RECENT PROGRESS IN IMPROVEMENT OF ATOMIC AND MOLECULAR PROCESS TREATMENT IN EIRENE-NGM

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1. INTRODUCTION

The EIRENE code [1][2] also known as Neutral Gas Module (NGM) is a multi-purpose Boltzmann-equation Monte-Carlo (MC) solver typically employed in an iterative scheme with a Computational Fluid Dynamics code (CFD) such as SOLPS-ITER [3] and EDGE2D-EIRENE [4] (also EMC3-, SOLEdge3X- etc.). It can track atomic and molecular (A&M) neutrals and ions kinetically, however ions are mostly handled on the CFD side. An essential part of the NGM are the collisional-radiative models (CRMs) treating A&M processes and involving both main-plasma species and impurities. This includes ionization-dissociation-recombination and elastic processes. Numerical simulations with EIRENE-NGM are indispensable for both understanding and predicting the fuel and impurity transport in the edge and divertor areas of fusion devices. The transport determines impurity penetration towards the core, plasma exhaust and plasma-surface interaction (PSI) issues largely determining the device duty cycle. The modelling insight into the interplay of transport and A&M processes is key for understanding detachment phenomena [4]. A main issue for simulations at the ITER or DEMO scales is the CPU cost, which is mostly on the kinetic side of the EIRENE-CFD packages, in that the A&M processes are responsible for complexity of particle histories. Another issue is the growing requirements for the A&M data, in both quantity and detail also type multiplicity which also affects the performance issues.

The focus of this work is on the general improvement of the A&M and CRM part in EIRENE as well on the associated external tools and data bases. Validation of reaction datasets (both structure and content) in the EIRENE-related CRMs, in view of the prominent role of A&M processes during detachment and of the necessary massive data extension to resolve rovibrational states. The data amount and complexity require improved tools for visualization, processing, and quality/consistency control. The web-based toolkit PLOUTOS is a standard pre-processing tool for EIRENE. It can provide automatically the EIRENE input. By CRM we mean both the A&M reaction rate dataset and the solver, which can be a part of EIRENE or an external tool mostly neglecting transport effects. The PLOUTOS solver is external, but related to the full-scale CFD-EIRENE simulations. The new ModCR code is aimed to eventually substitute both internal and external solvers as well as a significant part of the data processing (DP) (see below). The established alternative external CRM YACORA [5][6] is used as well as the neutral code EUNOMIA (similar to EIRENE but aimed at linear devices) [7] with high molecular background pressure. A large effort is given to harmonizing the data and assumptions in the various CRMs, as well as demonstration of various particular effects: significance of particular reactions, effect of resolving the vibrational states (available e.g. in mccc-db.org), isotopes, etc. The last significant development line is a photon tracing module and the effect of photon transport on opacity and the plasma ionisation balance.

2. PHOTON TRANSPORT AND OPACITY

The EIRENE photon transport model applied to JET-ILW L-mode plasma solutions from SOLPS-ITER has revealed the contribution of Ly-β opacity towards D_α emission relative to other processes [9]. The model has indicated local regions with high Ly-α and Ly-β opacity in high-recycling and detached conditions. This opacity effect is predicted to reduce the Ly-α and Ly-β signals from the low-field side divertor by at least a factor of 2. The contribution of Ly-β to the population density of D (n = 3) is mostly localized near the emission source. In low-recycling regime, Lyman opacity is negligible. Ly-β is dominant in the high-recycling regime with predicted doubling of D_α peak emission values. In the detached regime, contribution from atomic recombination is dominant, but Ly-β capture remains relevant with predicted doubling of D_α emission in the private flux region and 50% enhancement at the strike point. In conclusion, opacity effects must be considered for the analysis of Ly-α, Ly-β and D_α diagnostics in high-recycling and detached conditions. Earlier it was shown that the photon absorption can also have a ~20% effect on the ionisation.

3. MODCR DEVELOPMENT

The new module "ModCR" is under development [10]. It is intended to eventually replace both the related routines in the main loop of EIRENE as well as the standalone CRM solvers (e.g. in PLUTOUS), largely improving performance and providing new functionality. It is also aimed to meet the challenge of the exploding amount of molecular data due to the necessity to include the vibrational [6] (and even rotational) states and hydrogen isotopes or atomic states with matastables [8]. ModCR is also meant to provide:

- Dynamic changes in the state population instead of typically used local thermodynamic equilibrium (LTE). The resulting balance equations (ODEs) are solved numerically by CVODE or MC.
- Critical increases in performance due to the reduced number of MC species to be tracked, substituted by state population variables with a flexible border between both approaches.
- A realistic workload for the EIRON toy-model of EIRENE, used to evaluate parallelisation, domain decomposition, and fluid-kinetic hybridisation concepts.

4. SUMMARY

The presentation aims to give an overview of the recent development of A&M CRMs in EIRENE-NGM including the external DP tools and performance. This includes the new module ModCR, refining and extending the photon transport module within EIRENE, the web-based pre-processing tool PLOUTOS and assessment of the CRM effect on performance utilizing the EIRON toy-model for EIRENE. The overview includes application results for validation of the new features and data as well as demonstration of their significance.

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