarbon molecules  $(C_x D_y, x > 1)$  may represent a significant fraction of  $\gamma_C$  (for example, up to  $\sim$ 60% for  $T_i \sim$  10 eV [21]). Data for the relative formation of these molecules and the rate coefficients for their dissociation to smaller molecules is sparse and unreliable (particularly for the higher order molecules, C<sub>3</sub>D<sub>v</sub>, etc., which may still represent a significant fraction of  $\gamma_C$ ). As a result, models often assume only the production of lighter molecules such as CD<sub>4</sub>, for which more reliable data exists (e.g. [5,6,10] although there are exceptions, as in [12]). The role that formation and transport of these heavier molecules plays in prompt redeposition of carbon at the surface or the formation of hydrocarbon films is not yet known and their exclusion introduces significant uncertainties.

A third area in which fundamental data is lacking is the reflection probability for hydrocarbon molecules and ions arriving at the surface. Although some data have recently become available for a limited range of the lighter molecules [22] (see also Section 5.1), no data are yet published for hydrocarbon ions and heavier molecules. Since the adsorption of hydrocarbon molecules on the surface (the converse of reflection) is a precursor to the growth of hydrocarbon films, this is clearly a critical issue and more work is urgently required [23].

Lastly, although only a minor issue in existing tokamaks (which are predominantly fuelled by deuterium), the impact of isotopic effects on hydrocarbon chemistry (see, for example [24]) must be evaluated for next-step devices operating with a tritium mix.

# 3.2. Recycling of fuel species

The recycling of hydrogenic ions is reasonably well understood (e.g. [25]). With the exception of recycling from mixed materials (see Section 3.3) and the recycling of incident ions as molecules (D<sub>2</sub>). Molecular recycling becomes significant at target surface temperatures below  $T_{\rm surf} \sim 1400$  K and dominates over atomic recycling for  $T_{\rm surf} < 900$  K [26]. Considerable uncertainties still exist regarding the ratio of atomic to molecular recycling as a function of temperature, with some disagreement noted between measurements in ion beam and tokamak experiments [9]. Incorrect estimates of this ratio can lead to serious errors in the interpretation of the absolute surface efflux from  $D_\alpha$  measurements.

A more serious impact on modelling may arise from the usual assumption that dissociation of these molecules releases atoms with the Frank-Condon energy (a few eV), capable of penetrating deep into the background plasma. Recent measurements [26–28] have shown that recycled molecules may be in highly excited vibrational or rotational states which facilitate the dissociation process, releasing atoms with energies as low as 0.3 eV. However, rates for the formation of excited

molecules as a function of surface temperature and incident ion energy as well as for the release of low energy atoms from electron-impact dissociation as a function of electron temperature [29] are not well understood.

#### 3.3. Mixed materials

A mix of several different plasma facing materials is likely to be used in the next step device to meet the requirements of areas with different power and particle flux characteristics. Erosion, and the subsequent transport of impurities, will inevitably lead to a certain amount of material mixing between these components. For example, CFC surfaces will become doped with W or Be impurities and the metal surfaces will become contaminated with carbon or other metals [30].

The physical and chemical properties of doped surfaces may be significantly different to those of the substrate (e.g. [12,31,32]) and many surfaces within the vessel may also become coated by hydrocarbon layers [22], with varying degrees of thermal conductivity, adhesion and D/C ratio. Despite the fact that such doped and/or coated, mixed material surfaces may actually represent the bulk of the plasma facing surface in both existing and next-step devices, little or no data exists for their associated sputtering yields, reflection coefficients and so on.

# 4. Modelling

Current codes model the plasma-wall region as a series of discrete, but coupled physical systems (e.g. [5–7,10,11,13,33]). That is, the background plasma and impurity transport models provide the particle flux for input to the surface physics model which, in turn, provides the source of impurities and recycled fuel species. However, the coupling between the systems is often incomplete and features such as the impact of sputtered impurities on the background plasma parameters (e.g. through enhanced radiation) are not always accounted for [11]. A high confidence, predictive code will need to combine these systems into an integrated model fully accounting for the non-linear feed-back between the plasma boundary physics and the physics of materials.

