

## Assessment of fluid neutral models for high recycling divertor conditions

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### Abstract

We compare a Navier-Stokes neutral model as well as a reduced neutral model (only parallel momentum) with a Monte Carlo solution of the kinetic equation. The Navier-Stokes model with a separate neutral energy equation gives the most accurate results. The reduced model shows to provide slightly less accurate results at a reduced computational cost.

### Introduction

The plasma edge in tokamaks is governed by plasma interacting with neutral particles. These neutrals have a significant influence on the particle and energy flow towards the divertor targets. Therefore, neutral particle transport modeling is of utmost importance for divertor studies. To take into account all important microscopic processes, the neutrals are mostly modeled using a kinetic equation that is solved with a Monte Carlo (MC) method, e.g., the EIRENE code [1]. However, the fluid approach becomes valid in the charge-exchange (CX) dominated regions for typical ITER and DEMO relevant (detached) regimes. Fluid neutral models eliminate the MC noise, which hampers the convergence of the coupled system of plasma and neutral equations.

In this paper, we assess different fluid neutral models by comparing them to the results of an MC simulation of the kinetic equation. This is done for a fixed background plasma, which is representative for a simplified high recycling case.

### Fluid neutral models

Inspired by the Navier-Stokes equations as used in fluid mechanics, a similar set of equations (continuity and momentum) can be deduced for neutrals dominated by CX collisions [2]:

$$\nabla \cdot (n_n \mathbf{V}_n) = S_{n_n}, \quad (1) \quad \nabla \cdot (m n_n \mathbf{V}_n \mathbf{V}_n + \Pi_n) = -\nabla p_n + \mathbf{S}_m \mathbf{V}_n, \quad (2)$$

with  $m$  the particle mass and  $p_n = n_n T_n$  the neutral pressure, with  $T_n$  the neutral temperature. This set of equations is solved for the neutral density  $n_n$  and velocity  $\mathbf{V}_n$ . The right hand sides of Eqs. (1)-(2) contain the particle and momentum sources, respectively  $S_{n_n}$  and  $\mathbf{S}_m \mathbf{V}_n$ . The stress tensor  $\Pi_n$  is given by  $\Pi_n = -\eta^n (\nabla \mathbf{V}_n + (\nabla \mathbf{V}_n)^T - \frac{2}{3} (\nabla \cdot \mathbf{V}_n) \mathbb{I})$ , with  $\mathbb{I}$  the identity tensor. The viscosity is  $\eta^n = \frac{p_n}{v_{cx}}$ , with  $v_{cx}$  the CX collision frequency.

For the second model we only retain Eq. (1) and the parallel component of Eq. (2) [3]. The particle flux densities in the radial and diamagnetic directions are set to  $\Gamma_{r,\perp}^n = -D_p^n \nabla_{r,\perp} p_n$ ,

where subscripts  $r$  and  $\perp$  respectively indicate the radial and diamagnetic directions. The pressure-diffusion coefficient  $D_p^n$  is given by  $D_p^n = (m(v_{cx} + v_i))^{-1}$ , with  $v_i$  the frequency of ionization events.

Finally, we can add an energy equation to capture the neutral-ion temperature difference:

$$\nabla \cdot \left( \left( \frac{5}{2}T_n + m \frac{||\mathbf{V}_n||^2}{2} \right) n_n \mathbf{V}_n + \Pi_n \cdot \mathbf{V}_n + \mathbf{q}_n \right) = S_{E,n}, \quad (3)$$

solved for  $T_n$ , with  $S_{E,n}$  the energy source. The heat flux vector  $\mathbf{q}_n$  is given by  $\mathbf{q}_n = -\kappa^n \nabla T_n$ , with the heat conduction coefficient  $\kappa^n = \frac{5p_n}{2m v_{cx}}$ . We solve both the Navier-Stokes and reduced model with and without (equal neutral and ion temperatures) energy equation (Eq. (3)).

## Boundary conditions

Particle, momentum and energy fluxes are imposed as boundary conditions. These boundary fluxes correspond to the moments of the total neutral distribution  $f_{n,b}(\mathbf{v})$  at a particular position at a boundary, with  $\mathbf{v}$  the particle velocity, which can be written as

$$f_{n,b}(\mathbf{v}) = \begin{cases} f_{n,v-,b}(\mathbf{v}) & \text{if } \mathbf{v} \cdot \mathbf{v} \leq 0, \\ \int_{\mathbf{v}' \cdot \mathbf{v} \leq 0} (R_b^i(\mathbf{v}' \rightarrow \mathbf{v}) f_{i,v-,b}(\mathbf{v}') + R_b^n(\mathbf{v}' \rightarrow \mathbf{v}) f_{n,v-,b}(\mathbf{v}')) d\mathbf{v}' & \text{if } \mathbf{v} \cdot \mathbf{v} > 0, \end{cases} \quad (4)$$

with  $\mathbf{v}$  the inward pointing normal and  $f_{i,v-,b}(\mathbf{v})$  and  $f_{n,v-,b}(\mathbf{v})$  the distributions of respectively the incident ions and neutrals. The incident ion distribution is a half-sided Maxwellian (possibly accelerated by the sheath potential). The diffusion approximation from Ref. [4] is used to estimate the incident neutral distribution.

