

# A hybrid fluid-kinetic model for plasma-edge neutrals using kinetic-fluid condensation and its application to ITER cases

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## Introduction

The neutral atoms in the plasma edge of nuclear fusion devices are typically modeled either kinetically or as a fluid. The kinetic treatment is most accurate because there is no a priori assumption on the velocity distribution of the neutral particles. This kinetic model is usually solved using a Monte Carlo code, such as EIRENE [1]. The MC treatment has two major issues, namely the introduction of statistical noise and the high computational cost in the regions where charge-exchange (CX) collisions between ions and neutrals dominate. When a fluid description is used, no statistical noise is introduced, and the need to simulate individual CX collisions is avoided. However, the fluid approach is only valid if the collisionality is sufficiently high. For these reasons, different hybrid fluid-kinetic methods are under development [2–5], which aim to efficiently combine the benefits of both methods. In this contribution, we propose a novel hybrid method based on volumetric “condensation” transitions from kinetic to fluid treatment, depending on the local collisionality of the kinetic atoms. The accuracy and speed-up of the method is showcased for a simplified ITER case.

## Method description

The validity of the fluid approach is predicted by the Knudsen number (Kn), which is defined as  $Kn = \frac{\lambda_{CX}^n}{L}$ , where  $\lambda_{CX}^n$  is the average CX mean-free path of the neutral atoms, and  $L$  is a characteristic macroscopic length scale of the problem. The fluid approach is typically assumed to be strictly valid for  $Kn < 0.01$ ,  $Kn = 0.1$  is regarded as a transition point, and  $Kn = 1$  predicts the onset of dominant kinetic effects. Similar to Kn, we can define  $Kn^p = \frac{\lambda_{CX}^p}{L}$ , where  $\lambda_{CX}^p$  is the CX mean-free path of an individual kinetic particle. In the proposed method, neutrals can originate as fluid or kinetic, but we terminate a kinetic trajectory when  $Kn^p < Kn^t$ , where  $Kn^t$  is a spatially constant user-defined transition criterion. The mass, parallel momentum, and energy of the terminated particle are then provided as sources for the fluid neutral population. The kinetic particle is said to be “condensed” to the fluid model. The sources of particles ( $n$ ), parallel momentum ( $||m$ ) and energy ( $E$ ) transferred from the neutrals to the plasma are the sum of the contributions from the fluid and kinetic part:  $S_{pl}^{n,||m,E} = S_{pl,k}^{n,||m,E} + S_{pl,fl}^{n,||m,E}$ . The steady-state fluid neutral model consists of convection-diffusion equations:  $\nabla \cdot \Gamma_n^{n,||m,E} = S_{n,fl}^{n,||m,E} + S_{n,k}^{n,||m,E}$ .

Here,  $\Gamma_n^{n,||m,E}$  represents neutral fluxes, and  $S_{n,fl}^{n,||m,E}$  represents source terms due to interaction of the fluid neutrals with the plasma by means of ionization, recombination and CX reactions. Expressions for  $\Gamma_n^{n,||m,E}$  and  $S_{n,fl}^{n,||m,E}$  in the context of the SOLPS-ITER 2D mean-field plasma edge code [7], which is used in this work, are elaborated in [6].  $S_{n,k}^{n,||m,E}$  are the source terms originating from the terminated kinetic trajectories.

The proposed method is inspired by the earlier work on the two-phases hybrid model elaborated in [3]. However, the underlying fluid model is improved [6], and there is no “evaporation” from fluid back to kinetic in the plasma volume. Due to the latter, a higher speed-up can be achieved, and buffering issues, where particles often transition from fluid to kinetic and vice versa, in regions of intermediate collisionality, are avoided.

