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** See annex of F. Romanelli et al, "Overview of JET Results",*
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ABSTRACT.

The 2004 tracer experiment of JET with injection of $^{13}CH_4$ into H-mode plasma at the outer divertor has been modelled with the ERO code. EDGE2D solutions for inter- ELM and ELM-peak phases were used as plasma backgrounds. Local 2D deposition patterns at the vertical outer divertor target plate were obtained for comparison with post-mortem surface analyses. ERO also provides emission profiles for comparison with radially resolved spectroscopic measurements. Modelling indicates that enhanced re-erosion of deposited carbon layers is essential in explaining the amount of local deposition. Assuming negligible effective sticking of hydrocarbons, the measured local deposition of 20−34% is reproduced if re-erosion of deposits is enhanced by a factor of 2.5−7 compared to graphite erosion. If deposits are treated like the substrate, the modelled deposition is 55%. Deposition measurements at the shadowed area around injectors can be well explained by assuming there negligible re-erosion but similar sticking behaviour as on plasma-wetted surfaces.

1. INTRODUCTION

Tracer injection experiments in tokamaks provide information on material migration and deposition under constant plasma conditions. In plasma devices with carbon plasma- facing components a suitable tracer is the natural isotope ^{13}C that can be distinguished from ^{12}C in post-mortem surface analyses. The principal carbon migration can be investigated by injecting a tracer containing molecule such as $^{13}CH_4$ from a net erosion zone, which is a strong impurity source also in the absence of injection.

Carbon migration in plasma is a complex process starting from physical or chemical erosion of the surface by particle bombardment, followed by dissociation and ionization of molecules and atoms to ions and their transport under the influence of electromagnetic forces, plasma flow and diffusion. Finally, the eroded or injected particles are deposited on the plasma-facing surfaces, where re-erosion may occur, or on remote areas. The diagnostic capabilities for studying the details of this process are limited: The density distributions of impurity species in the plasma during the discharge can be obtained in situ by spectroscopic measurements of their light emission, and the final tracer distribution on plasma-facing components can be measured ex situ by e.g. ion beam techniques—for an overview, see [1]. Interpretation of these measurements for complete understanding of carbon migration requires in addition computer simulations.

The modelling of global migration of ^{13}C in JET injection experiments has been completed recently and is described in a comprehensive manner in [2]. The computational tool was the 2D fluid code EDGE2D supplemented with especially tailored postprocessors to extend the modelling to re-erosion. EDGE2D uses the Monte Carlo code NIMBUS to model neutrals. The present paper reports a more detailed modelling of the local effects at the divertor which are out of reach of EDGE2D. We use the 3D impurity transport code ERO [3, 4] that has a more comprehensive physics basis for plasma–surface interaction processes, can describe the break-up chain of methane, and can cope with the toroidal inhomogeneity of the injection. Some initial modelling results that support the EDGE2D work were already reported in [2], and, conversely, the plasma solutions computed with EDGE2D are used as input for ERO in the present work.

The geometry of the outer divertor implies a shadowed region around the injection location. The shadowing effect has been modelled with a simple model in the ERO code itself and with a more detailed gap deposition model developed recently for evaluating the deposition in the tile gaps and castellated structures planned for ITER.

2. EXPERIMENT

On the final experimental day of JET Campaign C14 in 2004, 31 identical discharges were run with $^{13}\mathrm{CH}_4$ injection from 48 injectors (GIM 10) located toroidally distributed around the outer divertor. The discharges were 1.4T, 1.4MA H-mode with 8MW NBI and 120Hz 30kJ ELMs. The total injected amount was 4.3 °— 1023 particles. The geometry is shown in figure 1 with the simulation volume and part of EDGE2D plasma also drawn. The gas injection module GIM 10 is located in the gap between tiles numbered poloidally as 7 and 8. Subsequent post mortem surface analysis produced deposition profiles along various measurement lines and the total amount of ^{13}C deposited on tiles 7 and 8 has been estimated to 7.3×10^{22} particles (17% of injection) [5].

