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Status of A&M database and data analysis for fusion edge plasma transport studies

Atomic and molecular data are of relevance in fusion boundary layer plasmas, because reactive processes actively influence (and even control) the plasma flow and divertor dynamics in the near target surface domain in reactors.

These data are an important ingredient in fusion transport simulations of advective-diffusive-reaction type (codes such as B2-EIRENE (SOLPS) in EU, UEDGE in the US or SONIC in Japan). Data at the most detailed level enter such transport simulations in kinetic (microscopic) model components, i.e. neutrals (atoms and molecules, molecular ions, and weakly ionized impurity ions such as e.g. W, N, C, Be, He), whereas the macroscopic (fluid) components use condensed, reduced information and atomic collision processes.

The database HYDKIN (www.hydkin.de) of the EIRENE Monte Carlo code has been set up and is currently being developed to publicly expose the unprocessed raw A&M data used in B2-EIRENE. The underlying A&M dataset has either been compiled at FZJ in the past (e.g. the current hydrocarbon, and silane cross section databases), or data have been taken from publicly available other datasets (e.g. ADAS) or CR codes (H, H2, He) from NIFS.

The second purpose of the online tool HYDKIN is processing and analyzing data, prior to their activation in complex transport models. 1D (either time or, recently, also 1 spatial coordinate) test cases are solved, based upon an eigenvalue analysis of the underlying reaction master matrix. This enables a forward sensitivity analysis (evaluation of sensitivity coefficients defined as logarithmic derivative of CR population density wrt. reaction rate coefficients.

The eigenvalue analysis carried out on plasma chemistry models in HYDKIN gives direct indications about the existence of underlying reduced chemistry models (e.g. by a separation of fast against slow modes). A targeted application here was a H/H2/H2+ CR model, because presence of vibrational excitation at least of ground state H2 (and isotopomeres) provides a rather continuous spectrum of time scales, strictly ruling out condensation of vibrational kinetics into bundled rates.

Recent extensions of HYDKIN datasets have started with respect to the Be, BeH, BeH+ system, and the N, N^+, N_2, N_2^+ N_2- system, the former because of its relevance due to the choice of Be as ITER (and JET) main chamber material, the latter because of its possible important role as active edge plasma cooler in case of all metal divertors. Whereas the database wrt. the Be-family is rather sparse, the issue wrt. N,N_2, and their ions is just opposite: the huge amount of data available (e.g. from atmospheric research, space vehicle re-entrance issues, etc., requires primarily a critical evaluation, condensation and recommendation for the fusion community.