KU LEUVEN

TSVV5 – Neutral gas dynamics in the edge

Progress report KUL-TME 2022 & Workplan 2023

W. Dekeyser, W. Van Uytven, N. Horsten, V. Maes, S. Carli, E. Loevbak, M. Blommaert, G. Samaey, M. Baelmans

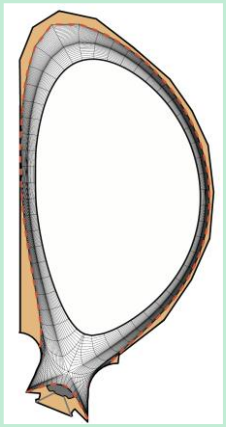
A hierarchy of neutral models

Advanced fluid neutral models

- Efficient (direct) coupling to plasma equations, no MC noise
- Basis for hybrid methods
- Good accuracy in highly collisional regimes

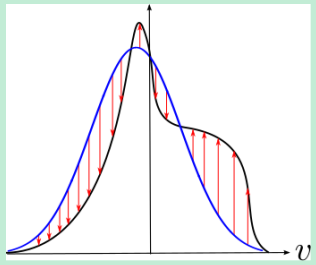
Hybrid fluid-kinetic models

Spatially (SpH)



- F-K transition based on location
- User-defined transition criteria

micro-Macro (mMH)



$$f_{\mathrm{n}}(v) = f_{\mathrm{n,f}}(v) + f_{\mathrm{n,k}}(v)$$

- Decomposition in velocity space
- Can be made **fully equivalent** to kinetic model

Kinetic model

- Most complete physical description
- Flexibility w.r.t. geometry, collisional processes, sources, boundary conditions,…
- Very expensive in highly collisional regimes

Model accuracy

Computational efficiency

CPU × 1/10?

KU LEUVEN

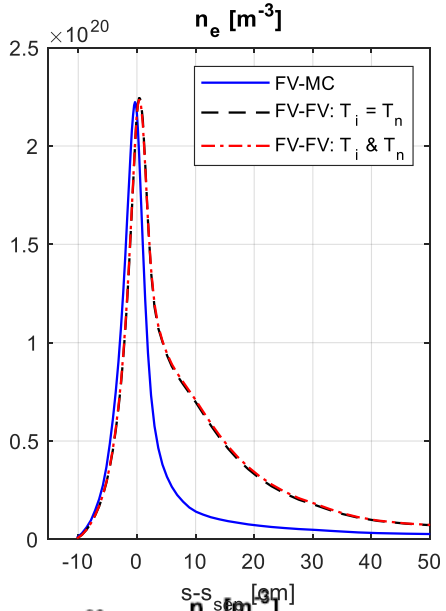
Summary of achievements 2022

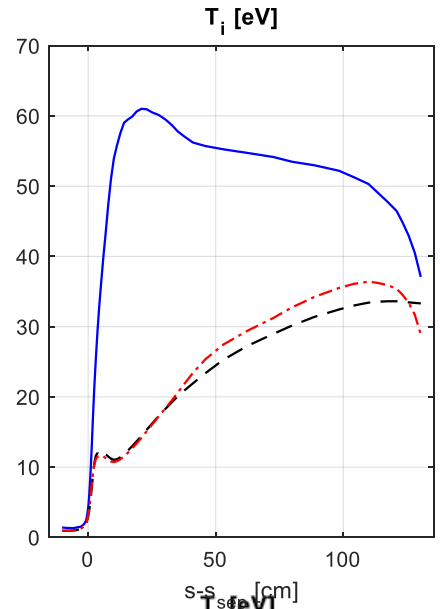
- Application Advanced Fluid Neutral models to ITER case, realistic wall materials [W. Van Uytven et al. NF 2022]
  - Consistent numerics essential for good agreement with kinetic results (9pt stencil, isotropic flux limits,…)
  - Impact wall material: more fast reflection with metallic wall (W) => larger kinetic corrections needed compared to low-Z materials (C, Be)