Tracer injection experiments avoid the complexities characteristic for long-term plasma–wall interaction studies in which various plasma configurations are involved over a period of months or years. However, some difficulties for modelling still arise from the uncertainties in the 2004 tracer injection experiment. It was found afterwards that part of the injected methane had been able to leak behind the divertor tiles and enter the vessel on top of the outer baffle, and possibly also in the PFR. The amount of leakage has been estimated in EDGE2D modelling [2] to be in the range 15–50%. Another significant fraction of the released methane is suspected to be deposited in the tile surfaces shadowed from the plasma, but there are no measurements from e.g. the top edge of tile 7. We have carried out preliminary modelling for this part with a gap deposition model, which is, however, still in the development phase and not extensively benchmarked to experiments. Therefore the fraction of carbon locally deposited on plasma-exposed surfaces remains relatively uncertain, and this uncertainty reflects to the quantitative code–experiment comparisons.

Relevant diagnostics in the present experiment include surface analyses and spectroscopy. Post mortem measurements of tile 7 cover the shadowed surface facing the plasma, several Rutherford Backward Scattering (RBS) measurements along toroidal lines, and SIMS measurements along two poloidal lines. We can compare the 3D gap modelling results against the first of these, and the actual ERO deposition pattern with the others. The KT3 spectrometer provides 12 radially separated, line integrated signals in front of the outer divertor target. Emission lines CII at 426.7nm, CH at 431.0nm, CII at 514.0nm and CI at 909,5nm were aquired prior to and during the puff.

3. SIMULATION METHOD

ERO is a 3D Monte Carlo impurity transport code originally developed at IPP Garching and FZJ. The code models the motion of impurity particles in plasma (e.g. tokamak SOL or linear plasma simulator) and accounts for plasma–wall interactions and relevant chemistry through external databases. The simulations proceed in discrete time steps during which the surface composition is kept constant. Within each (surface) time step a much shorter (particle) time step is used for particle tracing, which can be further decreased in the vicinity of the surface. The surface time step is limited by the requirement that one must not erode more particles than there are in the interaction layer of a surface cell. The divertor receives such a high particle flux at the strike point that (assuming a fixed 2% chemical erosion yield and 10-fold enhanced re-erosion of deposited amorphous carbon layers) we have taken a surface time step of 0.005 seconds. The simulation volume shown in figure 1 extends 750mm toroidally, encompassing two injector locations 560mm apart. We have applied a periodic boundary condition for the test particles in the toroidal direction to simulate the effect of 48 injectors located around the torus. The poloidal extent is 160mm (3mm into the PFR and 130mm into the SOL at target). Also the radial dimension of the volume is 160mm. In our modelling, we have selected as a starting point a “reference case” in which all parameters have been chosen according to best knowledge. We then carried out parameter variations in order to evaluate the significance of different assumptions and to find out whether the match to measurements could be improved. The reference case is defined by the following input parameters: We assume the effective sticking coefficient of hydrocarbons S to be zero, describing either reflection or prompt re-erosion of deposited particles. Reflection of atoms and ions is calculated from TRIM data. The chemical erosion yield is fixed to 2% for the substrate, but physical and chemical re-erosion of deposited material is enhanced by a factor of 10 (the effect of this number was studied with parameter variations). The temperature and flux dependence of chemical erosion have been neglected but will be later included by using the Roth formula. Particle reflection, sputtering by test particles and the background plasma, perpendicular diffusion and thermal force are included in the simulation. The total injected amount of 4.3×10^{23} molecules of $^{13}CH_4$ in the experiment was assumed to be distributed over 200 s of plasma time and evenly over the 48 injectors, giving an injection rate of 4.47×10^{19} particles/s for each source point. The plasma background is the intra-ELM EDGE2D solution. The external source is represented by 10 000 test particles and the eroded flux by 4800 test particles on each time step. Tracing of these particles in the plasma takes most of the computing time, totalling 1–3 hours per time step on a single core of a quad-core processor.

