Implementation of a consistent fluid neutral model in SOLPS-ITER and benchmark with EIRENE

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In the quest for computationally affordable plasma edge transport simulations of reactor-relevant plasmas, we consider fluid neutral models in this paper. To obtain good agreement with kinetic neutral models in charge-exchange dominated regimes, model equations, transport coefficients, and boundary conditions have to be derived consistently from the kinetic description. In this paper, we describe a fully-fluid plasma edge transport model that is aimed at reproducing the results of coupled finite-volume/Monte-Carlo runs with the kinetic Monte Carlo code EIRENE as closely as possible. To this end, we incorporate the rate coefficients from the AMJUEL reaction database and boundary conditions are based on the reflection data from TRIM. The fluid neutral model is implemented into the SOLPS-ITER code suite to compare the plasma sources with those of EIRENE on a simplified slab geometry. For a detached case, the results show a nearly perfect match between fluid and kinetic model, with errors locally ranging up to a maximum discrepancy of 10% for particle and electron heat sources, and 30% for parallel momentum sources. These very localized errors can be largely attributed to the discretization error, mainly near the ionization peak.

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1 Introduction

At present, (partially) detached divertor operation is considered as a necessity to obtain acceptable divertor heat loads in future fusion reactors, while maintaining an adequate Helium exhaust. The simulation of the edge transport under such conditions, however, poses severe challenges for current plasma edge codes. Especially the accurate simulation of neutral transport with a kinetic Monte Carlo (MC) code rapidly becomes inaccessible for such high-collisional cases because of the tremendous computational cost. It is exactly in these conditions that simple fluid models perform best and might provide a feasible alternative.

Although many plasma edge transport codes already feature a fluid neutral model, prior attempts to benchmark fluid neutral models with kinetic codes reported large discrepancies [1, 2]. Recent efforts of Horsten et al. therefore focused on deriving neutral model equations and boundary conditions starting from the corresponding kinetic description [3]. As such, transport coefficients were derived consistently with the underlying collisional data from atomic physics databases [4], and boundary conditions were formulated that include the effects of microscopic (partial) reflection of neutrals at solid surfaces [3]. In a benchmark of this new generation of fluid neutral models with an in-house kinetic code on a fixed background plasma, these models have proven to offer an accurate alternative for MC codes in high-collisional plasma edge regions.

Based on these promising results, we now couple such a fluid neutral model with a full-fledged plasma model in the SOLPS-ITER code suite [5]. In order to get best comparison to the kinetic neutral code EIRENE, the fluid neutral model incorporates the microscopic rate and reflection coefficients from respectively the AMJUEL-HYDHEL [6, 7] and TRIM [8] reflection databases. As such, a fluid neutral model is envisaged that is fully consistent with EIRENE in the limit of highly-collisional plasmas.

This paper is outlined as follows. Section 2 describes the implemented model equations and boundary conditions. Next, in section 3 a so-called ‘slab’ test case is set up on which the fully-fluid plasma edge transport model

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is solved and plasma sources are compared to those given by the EIRENE code. Finally, section 4 contains a discussion and an outlook to future work.

2 Fluid neutral model

2.1 Model equations

We start from the B2.5 plasma edge transport model [9]. The plasma is modelled with a drift-reduced plasma model from the B2.5 code. This plasma model is now augmented with a state-of-the-art fluid neutral model from Horsten et al. [3] that was consistently derived from the kinetic description for charge-exchange (CX) dominated regimes and is thus expected to compare well to results from the Monte Carlo code EIRENE. More specifically, let the subscripts $\parallel, \theta, r, \perp$ denote the parallel, poloidal, radial, and diamagnetic directions, respectively. The neutral density n_n is solved from the neutral continuity equation

$$\nabla \cdot (n_n \mathbf{V}_n) = S_{n_n}, \quad \text{with } [n_n \mathbf{V}_n]_{r,\perp} = -D_p^n \nabla_{r,\perp} p_n, \quad (1)$$

with $\mathbf{V}_n$ the neutral velocity vector, and $p_n = n_n T$ the neutral pressure.