### Application to ITER case

We test the method on two simplified D-only low-power ITER cases. 20MW of core power enters the domain, equally divided between ion and electron channels. Void regions are not included in the geometry and we use the same spatially constant anomalous transport coefficients as in [5, 6]. The core ion density ( $n_{i,c}$ ) is either  $3 \cdot 10^{19} \text{ m}^{-3}$  or  $6 \cdot 10^{19} \text{ m}^{-3}$  to achieve different levels of ion-neutral collisionality. Pumping is mimicked through a 2% neutral absorption coefficient at the private flux and main chamber wall boundaries. The target plates are made of tungsten while the other boundaries are modeled as beryllium. We assume perfect ion-neutral temperature equilibration for the fluid neutrals here. Figure 1 shows the resulting Knudsen numbers for the two standard coupled plasma-neutral simulations with  $n_{i,c} = 3 \cdot 10^{19}$  or  $6 \cdot 10^{19} \text{ m}^{-3}$ . For simplicity, we have used a spatially independent  $L = 0.1$  m, as a rough estimate for the gradient length scales in the divertor.

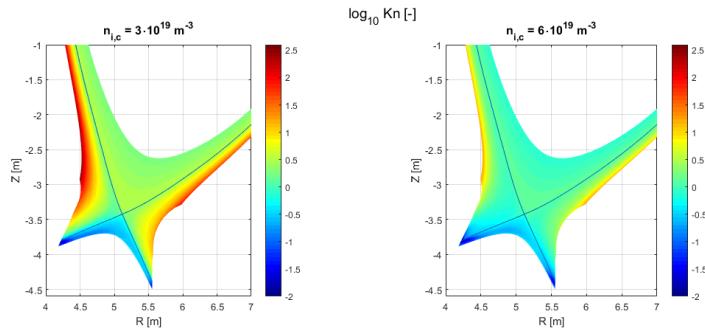


Figure 1: Knudsen numbers for the neutral particles for the standard coupled plasma-neutral solution with  $n_{i,c} = 3 \cdot 10^{19} \text{ m}^{-3}$  (left) and  $n_{i,c} = 6 \cdot 10^{19} \text{ m}^{-3}$  (right).

All ions that recycle as neutrals are launched kinetically here. The fluid neutrals incident on the vessel boundaries can either be reflected as fluid or relaunched kinetically. In general, the

edge modeler can choose the specific treatment at each boundary. Here, we opt for a kinetic treatment at the target plates. At the main chamber and private flux boundaries, we use fluid reflection. The former is justified due to the negligible presence of fluid neutrals near the main chamber boundary. The latter is possible due to the expected validity of the fluid approach in the cold private flux regions. Neutrals originating from volume recombination are directly treated as fluid, again due to the expected validity of the fluid approach in the cold regions where recombination occurs.

Figure 2 shows plasma profiles along the outer target. The agreement between the fully fluid and fully kinetic solutions is better for the higher density case, as expected. In both cases, there exists a clear mismatch between fluid and kinetic treatment at the upper part of the divertor, as could be expected from the Knudsen numbers shown in Figure 1. We observe that using  $\text{Kn}^t=1$  provides near-perfect agreement for all state variables. Even when we already allow kinetic particles to condense to the fluid population at  $\text{Kn}^t=10$ , a significant improvement compared to the fully fluid approach is obtained.