Although many codes have a 3D capability, the simplifying assumption of toroidal symmetry is often made. However, there is growing evidence (e.g. [2–4,34]) that impurity sources may be strongly influenced, even dominated, by toroidally localised erosion, resulting from effects such as increased power deposition on the leading edge of radially misaligned plasma-facing components.

Amongst the other features which must be included are a more thorough treatment of prompt redeposition of sputtered material. At the moment many codes (e.g. [6,7]) simply assume that the gross sputtering yield is

modified by a factor to account for rapid redeposition, close to the source. This factor is effectively chosen as a fitting parameter in these codes and yet may be quite significant (70–99% of gross sputtering may be locally redeposited). 3D gyro-orbit resolution, impurity following codes are a more accurate way to account for this effect and have already been used in some models [5,12].

#### 5. The way ahead

#### 5.1. Advancements in diagnostics

Diagnostic limitations are hampering progress. Long term wall samples, removed during maintenance procedures, have been used to measure long term erosion and surface modification but relating the data to specific plasma conditions can be very difficult [8].

Nevertheless, some of the data required for the validation and future development of current plasma-wall interaction models can still be obtained with these diagnostics providing that sufficient time is allocated to dedicated plasma-wall interaction studies on current fusion devices. However, significant advances in the future are likely to result from the use of more sophisticated diagnostics.

Removable sample probes have been employed on several devices (e.g. [5,29,32,35,36]) to make controlled measurements of local erosion and deposition from targeted experimental campaigns (e.g. diverted/limited, L-mode/ELMy H-mode, etc). Rotating sample probes have even been used [37] to provide a degree of intrashot time resolution.

Typically these probes have been used at a single divertor location. However, they are capable of providing invaluable data from other areas of the vessel including; the impact on erosion of leading edge misalignment between plasma-facing components, levels of erosion at the first wall resulting from charge exchange or ion fluxes and impurity flows in the SOL. Although their access to the vessel will always be limited by port availability, the full capabilities of this diagnostic are yet to be fully explored.

Quartz crystal microbalances were pioneered at TdeV [38] and have recently been installed on ASDEX-Upgrade [39], with systems also being planned for JET and the spherical tokamak NSTX. These devices are capable of measuring the growth of co-deposited films on a shot by shot basis, with immediate results, and can be mounted on many surfaces within the vessel (providing they are shadowed from high power or particle fluxes). Future microbalance designs are being considered [40] which may allow measurements with intra-shot time resolution and from high power loading regions.

Several other new diagnostic techniques, providing data complementary to that of microbalances, are also receiving attention at the moment. High power, pulsed lasers are being targeted at regions of film growth in JET to desorb co-deposited material [41]. Spectroscopy of the emission plume as the desorbed material enters the plasma may provide information on D/C ratios in the co-deposited films. Similar laser ablation experiments were done at the ASDEX-Upgrade central column for spectroscopic measurement of wall material erosion and of penetration probabilities [42]. So-called 'sticking probes' are also being tested on JET and other devices [22]. Although technically a long term sample, this diagnostic has the unique ability to discriminate between the efflux to the wall of different hydrocarbon radicals, providing information on the production, transport and redeposition of hydrocarbon molecules.

Passive, visible light spectroscopy of recycled species is in widespread use and often obtained with diagnostic arrays, allowing spatial inversion to provide poloidal reconstructions of both fuel and impurity radiation. The use of lines associated with low ionisation states such as  $D_{\alpha}$ ,  $C_{II}$  or  $W_I$ , can localise the measurements close to the particle source providing species-resolved data on particle influx from the wall.

Such measurements have already proved invaluable for model validation (e.g. [5,6,11,26]). However, in recent years, this technique has been expanded from atomic to molecular species by using high resolution spectroscopy to examine molecular bands (e.g. [9,10]). As mentioned in Section 3.2, measurements of the vibrational and rotational excitation states of fuel species recycled as molecules may provide an important input to future models [26–28].

More importantly, molecular spectroscopy of CD lines holds out the promise of providing a direct measurement of the total hydrocarbon efflux from surfaces. Unfortunately, this technique has yet to provide quantitatively reliable data due to continuing uncertainties over photon efficiencies (of CD band emission) for the various hydrocarbon molecules, as a function of plasma density and temperature (e.g. [43]). Indeed, to fulfil its full potential and provide species-resolved fluxes for the various desorbed hydrocarbon molecules, photon efficiencies for a greater range of molecular bands need to be evaluated.

