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Tracking of internal states in CRMs employed in the transport codes

The collisional-radiative models (CRMs) play a significant role in the Monte-Carlo (MC) transport codes used for edge and divertor plasma in fusion relevant devices. In turn, the codes like the impurity transport code ERO [1] or the more oriented on the main plasma species EIRENE [2] are indispensable for the understanding of the interplay of various processes in edge and divertor plasmas of fusion devices also in relation with the plasma-wall interaction and power exhaust. The study of detachment phenomenon including the dominating atomic and molecular (A&M) processes is of particular interest. EIRENE needs iterations with a fluid plasma codes like for instance Edge2D or B2.5 (making up the SOLPS-ITER package [3]) to produce a self-consistent simulations which are often used as a background plasma input for ERO. Therefore it is of great value to unify the CRMs in all the deeply interconnected codes. Both main plasma species containing hydrogen isotopes H/D/T including molecular neutrals and ions and main impurities like beryllium, tungsten, argon, etc. are to be included into simulations, thus in CRMs, including related spectroscopy as well as impact on particle, momentum and energy balance. Recently a large effort [4] is put into the improvement of the EIRENE code which includes restructuring and extension of the CRMs associated with it. This includes development of the PLOUTOS tool for A&M data pre-processing for EIRENE (allowing flexible setting of various model assumptions), which however also contains a stand-alone (SA) solver for CRM. Another SA CRM used is YACORA [5] containing a very established and up-to-date A&M data collection. It was shown multiple times that despite standalone CRMs neglect most part of transport effects they can produce insights into the physics and even practically useful simulation results [6].

The systematic challenges for any CRM employed inside the transport codes are a) the variety and amount, thus controllability of the data and b) decrease of the code performance. Both issues are addressed to a certain extent by the code structure in EIRENE providing much of the data preparation before entering the main loop –rates are pre-calculated for every volume cell inside which the plasma parameters (often taken from the fluid code) are fixed. The reaction data structure was further optimised to reduce the branching by the reaction types. Nonetheless, the upcoming dramatic increase of the data due to necessity to consider rovibrational states in molecules or simply very complex elements like tungsten (W) requires tracking the internal state of the species. This, however must not necessarily be the full-detailed CRM, but can be a reduced essence of it. Earlier, the ERO code has demonstrated the tracking of the internal states in beryllium (Be): just 2 BeI states (the ground and the metastable ones) allowing to capture mostly the population dynamics provided by the whole CRM - these are different options provided in ADAS [7]. Similar effort was provided for WI with various number and bundling assumptions of the tracked states. In case of 2 states tracked a fully analytical approach can be used for solution of the time-dependent evolution of the populations; for more states matrix exponent based solution is applied. The present work suggests how this approach can be used for molecular species. Tracking the vibrational states as independent species is demonstrated by Edge2D-EIRENE, however this leads to enormous CPU time demands if a decent MC statistic for each vibrostate is provided. Tracking of state populations as internal variables will remedy that on a price of negligible numerical bias error in case the ionisation and other processes impacting the specie transport are little dependent on its particular vibrational state. It is of importance to provide a flexible link and data pre-processing procedure between the SA CRM like PLOUTOS and the internal tracker inside the main loop of EIRENE.

The presentation is aimed to overview the already developed parts on the internal state (e.g. metastable) tracking with few illustrations for BeI and WI spectroscopy in edge plasma and to present a concept of how this experience can be used in EIRENE with PLOUTOS for molecules.

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