**CHARACTERIZATION OF ATOMIC AND MOLECULAR
IMPURITY SOURCES AND TRANSPORT
AT THE TOKAMAK EDGE**

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CHARACTERIZATION OF ATOMIC AND MOLECULAR IMPURITY SOURCES AND TRANSPORT AT THE TOKAMAK EDGE*

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ABSTRACT

The characterization of impurity sources in the tokamak edge is challenging because of the highly localized nature of impurity generation. Detailed, spatially resolved, diagnostic information is needed, and three-dimensional (3-D) modeling is required for interpretation. There is also a need for a more extensive atomic and molecular data base for the conditions encountered in this region. The availability of new measurements of photon efficiencies for some relevant hydrocarbon molecules for plasma conditions typical for the tokamak edge and the development of a 3-D Monte Carlo impurities code have enabled the successful modeling of spatially resolved measurements in the vicinity of the pump limiter neutralizer plate and near the inner wall of Tore Supra.

INTRODUCTION

Almost all major fusion plasma experiments are now increasing their emphasis on plasma material interaction, including impurity generation and edge impurity transport. This issue is even more complex than that of core-region impurity transport for several reasons: (1) Impurity generation at the edge is very localized. Measurements require a high spatial resolution in both the toroidal and the poloidal directions. A three-dimensional (3-D) description is essential for codes used in producing extrapolable models of the phenomena. (2) Modeling must include impurity neutral species and molecules, as well as working gas neutrals. This introduces uncertainties due to the very limited available atomic and molecular data bases. In this paper we will illustrate these issues using examples from our impurity studies on Tore Supra.

Tore Supra is a large, superconducting Tokamak designed for long-pulse operation.¹ All plasma-facing components are water-cooled and designed for continuous-power handling. Tore Supra typically operates with a major radius of $R = 2.35$ m, minor radius of $a = 0.75$ to 0.80 m, toroidal field $B_T = 4$ T, I_p in the

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range of 1 to 2 MA, and central electron density in the range of 1 to $8 \times 10^{19} \text{ m}^{-3}$. The maximum input power is about 8 MW, with 12 MW planned for the near future.

Currently, the primary limitation to pulse length is the power-handling capability of the plasma-facing components. As a result, there is a great deal of interest in examining the heat deposition profiles on these components and determining the location and causes for "hot spots." Associated with this effort is also a study to determine the impurity generation patterns on these surfaces.

Diagnostics

To meet the need of these two parallel programs, most of the optical diagnostic systems that view the plasma-facing surfaces can survey both the infrared and the visible regions of the spectrum. The surfaces that are best diagnosed are the inner bumper limiter and the outboard pump limiter (Fig. 1). Most of the inner wall can be viewed by means of both a CCD camera with interference filters and an infrared camera. At least half of the inner wall can be observed by a set of nine discrete fiber optic views that are relayed to a visible spectrometer equipped with a two-dimensional (2-D) camera detection system.

The outboard pump limiter (Fig. 1, inset) is a large surface (50- by 60-cm), pyrolytic graphite limiter.² It is equipped with a large number of internal diagnostics,

Fig. 1. Schematic of poloidal cross section of Tore Supra showing optical views of primary plasma-facing components. (Inset: schematic of toroidal cross section of half of the outboard pump limiter and associated diagnostics.)

including a set of optical fibers to view the neutralizer plate and to relay the light to a dedicated visible spectrometer. The front face of the limiter is observed by means of a periscope system, which allows simultaneous fiber optic and CCD camera views. The latter provides the good spatial resolution, while the former provides good spectral resolution and absolute intensity calibration for specified locations on the front face.

The BBQ Code: Scrape-Off Layer Impurity Transport Model

A goal of the work is to produce extrapolable models for impurity generation and transport to predict suitable conditions for long-pulse and steady-state operation in next-step (e.g., Tore Supra Continu) and next-generation machines [e.g., International Thermonuclear Experimental Reactor (ITER)]. This requires the use of codes that incorporate measured values of background plasma parameters and yield estimates for the generation-rate and spatial distributions of impurities for comparison with experimental observations. To do this, a 3-D Monte Carlo code has been developed that is patterned after the LIM code of Stangeby et al.³ The code incorporates an impurity generation model based on the physical and chemical sputtering processes described in the review by Roth et al.⁴ Detailed geometric models for the Tore Supra plasma-facing components are used to produce a spatial and velocity distribution of C⁰ atoms (or CH₄ in the case of chemical sputtering) that is then tracked through ionization, recombination, and diffusion parallel and perpendicular to the flux surfaces. Carbon self-sputtering is treated by recording the impact position, energy, charge state, and angle of incidence of carbon ions returning to the plasma-facing components and then making a subsequent calculation with the emission source of neutral impurities created by this process. Estimates of the expected wall temperature are required for the treatment of chemical sputtering. The basis for these estimates is described below. Typically, 1,000 to 20,000 flights are used to obtain spatial distributions, with the larger numbers used in cases where an accurate accounting of high charge states is required.