These data are clearly closely related to the need for accurate estimates of the chemical erosion yield,  $\gamma_{\rm C}$ , and rate coefficients for the dissociation of higher order hydrocarbon molecules in the plasma, for input to modelling (see Section 3.1), and will only be provided by controlled environment, dedicated experiments (see Section 5.2). The availability of accurate photon efficiencies will also improve the quantitative accuracy of related experiments to investigate the transport and screening of hydrocarbons by gas puffing of CD<sub>4</sub> and higher order hydrocarbon gases into the plasma edge.

Reliable tools for better characterisation of the background plasma already exist. More widespread use of divertor Thomson scattering systems, lithium or helium beam diagnostics, reciprocating Mach probes (for determination of SOL flows) and so on are strongly recommended, to support density and temperature data from target Langmuir probes and improve confidence in models of the background plasma. In turn this will improve confidence in the derived efflux from the plasma to material surfaces. However, obtaining reliable diagnostic measurements of this flux presents a greater challenge.

Embedded thermocouples have been used to provide measurements of incident power flux in regions of codeposition [14], overcoming problems associated with IR thermography in these areas and helping to determine the power split between ion and electron channels (as derived from target probes). Solid-state microsensors have been used [16,17] to determine the fluence and energy distribution of the hydrogenic particle flux to surfaces but further improvements, such as measurements of the species composition of the impacting flux, will require development of new diagnostics.

Candidate techniques for measuring the flux of atomic and molecular impurity ions might be active spectroscopy, such as Doppler laser-induced fluorescence (e.g. [44]) of ionic impurity lines, or some form of ion mass spectrometer embedded in the target surface and utilising the toroidal field (a target adaptation of the PIMS probe [45]).

# 5.2. Dedicated experiments

Dedicated tokamak experiments are required to develop realistic plasma-wall models for next step devices.

Magnetised linear plasma devices, such as PISCES [46], NAGDIS [47] and PSI-1 [48] come close to the next-step relevant regimes and have simulated many features of the tokamak divertor plasma, including such complex effects as detachment. However, they can never hope to simulate either the full 3D geometry of a divertor or its 'closed' nature, in which impurity source and sinks are in approximate equilibrium (erosion being balanced by redeposition and co-deposition).

A tokamak with an adequate power input (so that erosion levels were measurable), plasma-facing component materials matching those in a next-step device (e.g. beryllium, tungsten and CFC in the case of ITER) and good control over plasma-facing component temperatures is required. Measurement of physical and chemical sputtering yields from mixed material surfaces, CD-band photon efficiencies, rate coefficients for dissociation of heavy hydrocarbons and so on would require a comprehensive range of dedicated diagnostics with easy access to the divertor.

Sufficient operational time must be allocated to dedicated plasma—wall interaction studies on this device and to rigorous inter-machine comparison of divertor and wall behaviour, which has yet to be done in a similar manner to that for core parameters. Such a device would provide the ideal test-bed for model validation and benchmarking.

# 6. Conclusions and acknowledgements

Significant advances have been made over the last 5–10 years in modelling of the intrinsically complex plasma–wall interaction region. However, the goal of developing a high confidence, predictive model, capable of bridging the wide gap between plasma–wall conditions in existing and next-step devices will only be achieved if code developments are matched by significant improvements in the range and quality of diagnostic information available from the plasma–wall region, as well as enhanced data on a range of fundamental physical properties.

Extensive validation efforts on existing codes have highlighted the key requirements. Some progress can be made to meeting these with existing diagnostics on current fusion devices but there is a strong case for the development of new, more advanced diagnostic techniques and substantially increased operational time allocated to dedicated plasma—wall interaction studies on relevant devices.

Many techniques for obtaining the necessary data actually already exist but are not routinely used. In part this is because they tend to be labour intensive but is mostly because a causal link between wall conditions and key core phenomena, such as the formation and support of H-modes or internal transport barriers, has yet to be clearly established (although evidence of a link to wall recycling is beginning to appear [49]). This will be an important aim of future plasma—wall interaction studies.

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