The radial and diamagnetic components of the neutral flux density $n_n \mathbf{V}_n$ are modelled using a pressure-diffusion relation, which assumes the momentum equation reduces to a balance between reaction sources and pressure gradient in these directions [10]. Remark that because of toroidal symmetry, the diamagnetic pressure gradient can be simply projected onto the poloidal plane as $\nabla_\perp p_n = b_\phi \nabla_\theta p_n$, with b_ϕ the toroidal magnetic field pitch. Conversely, the parallel component $u_{n\parallel}$ of the neutral velocity $\mathbf{V}_n$ is solved from the parallel momentum equation

$$\nabla \cdot (m n_n u_{n\parallel} \mathbf{V}_n - \eta_n \nabla u_{n\parallel}) = S_{m u_{n\parallel}} - \nabla_\parallel p_n + S_c, \quad (2)$$

with m the atomic mass, η_n the isotropic neutral viscosity, and S_c a centrifugal force term that partially accounts for the additional terms that arise when taking the parallel component of the vector momentum equation in a curvilinear coordinate system. The expression of this latter term can be found in [3].

Finally, the ion-neutral temperature T is solved from the combined ion-neutral internal energy equation

$$\nabla \cdot \left(\frac{5}{2} \sum_{a=i,n} n_a \mathbf{V}_a T - \kappa \nabla T \right) = S_{E_{n,i}} + Q_{ei} + \sum_{a=i,n} u_{a\parallel} \nabla_\parallel p_a - \sum_{a=i,n} \nabla u_{a\parallel} \cdot \eta_a \cdot \nabla u_{a\parallel}, \quad (3)$$

with $\kappa = \text{diag}(\kappa_i^\theta + \kappa_n, \kappa_i^r + \kappa_n)$ the heat conductivity tensor. In these equations, the subscripts i, e , and n refer to the ion, electron, and neutral species, respectively, and the superscripts θ and r refer to the components in the poloidal and radial directions. Q_{ei} is a source term representing temperature equilibration between electrons and ions.

In these equations the sources due to ionization, recombination, and CX reactions are given by

$$\begin{aligned} S_{n_n} &= n_i n_e K_r - n_n n_e K_i, \\ S_{m u_{n\parallel}} &= m (n_i n_e K_r + n_n n_i K_{cx,m}) u_{\parallel} - m (n_n n_e K_i + n_n n_i K_{cx,m}) u_{n\parallel}, \text{ and} \\ S_{E_{n,i}} &= m \left(\frac{1}{2} K_i n_e n_n + \frac{1}{2} K_r n_i n_e + K_{cx,m} n_i n_n \right) (u_{\parallel} - u_{n\parallel})^2. \end{aligned} \quad (4)$$

Here, K_i and K_r are the rate coefficients for ionization and recombination, respectively, and $K_{cx,m}$ is the so-called *momentum-linearized* CX rate, as defined in [4]. The latter is obtained from the microscopic CX rate by linearizing the charge-exchange term of the momentum source w.r.t. the difference in drift velocity between ions and neutrals, and assuming a Maxwellian distribution for both species. To obtain the same physics as in EIRENE, all rates appearing in the plasma sources are extracted in this neutral model from the AMJUEL database [6]. For later use, we also define the electron energy source due to electron-neutral interactions as

$$S_{E_e} = -n_i n_e K_r \bar{E}_r - n_n n_e K_i \bar{E}_i, \quad (5)$$

with $\bar{E}_r$ and $\bar{E}_i$ the total electron energy loss per recombination or ionization event, respectively. These loss rates include the line and continuum radiation, kinetic energy of products, and potential energy contributions as tabulated in the AMJUEL database, as well as losses due to Bremsstrahlung.

Essential for the asymptotic similarity of the fluid neutral model with kinetic models in strongly CX-dominated regimes is that the choices of transport coefficients are based on the kinetic model. Using the Chapman-Enskog theory, the following transport coefficients are thus obtained: $\eta_n = n_n T \tau_n$, $\kappa_n = \frac{5n_n T \tau_n}{2m}$, with $\tau_n = (n_i K_{cx,m} + n_e K_i)^{-1}$ a collision time for neutrals. With this definition, the pressure-diffusion coefficient is given by $D_p^n = T \tau_n m^{-1}$. Finally, also the sources of the electron energy equation S_{E_e} have to be adjusted to incorporate electron heat loss rates for ionization and recombination from AMJUEL H.10. Since these reaction rates exclude energy losses from Bremsstrahlung and the energy source from potential energy of recombination reactions, their rates have to be added separately.

2.2 Boundary conditions

The most important cornerstone for improved neutral fluid modelling by Horsten et al. [3] w.r.t. earlier fluid neutral models is situated in the boundary conditions. These boundary conditions account for the first time for the angular and energy dependence of particle reflection probabilities, and consistently obtain particle, momentum, and energy boundary conditions for neutral transport. Here, we give only a short overview of the principles on which these boundary conditions are based. For details, we refer to Refs. [4, 3] and references therein.