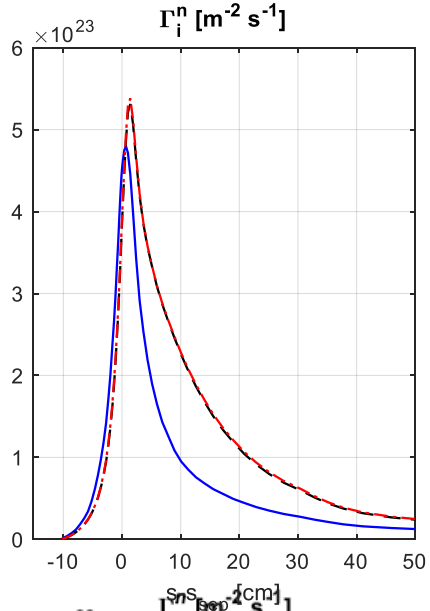
- Extension Advanced Fluid Neutral models to account for drifts [W. Van Uytven et al. NME 2022]
  - Additional advective transport term in AFN model
  - Correctly includes effect of drifts on neutral transport compared to kinetic simulation (link with ion neutral current)
  - But: impact of drifts on background plasma solution is by far most dominant contributor compared to direct impact of drifts on neutral transport

Application AFN to ITER case, W-Be wall

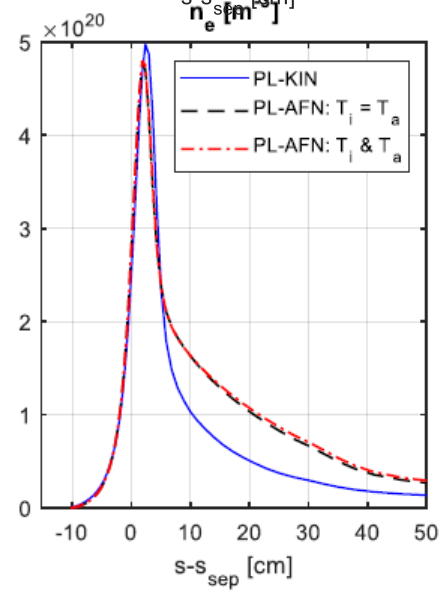