We use a simplified model for the reflection kernels  $R_b^i(\mathbf{v}' \rightarrow \mathbf{v})$  and  $R_b^n(\mathbf{v}' \rightarrow \mathbf{v})$ . Half of the incident ions and neutrals are recycled or reflected as fast atoms with half of the incident particle energy and the remaining fraction are dissociated molecules (Franck-Condon dissociation).

The corresponding moments of Eq. (4) lead to the particle flux density  $\Gamma_b^n$ , momentum flux density tensor  $\Gamma_{m,b}^n$  and energy flux density  $\mathbf{Q}_b^n$ :

$$\begin{pmatrix} \Gamma_b^n & \Gamma_{m,b}^n & \mathbf{Q}_b^n \end{pmatrix} = \int \begin{pmatrix} 1 & m\mathbf{v} & \frac{m}{2}||\mathbf{v}||^2 \end{pmatrix} \mathbf{v} f_{n,b}(\mathbf{v}) d\mathbf{v}, \quad (5)$$

where the integral is taken over the whole velocity space. These boundary conditions are robust without any user-defined fitting parameters.

## Results

Fig. 1a shows a sketch of the simulation domain. We simulate a single divertor leg, which is rectified such that the poloidal direction ( $\theta$ ) is parallel to the  $Z$ -direction. The fixed background plasma (typical for a high recycling regime) is shown in Figs. 1b-d. We compare the profiles of the sources at the poloidal distances  $Z_t$  from the target indicated in Fig. 1a.

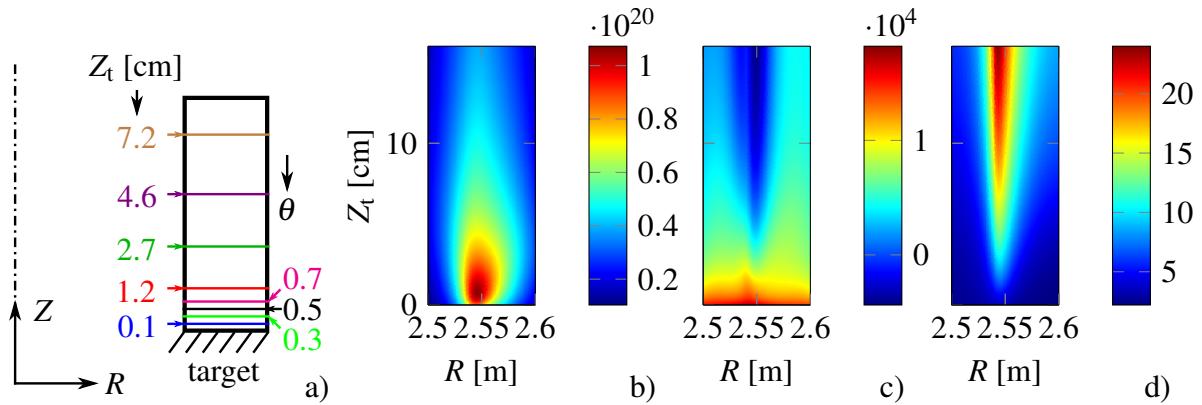


Figure 1: a) Sketch of the domain, b)-d) background plasma state: b) ion density ( $m^{-3}$ ), c) plasma parallel velocity (m/s) and d) ion temperature (eV). We assume equal ion and electron temperatures.

Fig. 2 shows the results for the different plasma sources (particle ( $S_{n_i}$ ), parallel momentum ( $S_{mu_{||}}$ ) and ion energy ( $S_{E,i}$ )). The particle source is plotted for  $Z_t = 0.1, 1.2, 2.7, 4.6$  and  $7.2$  cm. The momentum and energy source are dominant in a region much closer to the target and are therefore plotted for  $Z_t = 0.1, 0.3, 0.5$  and  $0.7$  cm.