The net neutral continuity, parallel and total momentum fluxes at the boundary are given by the moments of the neutral kinetic distributions at the wall. These distributions are a combination of one-sided kinetic distributions of incoming particles, reflected neutrals and recycled ions. Let Γ_j^n denote the flux densities with index j denoting a particular moment: 0 for the particle flux density, 1 for the parallel momentum flux density and 2 for the total energy flux density. The net flux densities can then be decomposed as

$$\Gamma_j^n = -\Gamma_{j,in}^n + \Gamma_{j,refl}^n + \Gamma_{j,rec}^n, \quad (6)$$

with the subscripts in , $refl$, and rec referring to the incident, reflected, and recycled neutral flux densities, respectively. In a fluid approach, of course, these one-sided distributions are not readily available. Therefore, the so-called *diffusion approximation* is used to estimate the incoming neutral flux at the walls, assuming neutrals originate from CX reactions close to the wall, where they inherit their velocities from the plasma distribution that is assumed to be a drifted Maxwellian. For the incident ions, we assume that a one-sided drifting Maxwellian is accelerated with the sheath potential.

Using these distributions of incident particles, we can now calculate the kinetic distributions of the recycled and reflected neutral fluxes. These consist of two parts. The first part are the fast reflected/recycled atoms, for which the distributions are given by multiplying the incident distribution with the angular and velocity dependent fast reflection probabilities p_F from the TRIM [8] tables. The second part are the thermally released molecules, that stick to the walls and are isotropically re-emitted. Since molecules are not modelled within this approach, it is supposed that they dissociate instantly and they are therefore emitted as mono-energetic atoms with a Franck-Condon dissociation energy of 2 eV. Like in EIRENE, the thermal emission probability p_T is reduced by the effective recycling coefficient R_T as $p_T = R_T - p_F$ ¹. This effective recycling coefficient as such effectively models the pump.

In practice, the determination of the distribution and their moments is too expensive to do at runtime. Therefore, the integration over angles and velocity in the evaluation of the moments is done in a preprocessing step and tabulated as function of ion Mach number M_i , ion temperature $T_i = T$, and the value of the sheath potential drop δ_{sh}^{pot} divided by the ion-electron temperature ratio $\tau_{i,e} = T_i/T_e$. Since these integrals include the fast reflection probabilities from the TRIM tables, these tables are set up for a specific combination of wall material and plasma species. To reduce the number of dependencies in these integrals, referred to symbolically here as I_j^k , it was hereby assumed that only the toroidal plasma drift velocity is significant. The reflected and recycled

¹ Remark that the fast reflection probability might be reduced as well at very low effective recycling coefficients, as done in EIRENE [8].

Fig. 1 The slab geometry used for the neutral model benchmark. The horizontal blue lines indicate the *cuts*, which enclose the core region. The flux tubes indicated in purple are those on which the plasma sources are compared in this paper.

flux densities can then be written succinctly as [3]

$$\Gamma_{j,\text{refl}}^n = B_j^1 n_n I_j^{\text{refl},1} + B_j^2 \frac{\partial n_n}{\partial \tau} I_j^{\text{refl},2} + B_j^3 \frac{\partial n_n}{\partial \nu} I_j^{\text{refl},3} \quad (7)$$

$$\Gamma_{j,\text{rec}}^n = A_j I_j^{\text{rec}}, \quad (8)$$

with the coefficients A_j^k , $k = 1 \dots 3$ and B_j including all coefficients that can be pulled in front of the integral, and $\partial n_n / \partial \tau$ and $\partial n_n / \partial \nu$ the gradients of the neutral density, tangential and normal to the wall, respectively. Finally, it should be remarked that an internal energy equation for neutrals and ions is solved. The neutral contribution to the internal heat flux at the boundary Q_b^n can then be obtained from the total heat flux Γ_2^n as

$$Q_b^n = \Gamma_2^n - u_{n\parallel} \Gamma_1^n + \frac{m u_{n\parallel}^2}{2} \Gamma_0^n. \quad (9)$$

3 Comparison to EIRENE kinetic simulation of neutrals

The standard approach to perform plasma edge transport simulations in SOLPS is to run the coupled B2.5-EIRENE simulation. Hereby, the B2.5 finite volume code computes the neutral sources for EIRENE and the Monte Carlo code EIRENE returns the plasma sources to B2.5. This process is iterated until a statistically steady-state solution is reached. In this section, we will now compare the results of the newly implemented fluid neutral model with the EIRENE code. It is understood that the solution of the fluid neutral model is at least an order of magnitude faster than the simulation with EIRENE.