Tile 8 shadows the top edge of tile 7 from plasma so that the injected methane can possibly form a gas pocket in front of the injection location. The dimensions of the shadowed region are a few millimetres. Significant, toroidally symmetric deposition has been found at the upper part of tile 7 [6]. To model this deposition ERO would require a plasma background for particle tracing, but it is not straightforward to extend the EDGE2D plasma solution to the shadowed region and into the gap between tiles. Therefore we have reduced the tile shapes planar and applied a modified plasma background in ERO. Re-erosion is prevented on a surface region representing the shadow by setting the plasma temperature and density essentially to zero. More realistic modelling of this region with the 3DGap code [7] has been initiated and the results will be reported in a subsequent paper.

4. SIMULATION RESULTS

4.1. REFERENCE CASE

Starting from a clean carbon surface, injected ^{13}C starts building up layers mainly downstream of the injection points. At the beginning of the simulation 79% of the injected carbon is deposited. The rest escapes into the PFR and SOL. As the layer builds up, re-erosion starts releasing some of the deposited carbon and the loss rate increases. After about 0.3 seconds of simulation time an equilibrium surface concentration distribution is reached and the net deposition rate levels off at about 17% of the injection rate. The preferable escape route is into the PFR, some carbon still ending up into the SOL.

Figures 2 and 3 show the temporal evolution of deposition efficiency towards equilibrium and the deposition profiles along lines used in post mortem analyses, respectively. The 2D deposition pattern for the reference case is shown in figure 4 and is relatively similar in the other cases. One can see that the plasma flow along B drags the carbon downstream and that it is mostly deposited within some tens of centimetres from the source. The toroidally extending deposition stripe between injectors represents the accumulation of ^{13}C in the shadow.

4.2. ELMS

As a result of the investigations of global migration [2] there are EDGE2D plasma backgrounds available both for the inter-ELM phase and for the ELM peak. In the present work we used these plasma solutions to perform a simple study of the effect of ELMs on local migration. Once our reference case reached its equilibrium (with the inter-ELM plasma background), successive short time steps with alternating ELM-peak and inter-ELM plasma backgrounds were simulated. The lengths of the time steps were chosen to be 0.1ms for the ELM peak and 5ms for the inter-ELM phase, matching roughly the real durations of these phases. The onset of ELMs leads to redistribution of deposited carbon, and after a short transient a new equilibrium surface distribution is obtained, however, at the SIMS measurement lines the difference between equilibria is hardly visible. The net deposition drops from the equilibrium value of 17% to about 8% during this transient but raises quickly back to about 16%. In the simulation the duration of the transient is about 0.3 seconds.

4.3. PARAMETER STUDIES

Several modelling studies with the ERO code indicate that deposited soft carbon layers would be 3 to 5 times more prone to erosion than graphite [8, 9, 10]. Therefore we used a re-erosion enhancement factor fre, and its value was set to 10 in our reference case. We investigated the effect of varying fre by scanning through the range f_{re} = 1...10 and it turned out that best match to measured local deposition is achieved with f_{re} = 2.5...7. This is illustrated in figure 5 (red bars) where the experimental range accounts for the uncertainty due to methane leakage. Local deposition in other simulation cases is also included in the figure (blue bars, see below).

In the EDGE2D/NIMBUS work [2] it was assumed that the injected $^{13}CH_4$ can be described as ^{13}C atoms. To estimate the validity of this assumption we have run ERO also by injecting atoms instead of molecules. ERO uses by default a thermal distribution of molecules whereas in fluid codes the emission energy of atoms is typically of the order of surface binding energy. Moreover, the sticking assumption S = 0 for hydrocarbons in the case of CH_4 injection is to be compared with the typical sticking behaviour of atoms, given by the TRIM data. The typical reflection coefficient is 0.3, so a comparison was run with S = 0.7 for hydrocarbons. With this assumption the deposition pattern becomes much more peaked than the measured one. However, the bars 5 and 6 in figure 5 show that the difference in local deposition between atomic/molecular injection is small. With a higher injection energy (EDGE2D assumption, bar 7) the local deposition drops by some 50%, which compensates for the higher sticking, and the locally deposited fraction in fact coincides with measurements. On this basis the assumptions used in EDGE2D provide a reasonable starting point for modelling global migration.