$n_{i,c} = 4 \cdot 10^{19}\ m^{-3}$

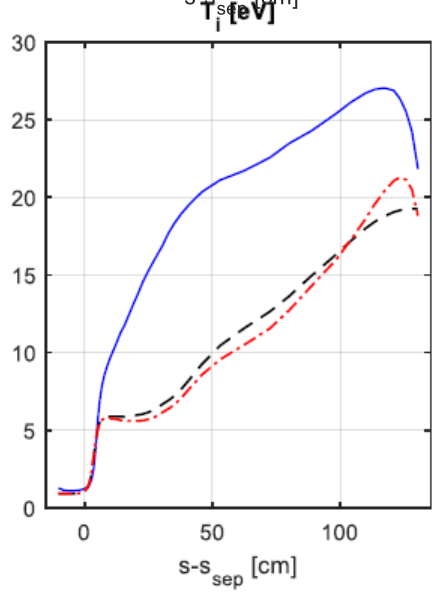


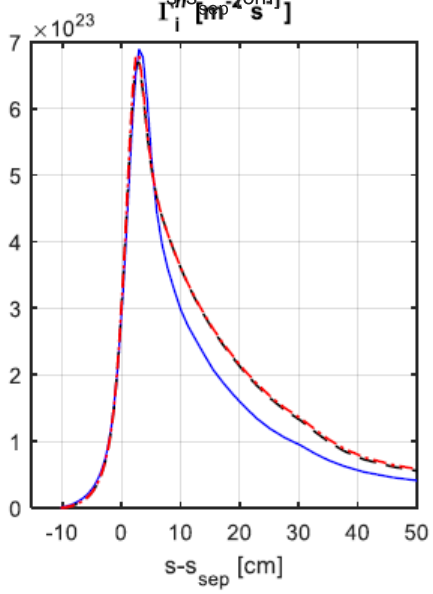


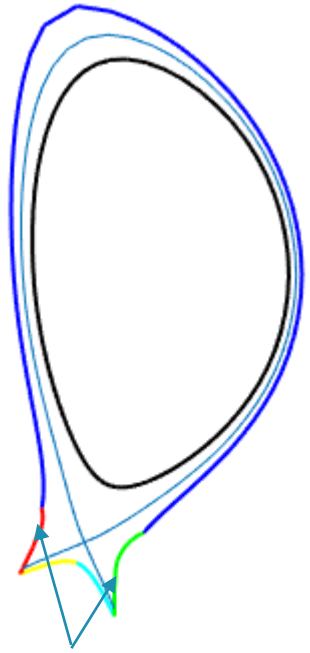


$n_{i,c} = 8 \cdot 10^{19}\ m^{-3}$





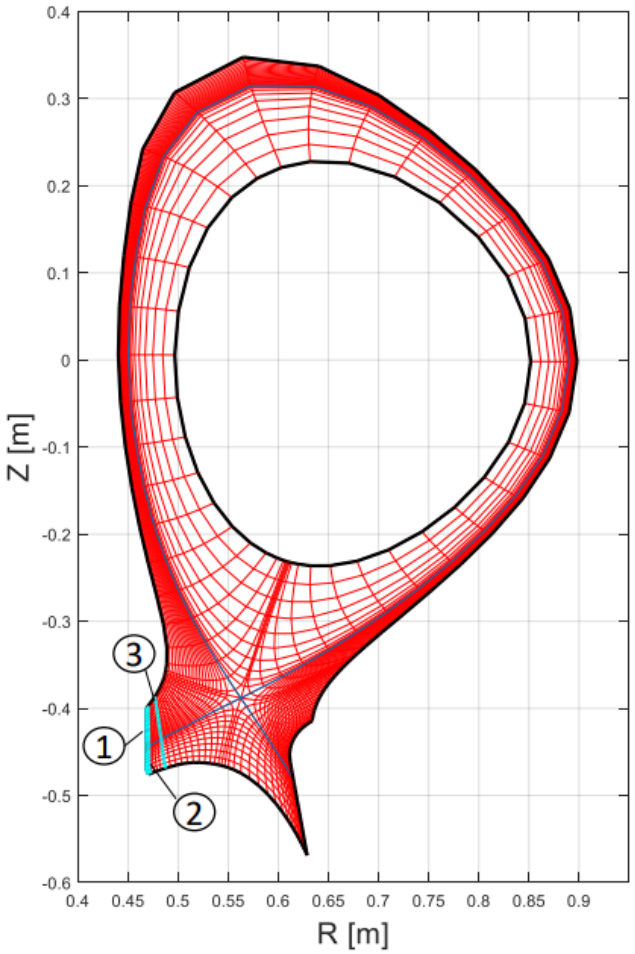




Tungsten

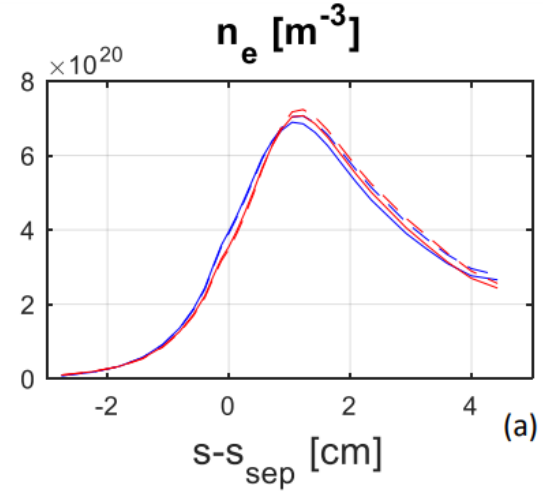
Tungsten
→ *more fast reflection*
→ *higher T and Kn*
→ *reduced validity fluid neutrals*
→ *correct with hybrid approach*

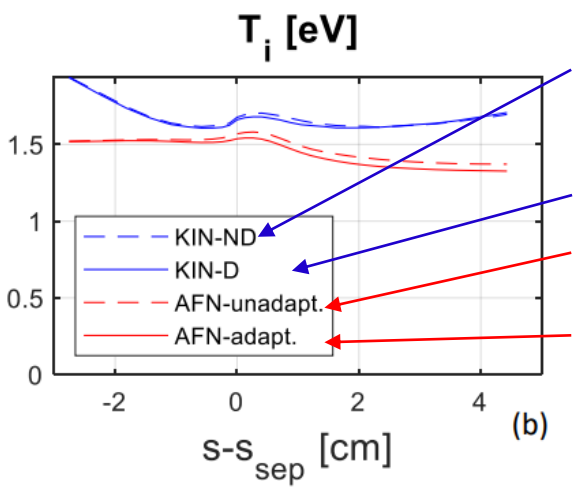
Application AFN to Alcator C-mod case with drifts