LOCALIZATION OF EDGE IMPURITY PROCESSES

A good example of the localized nature of the edge impurity generation and transport processes is seen in the study of the inner wall. This plasma-facing surface, which covers about 60° above and below the equatorial plane, is composed of about 7500 graphite tiles, each individually aligned and brazed to the water-cooling manifold.

Figure 2 shows a CCD camera picture of a toroidal segment of the inner wall that was made with an interference filter centered at about 8900 Å in wavelength. The picture thus shows the relative spatial distribution of the temperature, which is proportional to that of the incident heat flux. Close examination of this picture, neglecting the hottest regions, shows that there is a periodic pattern of the heat flux in the poloidal direction. This pattern can be attributed to the discrete nature of the tiles on the inner wall and has been reproduced successfully with the BBQ code, using a complex "exponential sine" model,⁵ in which

$$q = q_{\parallel} \exp(-\rho/\lambda) \sin\phi + q_{\perp} \exp(-\rho/\lambda) \cos\phi ,$$

Fig. 2. CCD camera view of inner wall made with 0.89- μm interference filter for shot 10322.

or

$$q = q_{\parallel} \exp(-\rho/\lambda) \sin(\phi + \alpha) ,$$

where $\alpha = \tan^{-1}(q_{\perp}/q_{\parallel})$, the minimum angle of incidence due to the nonzero cross-field heat flux.⁶

Figure 3 shows the predicted angle of incidence and SOL depth as a function of poloidal angle and scrape-off layer distance. The predictions for the case of an ideally smooth (nondiscrete) surface are overlaid in the plots. The experimental observations show the effects of tile misalignments, but in regions where the flux impinging on the first wall is relatively unaffected by misalignments, the poloidal distribution is consistent with the distribution predicted by BBQ if $q_{\parallel}/q_{\perp} \sim 2.5$.

Once the heat deposition is described, the spatial distributions of the impurity sources are also computed with BBQ. In Fig. 4, the radial and poloidal distributions of the various ionization stages of carbon are shown for the case of Tore Supra shot 10318. As expected, the lower ionization stages exhibit more structure, similar to that of the heat flux profiles, than the higher ionization stages.

It is much easier to make quantitative comparisons of modeling with measurements for the one-dimensional (1-D) spectrometer views of the innerwall than for the 2-D CCD camera data. In Fig. 5 we show the predicted CII poloidal profile, averaged over the viewing angle of each fiber view. We also show the measured values. Note that the spatial distributions compare well, except for the central peak, which is

Fig. 3. Predicted angle of incidence and SOL depth as function of poloidal angle for case of Tore Supra shot 10318.

predicted by the code but not seen in the measurement. We have found that the central peak goes away in the model, if the elongation is changed slightly, within the uncertainties of the shape of the plasma.

MODELING OF MOLECULAR SOURCES FROM THE NEUTRALIZER PLATE

The simultaneous presence of various ionization stages and various molecular species and the resulting dependence of modeling on the atomic and molecular data base is well illustrated in the case of the throat region of the pump limiter. As indicated previously (Fig. 1, inset), the neutralizer plate of the pump limiter can be viewed with a set of optical fibers at the back end of the pumping chamber. The collected light is relayed to a visible spectrometer.

Fig. 4. Inner wall radial and poloidal distributions of various ionization stages of carbon for case of Tore Supra shot 10318.

When viewing the neutralizer plate, we obtain spectra that are dominated by molecular bands of hydrocarbon radicals. For example, Fig. 6 shows two spectra, one containing the CD band at $4310 \text{ \AA}$ and the other the C_2 band at $5161 \text{ \AA}$. Note that singly ionized carbon atomic lines are also seen in these spectra. In fact, doubly ionized carbon is also usually observed. Under certain conditions, even hydrogenic carbon has been seen in the throat of the pump limiter.⁷ Note that the continuum in these spectra is also dominated by molecular features.

The presence of molecules is a result of chemical sputtering at the neutralizer plate, which is made of pyrolytic graphite, by the deuterium ions in the throat region that are accelerated by the plasma sheath to ~ 100 to 150 eV ($\sim 5 \times T_e$). The temperature of the neutralizer plate is estimated to be in the range of 450 to 550°C . In that range, chemical sputtering yields are known to peak.⁴ However, in the past, such yields have been measured primarily with ion beam experiments, and the available data base is limited to ion fluxes that are substantially lower than those at the neutralizer plate of this limiter. The presence of the Langmuir probe, which measures the ion flux directly, allows us to estimate the sputtering yield.

Fig. 5. Predicted CII poloidal profile averaged over viewing angle of each spectrometer view of inner wall.

Global Estimate of the Chemical Sputtering Yield

Typically, molecular bands are difficult to model quantitatively because the available base of recommended data is severely limited. However, in the case of the specifically observed molecular bands, photon efficiency data are available in the literature. They were obtained by means of hydrocarbon injection experiments by Pospieszczyk and coworkers on the PISCES-A plasma facility.⁸ Absolute measurements of the molecular band emissions were related to the calibrated injection rates to obtain the ratio of molecular dissociations per photon emitted.