If the shadow model is disabled, the deposition pattern peaks strongly in the vicinity of injectors. Therefore the high measured deposition in the shadow along “SIMS A” measurement line cannot reproduced. Also the amount locally deposited (about 7%) remains much below the measured value.

Finally, the calculation of test particle motion in ERO is based on a relaxation time approximation of the Fokker-Planck equation and requires that one explicitly specifies the distribution functions for all plasma particle species. In the derivation it is assumed that these distributions are Maxwellian. Due to parallel temperature gradients in the plasma, higher-order corrections, thermal forces, are needed for a more accurate description. We have implemented the calculation of thermal forces for the divertor version of ERO. The temperature gradients are directly evaluated from the EDGE2D plasma solution by a preprocessor. In the present simulation cases the gradients are of the order 6×10^{-2} eV/mm in the poloidal plane, but B is nearly toroidal. Therefore the gradients projected along B are as weak as 4×10^{-3} eV/mm and the effect of thermal force remains negligible.

CONCLUSIONS

Local deposition in the 2004 JET divertor tracer injection experiment was carried out with the ERO code using EDGE2D plasma backgrounds. Measured 13C distributions can be closely reproduced by assuming enhanced re-erosion of deposits and negligible re-erosion in the shadowed areas. Sensitivity of the results was studied with parameter variations and the effect of ELMs addressed by using different fluid plasma solutions in ERO. The analysis will be continued with a comparison to spectroscopic measurements, which helps validating the ionisation/dissociation data used in ERO. Modelling of gap deposition will be carried out by interfacing ERO with the 3DGap code for more realistic geometry description. The results of these more detailed analyses will be published in a subsequent paper.

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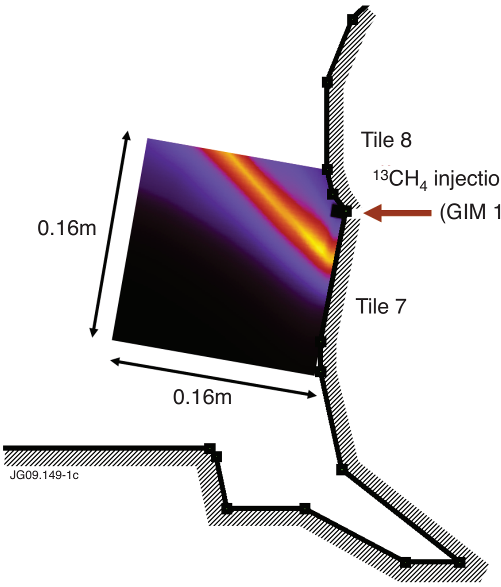

Figure 1: Simulation volume.

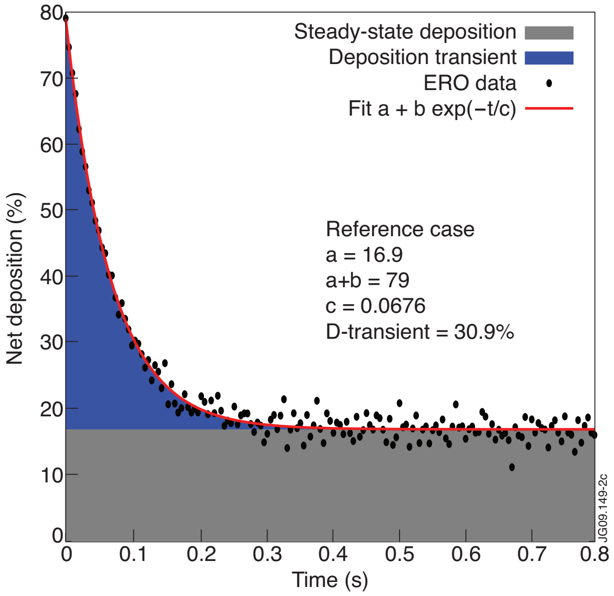

Figure 2: Time evolution of net deposited fraction (relative to the injection rate) in the reference case. The initial transient deposition (blue area) increases the simulated tarcer accumulation shown in figures 3 and 4. After 0.8s (end of simulation) the excess amount of 31% above the deposition obtained at the steady-state rate over the same time interval (grey). Because the homogeneous material mixing surface model is used, the actual time scaling may not be realistic but depends on the selected interaction layer thickness, which is 5nm here.

