TSVV-K : Plans for 2026

Contributions from Aalto University

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Work plan for 2026: obtain and assess first SOLPS-ITER predictions with dedicated reaction rates for deuterium and tritium molecules

- Technical implementation and testing of inline CRM (Sawada model) in EIRENE for hydrogenic molecules (H2_COLRAD) for multiple-parameter reaction rates (beyond current 2-parameter fitted rates as function of n_e and T_e)

→ Separation of hard-coded reaction rates and other inputs in easily interchangeable data entries (input files → subroutines → "something better" for computational speed)

→ Revision of critical reactions for **deuterium and tritium**, e.g., proton charge transfer rate $H^+ + H_2(v) \rightarrow H + H_2^+$, AMJUEL H.3 3.2.3, dissociative attachment rate $e^- + H_2(v) \rightarrow H_2^- \rightarrow H + H^-$, AMJUEL H.2 2.2.17

- Validation of impact of inline CRM (and Ly-alpha opacity, post-processing using Cherab for synthetic JET diagnostics) in SOLPS-ITER simulations (standard → wide grid) for JET-ILW hydrogen, deuterium and tritium plasmas → R. Chandra, PSI 2026 invited

- Assessment of impact of Ly-alpha opacity and inline CRM in SOLPS-ITER simulations for JT-60SA and ITER → DEMO

Work plan for 2026: revise CRM input data, assess differences in rates and impact on predicted divertor conditions

- Assessment/revision/replacement/update of outdated (H2VIBR) rates for vibrationally resolved molecules (ground and excited states) using interchangeable data entry formats
  - E.g., with Scarlett (MCCC, Scarlett, Atoms 2019) and Laporta rates ('local-complex-potential' method, Laporta et al., PPCF 2021) as in Bergmayr et al., using Yacora H2($X^1\Sigma_g^+$,v) model (Eur. Phys. J. D 77 (2023), 136. for hydrogen → **deuterium and tritium**
- Assessment of application of Sawada 2015 (Sawada et al., Atoms 2016) or Yacora H2(v,N) models (Bergmayr et al., JQSRT 2025) to predict measured Fulcher band