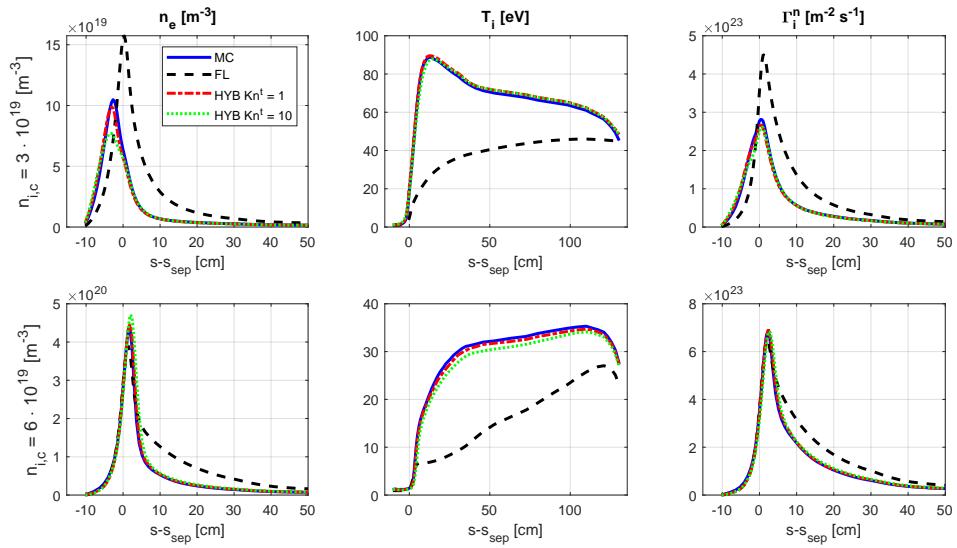


Figure 2: Plasma density, ion temperature and ion particle flux density along the outer divertor target for  $n_{i,c} = 3 \cdot 10^{19} \text{ m}^{-3}$  (top row) and  $6 \cdot 10^{19} \text{ m}^{-3}$  (bottom row). The plasma model is coupled to either the fully kinetic neutrals (blue solid line), the fully fluid model (black dashed line), the hybrid model with  $\text{Kn}^t=1$  (red dashed-dotted line) or  $\text{Kn}^t=10$  (green dotted line).

Table 1 shows the computational times needed by EIRENE for both the MC and hybrid cases, for the same number of launched particles. A total of 200 000 particles is launched, divided over the different boundary regions according to the ratios of the incident particle fluxes. For the full MC cases, the CPU time increases by a factor 3 when going from  $n_{i,c} = 3 \cdot 10^{19} \text{ m}^{-3}$

to  $6 \cdot 10^{19} \text{ m}^{-3}$ , demonstrating the dependence on the collisionality. Only the hybrid case with  $\text{Kn}^t=1$  and  $n_{i,c} = 3 \cdot 10^{19} \text{ m}^{-3}$  does not provide a speed-up, because there is only a very small region with fluid validity. In the other cases, a speed-up between 2.7 and 26.5 is achieved. A more rigorous assessment of the computational speed-up [8], also taking into account the reduced statistical noise of the hybrid method for the same number of particles, is left for future work.

	$n_{i,c} = 3 \cdot 10^{19} \text{ m}^{-3}$			$n_{i,c} = 6 \cdot 10^{19} \text{ m}^{-3}$		
	MC	HYB $\text{Kn}^t = 1$	HYB $\text{Kn}^t = 10$	MC	HYB $\text{Kn}^t = 1$	HYB $\text{Kn}^t = 10$
Tot. CPU time [s]	58.9	60.4	17.2	177.2	66.7	6.6
Speed-up		0.98	3.4		2.7	26.5

Table 1: Computational times required by EIRENE.

## Conclusion and outlook

A hybrid fluid-kinetic method based on kinetic-fluid condensation has been presented, and the accuracy was demonstrated on a simplified ITER case. Given the significant speed-up compared to fully kinetic simulations, the method is promising towards simulation of complex ITER and DEMO cases. We envisage to further extend this method to treat void regions [5] and include molecular processes [9].

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## References

- [1] D. Reiter, et al. Fusion Science and Technology 47.2 (2005): 172-186.
- [2] N. Horsten et al. Contributions to Plasma Physics 60, no. 5-6 (2020): e201900132.
- [3] M. Valentiniuzzi et al. Nuclear Materials and Energy 18 (2019): 41-45.
- [4] B. Mortier et al. Contributions to Plasma Physics 60, no. 5-6 (2020): e201900134.
- [5] M. Blommaert et al. Nuclear Materials and Energy 19 (2019): 28-33.
- [6] W. Van Uytven et al. Contributions to Plasma Physics 60, no. 5-6 (2020): e201900147.
- [7] S. Wiesen, et al. Journal of nuclear materials 463 (2015): 480-484.
- [8] K. Ghoos et al. Journal of Computational Physics 322 (2016): 162-182.
- [9] N. Horsten et al. Nuclear Materials and Energy 27 (2021): 100969.