All models give accurate results for the particle source with the maximum relative error for the parallel momentum model without energy equation (about 30%). The Navier-Stokes model with the three components of the momentum equation gives the better results. Adding an energy equation further improves the results with almost no distinction between the kinetic solution and the results from the Navier-Stokes model with energy equation. The momentum and energy sources are only significant in a very thin region near the target. It seems that the introduction of the radial and diamagnetic components for the Navier-Stokes model decreases the accuracy. This is due to the necessity of extra boundary conditions, which introduce errors in this narrow region adjacent to the target. After all, the boundary conditions of Eq. (5) are approximations whose validity increases with the number of neutral-ion collisions. The neutral energy equation has a significant influence on the results for the Navier-Stokes model. The energy equation also improves the ion energy source further away from the target (magenta and black) for both the Navier-Stokes and parallel momentum model. The fluid approach is no longer valid in the low-collisional region close to the private flux and wall boundary ( $R = 2.5$  and  $2.6$  m).

## Conclusions

The plasma sources from the fluid neutral models are within the same order of magnitude as the sources from the kinetic model. Moreover, the results will become even better for more CX dominated (detached) regimes, relevant for ITER and DEMO and the distinction between the full Navier-Stokes model and the parallel momentum equation will become smaller. In Ref. [5]

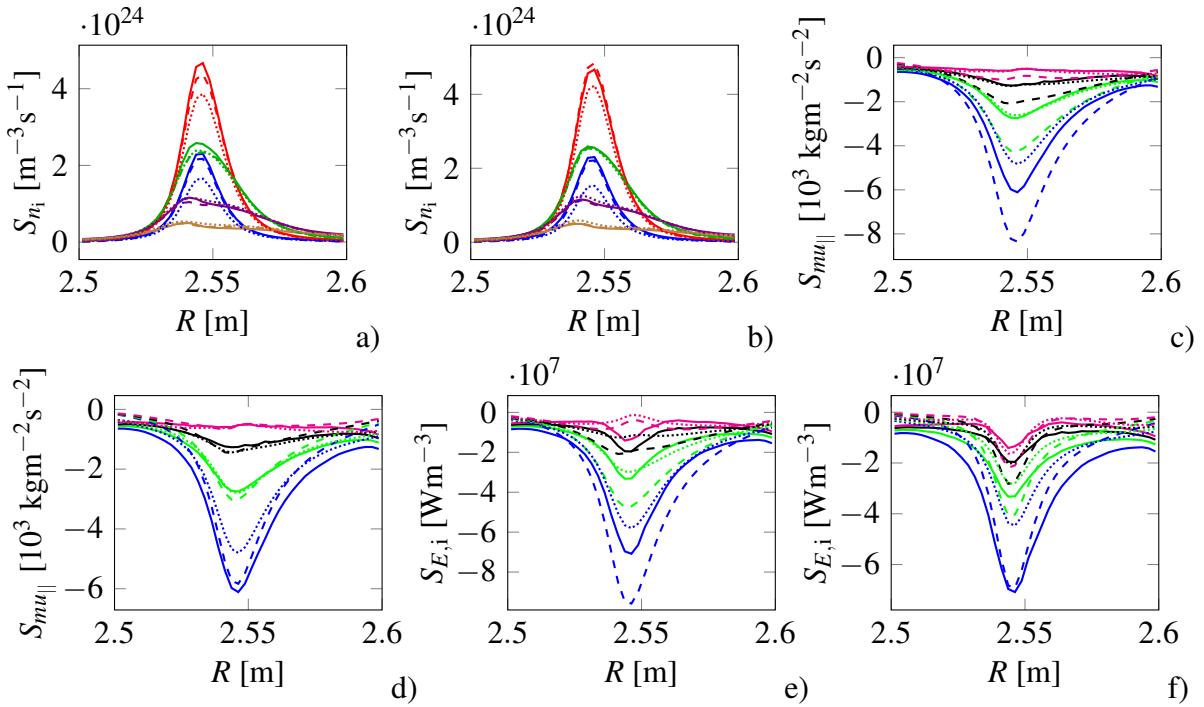


Figure 2: *Plasma sources: MC (solid), Navier-Stokes (dashed) and parallel momentum with radial and diamagnetic pressure diffusion (dotted). a)-b) Particle, c)-d) momentum and e)-f) ion energy source. For a), c) and e) equal neutral and ion temperatures are assumed, whereas an energy equation is added for b), d) and f). The colors correspond to the locations  $Z_t$  of the profiles as indicated in Fig. 1a.*

it is shown that the parallel momentum equation in combination with the pressure-diffusion equation gives very accurate results for an ITER detached case. As it is computationally costly to solve the full Navier-Stokes model, it is recommended to use a more reduced model.

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