In the case of medium chord-averaged density discharges in Tore Supra ($\langle n_e \rangle \sim 4 \times 10^{19} \text{ m}^{-3}$), the average ion flux measured by the Langmuir probes in the throat of

Fig. 6. Two spectra from pump limiter throat region, one containing the CD band at 4310 Å and one the C₂ band at 5161 Å.

the outboard pump limiter were $\sim 2 \times 10^{19}$ ions/cm²/s. If Γ is the average ion flux to the plate, B is the irradiance (photons/cm²/s) at the plate, and α is the ratio of molecular break-up events/photon from Pospieszczyk's study, then the sputtering yield is given by

$$Y = \frac{\alpha B}{\Gamma} .$$

For the case of the CD band, assuming it originated solely from breakup of CD₄, we estimate

$$Y = 1 \times 10^{-2} \text{ C-atoms/ion} .$$

For the case of the C₂ band, assuming that it originated from breakup of either C₂D₂ or C₂D₄, we estimate

$$Y = 2 \times 10^{-2} \text{ C-atoms/ion} .$$

Estimate of the Chemical Sputtering Yield via Modeling

The above are global estimates of a 3-D generation and transport process. No profile effects are included. For example, such a calculation cannot take into account the fact that T_e varies across the neutralizer plate, changing the expected chemical sputtering yield. Also, one must consider that chemically sputtered molecules undergo a complex breakup chain along the field (axially) before producing CD as a final product. Modeling allows us to incorporate these profile and rate effects and make an independent estimate of the hydrocarbon production rate at the neutralizer plate by matching the observed intensity.

Figure 7 shows the spatial profiles, from the BBQ simulation, of the most significant breakup products of CH_4 along the axial direction, that is, along the toroidal magnetic field direction. The single dashed line corresponds to the location where the neutralizer plate ends. The double dashed lines correspond to the location of the Langmuir probes where the ion flux and the plasma parameters are measured.

The BBQ simulation, which uses the Langmuir probe data and estimates of the neutralizer plate temperature as inputs, shows that 40% of the sputtered carbon flux

Fig. 7. Spatial profiles, from BBQ simulation, of most significant breakup products of CH_4 along axial direction, that is, along toroidal magnetic field direction, in pump limiter throat.

ends up going into the pumping chamber of the limiter, while 50% ends up redeposited on the floor of the throat region, 3% on the roof, and 1% on the sidewalls; 6% escapes into the plasma outside the throat. A sputtering yield of ~ 0.01 is computed, in agreement with the global estimates. The values obtained by the global estimate and by spatially resolved modeling are consistent with extrapolations of the chemical sputtering data base, which is limited to much lower ion fluxes.⁴

However, it is found that the results are very sensitive to the electron temperature. Sensitivity studies, in which T_e was varied from 20 to 35 eV, resulted in sputtering yields from 0.005 to 0.012. In addition, the simulation results are sensitive to the assumed molecular rate coefficients. These coefficients are taken from the Ehrhardt-Langer data base,⁹ which is included in many present magnetic fusion codes. However, many of the coefficients in this data base are rough estimates due to the absence of accurate recommended data. Sensitivity studies in which these rates were doubled produced approximately a doubling of the resulting sputtering yield (Fig. 8).

Fig. 8. Effect of doubling molecular rates in Ehrhardt-Langer (E-L) data base by 2 on the predicted hydrocarbon breakup products. (I) BBQ code results using E-L rates. (II) Results with doubled E-L rates.

DISCUSSION AND CONCLUSIONS

Using examples from our impurity studies program in Tore Supra, we have shown that the generation and transport of impurities at the tokamak edge is complicated by both the localized nature of the problem and by sensitive dependence on a limited atomic and molecular data base.

Modeling of the visible and infrared measurements on the inner wall shows clearly the problem of localization. Even the multichord spectrometer, which views the inner wall, cannot resolve all the features seen in the CCD camera views. The 3-D aspect of the BBQ code is essential for modeling these features because they are dependent on the shape of the individual graphite tiles and on the shadowing between tiles and, therefore, on the magnetic field topology. Including all these effects, the code successfully reproduces some of the features of the 2-D CCD camera images when cross-field transport is included.

In the modeling of the molecular fluxes from the neutralizer plate of the pump limiter, we have shown the importance of atomic and molecular data to obtain quantitative information from the measurements. Because some recommended cross sections of the CH_x molecules and radicals are available (note that *none* is available for the case of CH), we were able to model the measurements of the CD band. No recommended cross-sectional data are yet available for modeling the case of the C_2 band.

Finally, the availability of photon efficiency data for the molecular bands of CD and C_2 for plasma conditions similar to those of the pump limiter throat made it possible to make global estimates of the sputtering of CD_4 and C_2H_x from the neutralizer plate. Because until now no measurements of the chemical sputtering yield were available for the high ion fluxes ($\Gamma > 1 \times 10^{19}$ ion/cm²/s), these measurements provide the only such information (Fig. 9).¹⁰

Fig. 9. Comparison of sputtering yield estimates with available data base. Source: J. Roth, to appear in Atomic and P.M.I. Processes in Controlled Thermonuclear Fusion, Ed. R. K. Janev (Elsevier, 1993).

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