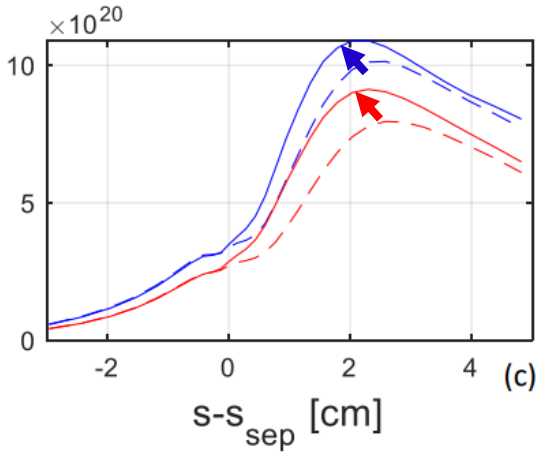


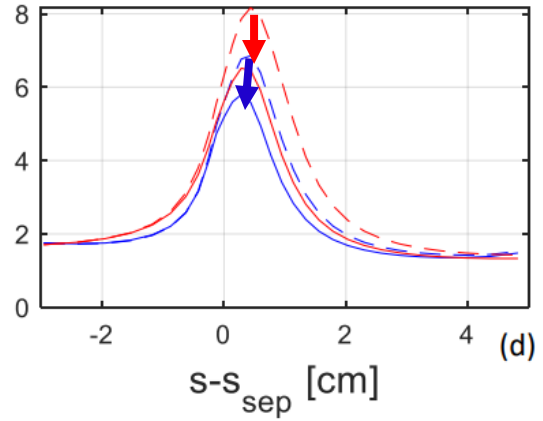
1

3









Kinetic solution, but drifts removed from ion background for EIRENE

Kinetic solution

AFN without drift corr.

AFN with drift correction

Summary of achievements 2022

- Validation fluid, (SpH) hybrid and kinetic neutral models for JET ILW L-mode plasmas [N. Horsten et al., NME 2022]
  - Realistic tokamak configuration, incl. voids, molecules,…
  - Large fluid-kinetic discrepancies at low density (factor 2), but smaller discrepancies at higher density (50%)
  - Fluid-kinetic discrepancies in both density regimes successfully corrected by hybrid approach
- Alternative hybrid approach that avoids cancellation errors by construction under development
  - Hilbert expansion based fluid model derived; both diffusive & hydrodynamic scaling investigated [V. Maes, in preparation]
  - Corresponding kinetic correction model: WIP
- Release of fluid and hybrid approaches in extended grids version of SOLPS-ITER to the community during dedicated workshop hosted @ KU Leuven, November 14-18, 2022

KU LEUVEN

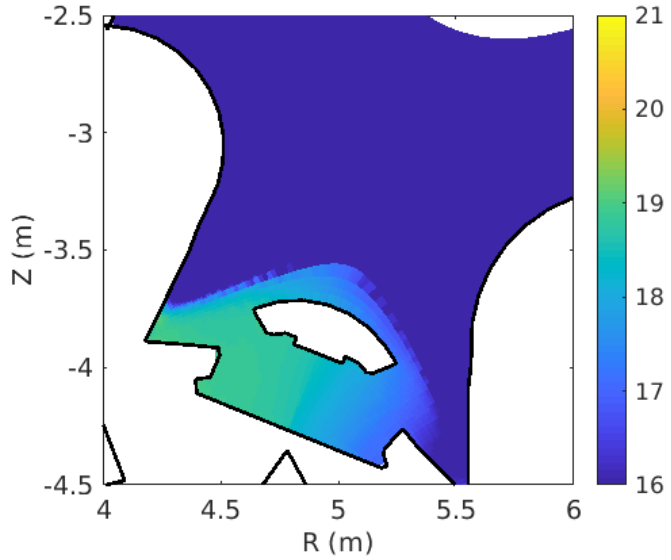
Summary of achievements 2022

- Progress towards implementation of derivatives based on algorithmic differentiation (TAPENADE) into EIRENE
  - SOLPS-ITER extended grids version selected for implementation (also differentiated B2.5 available)
  - Integration of updated EIRENE version (v3.0.8) ongoing; further removal of ‘old’/unsupported FORTRAN features not supported by TAPENADE
  - Initial processing of the code by TAPENADE successful