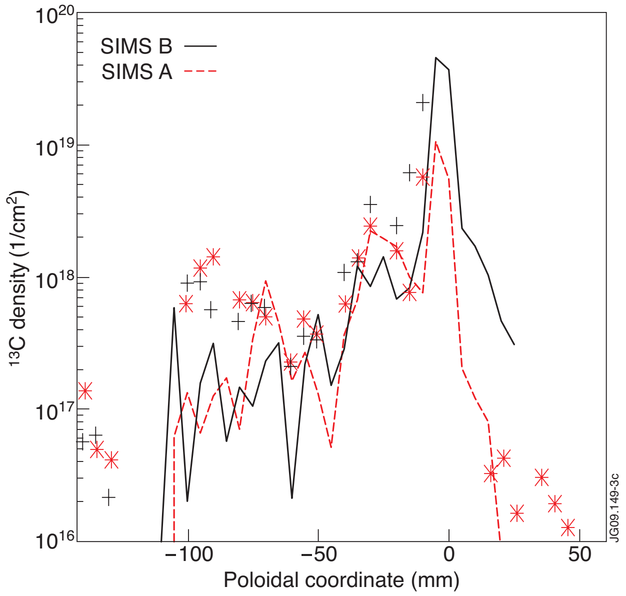

Figure 3: Poloidal profiles of the deposition along SIMS measurement lines in the reference case. Lines: ERO simulation, markers: SIMS measurement.

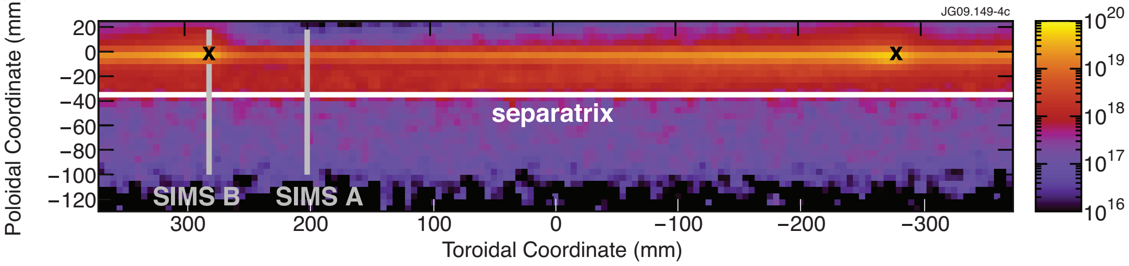

Figure 4: Deposition pattern in the reference simulation. Injector locations are marked with "x" and SIMS measurement lines shown in grey.

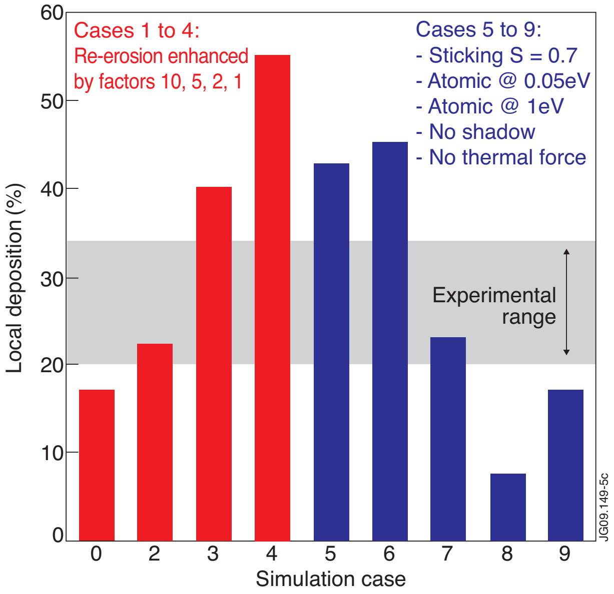

Figure 5: Local deposition with different values of the f_{re} erosion enhancement factor f_{re} and for various cases with other modelling assumptions (all with f_{re} = 10). Match to experiment is achieved with f_{re} = 2.5...7.