Kinetic Modelling of Carbon Migration in Scrape-Off Layer Plasmas and Comparison with Experimental Data

J Seebacher¹, S Kuhn², D Reiter³, S Lisgo⁴, P Börner³

¹ Institute for Ion and Applied Physics, Association EURATOM-ÖAW, University of Innsbruck, A-6020 Innsbruck, Austria
² Institute for Theoretical Physics, Association EURATOM-ÖAW, University of Innsbruck, A-6020 Innsbruck, Austria
³ Institute for Energy Research – Plasma Physics, Forschungszentrum Jülich GmbH, EURATOM Association, Trilateral Euregio Cluster, D-54245 Jülich, Germany
⁴ EURATOM/UKAEA Fusion Association, Culham Science Centre, Abingdon, UK

1. Introduction

Studying carbon migration and the deposition of carbon in the scrape-off layer plasma of modern tokamaks is an important issue, because carbon is one of the favored materials in the design of divertor targets. ITER will start its operation with a divertor target made from carbon fibre composite materials, and hence erosion and transport of carbon atoms and ions have to be considered for ITER as well. For describing the physics of transport of carbon ions the B2-EIRENE [1] code package is widely used in fusion research for various applications. Therein carbon impurity ions are treated in the fluid picture, which is correct for higher charge states of carbon but becomes inaccurate for the lower charge states. Moreover, short living molecular ions, e.g. CH₄⁺, x=1,…4, cannot be treated in the fluid picture and always require a kinetic description. For this purpose the EIRENE code has been recently expanded by a new physics module which allows treating short living ions more accurately on a kinetic level. The particular reason for this improvement was to enable B2-EIRENE to treat the break up and transport of hydrocarbons and their molecular ions simultaneously in one unified kinetic code. Currently the expanded EIRENE code does not contain a transport model in real space for taking into account diffusive (anomalous) transport effects perpendicular to the B-field, which currently still limits the application range to cases where neo-classical transport effects (drift orbits plus Fokker-Planck collisions in velocity space) are strong. This is for example the case for the spherical tokamak MAST [2] scrape-off layer plasma where magnetic field non-uniformity is pronouncing the newly included effects in EIRENE, because of its low aspect ratio. Therefore this machine is particularly well suited for first verification and validation applications of the extended code model.

2. The new TRACE ION MODULE for EIRENE

The kinetic Monte Carlo transport code EIRENE [1] is a well established tool for modelling
neutral gas, radiation and, in very crude approximations, also trace ion transport phenomena in Scrape-Off Layer plasmas. A new and far more detailed transport module for guiding centre averaged ionised particles, referred to as Trace Ion Module, has been developed over the last years for the EIRENE code. The details of the new code module have been described in Ref. [3]. This now allows a substantially refined unified treatment of neutrals, ions and PWI effects, which is important, e.g., for modelling the break up and transport of hydrocarbons (and their molecular ions) in the edge plasma region. The Trace Ion Module contains a full Fokker Planck collision operator, which takes into account classical relaxation processes as well as the thermo effect and pressure gradient force. Moreover, a guiding centre–orbit integration technique has been incorporated into EIRENE, replacing the former 0th order model in which trace ions directly followed the magnetic field lines. This now allows solving the drift kinetic equation for impurity ions in 3d2v inside the Monte Carlo framework of the EIRENE code. The updated EIRENE code is currently being verified and validated in order to enable, in the near future, simultaneous treatment neutral transport (atoms and molecules), radiation transport (by photon gas simulation) as well as transport of charged particles (atomic and molecular ions, guiding centre approximation), all on the same footing. In the present contribution we describe first modeling applications to geometrical and plasma conditions relevant for MAST

3. Modelling Methane Break Up and Transport in MAST

The extended EIRENE code has been applied to carbon migration studies as well as methane gas puff modelling for the TEXTOR and MAST tokamaks. In the present work only the results from methane gas puff modelling in MAST will be considered. From the simulation results line radiation profiles of the most prominent lines of carbon, CII (C⁺) and CIII (C⁺⁺), have been calculated, which then have been confronted with CCD camera images from experiments. The EIRENE code requires 2D or 3D background plasma fields as input, which can be either provided by a plasma fluid code, e.g. B2, EMC3, or directly from measurement. Here the edge and SOL plasma solution for MAST-discharge #13949 has been obtained with 2D OSM code modeling [4]. During this discharge methane has been puffed into the plasma from the lower inboard side (exact location r=0.281, y=-1.22). This puffing was toroidally symmetric, thus a 2D simulation is sufficient. The break up of methane in the simulation has been described by the METHANE data base [5], ionisation and recombination cross sections of the resulting atomic carbon ions have been taken from the ADAS data base (adf11, scd94 and acd94) [6]. The final dissociation fragments of CH₄, are the atomic carbon atoms and
ions. The emissivity of $C^+$ at 514nm (CII) and $C^{2+}$ at 465nm (CIII), respectively, have been measured during this discharge with a filtered CCD camera system. The raw images of the CCD camera have been inverted via ray tracing methods to enable direct comparison with the simulation results. The simulation of the methane gas puff with EIRENE has provided complete edge and SOL density and temperature profiles of all methane fragments and the related carbon ions. The radiation emission profiles of $C^+$ and $C^{2+}$ from simulation have been obtained in a post processing step. Photon emissivity coefficients for the specific wave lengths have again been taken from ADAS (pec96#c_vsuc1, pec96#c_vsuc2) to convert density profiles into line emissivities.

4. Comparison of Simulation Results with Spatially Resolved CCD Camera Images

In the simulations the impact of each of the included effects has been studied and it turned out that reasonable matching between simulation and measurement can be achieved with the extended code, which now includes gradient and curvature drift effects, a model for parallel and radial electric field, the mirror force and the full Fokker Planck collision operator, which has been extended to simulate the thermal force effect on a kinetic level. Not all these new effects are crucial for this particular comparison, e.g. the contribution of the thermo effect was negligible here because of the relatively flat temperature gradients in the region where carbon ions have deposited. This, and the other newly included effects are currently being tested independently on dedicated test-model cases.

![Emissivity of $C^{2+}$, 465nm: CCD image (uncalibrated) vs. EIRENE simulation](image)

Figure 1: Emissivity of $C^{2+}$, 465nm: CCD image (uncalibrated) vs. EIRENE simulation

An example of the MAST simulation is shown in Figure 1, where the emissivity of $C^{2+}$ at 514nm (CII) from simulation is compared with the corresponding inverted CCD camera
image. While satisfactory agreement between simulation and measurement has been achieved for the radiation of $C^{2+}$ at 465nm the simulated CII pattern does not match very well the CCD image. This discrepancy might be related to the very short life time of $C^-$, where the initial source distribution of $C^-$ (in the present case coming from the methane fragmentation exclusively) may be more important for the final distribution than the transport of the $C^-$ ions. This is the only source of carbon in this case, because intrinsic sputtering has been turned off in the simulation and the light from intrinsic carbon has been subtracted in the measurements. With the expanded EIRENE code the release, brake up of methane and transport of resulting atomic carbon ions in the MAST SOL has been studied on a kinetic level. First applications discussed here look reasonable and indicate that kinetic trace ion transport can indeed be carried out within the framework of the EIRENE Monte Carlo Code.

If further verification and validation of the newly added trace-ion-transport options in EIRENE is successful, then this tool will allow a significantly improved treatment of kinetic effects in edge transport codes without requiring additional code interfaces or code-to-code data transfer.

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**References:**