KU LEUVEN

Workplan 2023

- Further enhancements & application AFN & SpH to ITER/DEMO [W. Dekeyser; W. Van Uytven]
  - Introduction of n-n collisions in AFN model
  - Application to ITER case, extended grids, incl. sub-divertor area
  - Application to DEMO SN case
- Algorithmic differentiation w. TAPENADE [N. Horsten, S. Carli]
  - Investigation of memory issues for differentiation forward mode
  - Forward sensitivity computations in standalone EIRENE cases
  - Investigation of differentiation of coupled B2.5-EIRENE code, forward mode
- Kinetic-diffusion scheme [E. Loevbak, G. Samaey]
  - Investigation of estimators for diffusive Monte Carlo schemes
  - Implementation of kinetic-diffusion scheme in EIRON
  - Study of feasibility of implementing kinetic-diffusion scheme in EIRENE



References

- Van Uytven, W., Dekeyser, W., Blommaert, M., Horsten, N., Baelmans, M. (2022). Effect of drifts and currents on the validity of a fluid model for the atoms in the plasma edge. Nuclear Materials And Energy, 33, Art.No. 101255. doi: 10.1016/j.nme.2022.101255
- Horsten, N., Groth, M., Dekeyser, W., Van Uytven, W., Aleiferis, S., Carli, S., Karhunen, J., Lawson, K., Lomanowski, B., Meigs, A., Menmuir, S., Shaw, A., Solokha, V., Thomas, B., JET Contributors, (2022). Validation of SOLPS-ITER simulations with kinetic, fluid, and hybrid neutral models for JET-ILW low-confinement mode plasmas. Nuclear Materials And Energy, Art.No. 101247. doi: 10.1016/j.nme.2022.101247
- Van Uytven, W., Dekeyser, W., Blommaert, M., Carli, S., Baelmans, M. (2022). Assessment of advanced fluid neutral models for the neutral atoms in the plasma edge and application in ITER geometry. Nuclear Fusion. doi: 10.1088/1741-4326/ac72b4
- Maes, V., Dekeyser, W., Koellermier, J., Baelmans, M. Samaey, G. Hilbert expansion based fluid models for kinetic equations describing neutral particles in the plasma edge of a fusion device. In preparation for submission.
- Loevbak, E., Vandewalle, S., Samaey, G. Multilevel Monte Carlo for diffusive Kinetic Equations in Plasma Edge Simulations. NumKin 2022, Date: 2022/11/07-2022/11/10, Location: Garching, Germany.

KU LEUVEN

References

- Van Uytven, W., Dekeyser, W., Blommaert, M., Horsten, N., Marandet, Y., Baelmans, M. (2022). Advanced spatially hybrid fluid-kinetic modelling of plasma-edge neutrals and application to ITER case using SOLPS-ITER. Contributions to Plasma Physics, 62 (5-6), Art.No. ARTN e202100191.
- Horsten, N., Groth, M., Dekeyser, W., Van Uytven, W., Carli, S. (2022). Combination of micro-macro and spatially hybrid fluid-kinetic approach for hydrogenic plasma edge neutrals. Contributions to Plasma Physics, 62 (5-6), Art.No. ARTN e202100188.
- Bringmans, L., Maes, V., Koellermeier, G., Samaey, G. (2022). On the mitigation of cancellation errors in hybrid fluid-kinetic methods for solving kinetic equations describing neutrals in the plasma edge. Contributions to Plasma Physics, Art.No. ARTN e202100183
- Mortier, B., Baelmans, M., Samaey, G. (2022). Kinetic-diffusion asymptotic-preserving particle schemes for the Boltzmann-BGK equation in the diffusive scaling. SIAM Journal on Scientific Computing 44 (2), A720-A744.
- Mortier, B., Robbe, P., Baelmans, M., Samaey, G. (2022). Multilevel asymptotic-preserving Monte Carlo for kinetic-diffusive particle simulations of the Boltzmann-BGK equation, Journal of Computational Physics 450, 110736.
- Mortier, B., Maes, V., Samaey, G. (2022). Estimation as a post-processing step for random walk approximations of the Boltzmann-BGK model. Contributions to Plasma Physics, e202100197.

KU LEUVEN