3.1 Case set-up

It should be noted that in contrast to the plasma, neutrals are transported isotropically, requiring therefore a 9-point stencil for their discretization [11]. Since this feature is currently absent in the SOLPS-ITER code, we perform this benchmark on an orthogonal grid, using a so-called *slab* case. In this simplified geometry, it is assumed that θ and r -directions coincide with the vertical and radial coordinates of a cylindrical coordinate system with the origin at the central symmetry axis of the tokamak, as depicted in figure 1. The geometry has been given a size that roughly corresponds to the JET tokamak. *Cuts* are introduced to create a confined core region, by imposing periodicity at the inner side of these cuts and ‘teleportation’ from one private flux region to the other. It is discussed in Ref. [3] that a sufficiently fine grid is needed to accurately resolve the neutral physics. A computational grid of dimensions 140×40 is used here as a compromise between accuracy and computational cost. To increase the resolution in the divertor region, the grid is poloidally refined towards the target plates with poloidal cell lengths decreasing up to 1.9 mm.

Fig. 2 a) The electron temperature profile at the targets for $n_c = 2 \cdot 10^{19} \text{ m}^{-3}$ and $n_c = 5 \cdot 10^{19} \text{ m}^{-3}$, as a function of grid cell number y . b) The ion saturation current to a single target as a function of core density n_c .

At the core boundary 4.28 MW of heat is imposed as a boundary condition, equally divided over the ion and electron channels. At private flux and wall regions, decay lengths are imposed for n_i and T and an effective recycling rate $R_T = 0.98$ is used for the neutrals. At the targets, typical sheath conditions are used for the plasma and $R_T = 1.0$ is used for the neutrals. We assume that the plasma is pure deuterium and that the entire vessel is made from carbon. The radial plasma transport is determined by a radial diffusivity coefficient $D^i = 1.0 \text{ m}^2 \text{ s}^{-1}$, radial ion/electron conductivity coefficients $\chi^i = \chi^e = 1.0 \text{ m}^2 \text{ s}^{-1}$, and a radial ion parallel viscosity coefficient of $\nu^i = 0.2 \text{ m}^2 \text{ s}^{-1}$. The potential equation is kept at a spatially constant 3.1 eV for simplicity.

To estimate the expected validity region of the fluid neutral model, we examine the plasma regime for core densities n_c varying from $2 \cdot 10^{19} \text{ m}^{-3}$ to $5 \cdot 10^{19} \text{ m}^{-3}$ using the fluid neutral model². In figure 2a, the target profiles of the electron temperature T_e show a clear decrease when going from $2 \cdot 10^{19} \text{ m}^{-3}$ to $5 \cdot 10^{19} \text{ m}^{-3}$. In fact, with a steadily low T_e of around 0.5 eV over the whole target area, the target seems to be at the onset of detachment. This is confirmed from the ion saturation current in figure 2b that clearly shows a roll-over to detachment as a function of the core density. Furthermore, it can be seen here that $n_c = 2 \cdot 10^{19} \text{ m}^{-3}$ is still in a state of low recycling. To check how good the neutral fluid model performs both inside (CX-dominated) and outside (few CX-collisions) its validity region, we will now benchmark it with EIRENE for the cases with $n_c = 2 \cdot 10^{19} \text{ m}^{-3}$ and $n_c = 5 \cdot 10^{19} \text{ m}^{-3}$.

In this benchmark, we choose deliberately to run EIRENE without molecules and let the thermally emitted fraction be born as mono-energetic atoms at 2 eV, just like in the fluid neutral model. Furthermore, we circumvent teleportation of particles at the cuts by making them reflective and thus exploiting the symmetry of the test case.

3.2 Comparison of plasma sources

To compare the results of a plasma edge transport simulation with the new fluid neutral model with the coupled B2.5-EIRENE code, it suffices to compare the plasma sources of both neutral models on the plasma background of the converged plasma edge transport simulation. The reasoning of this approach is that if the sources given by both neutral models are the same, the steady state plasma solution is maintained. Additionally, many particles can then be launched in EIRENE to suppress the statistical noise on the resulting plasma sources, without need for excessive computational time. Here, 5.88 million particles were used to obtain the EIRENE sources.

Let us now compare the continuity, momentum, and electron energy sources, S_{n_i} , $S_{mu_{\parallel}}$, and S_{E_e} , respectively, from plasma-neutral interactions. Consider three flux tubes positioned at the separatrix and at a distance of about a half power decay length from the separatrix into the SOL and PF regions, as indicated in figure 1. Figure 3a-c then show the sources for the low recycling case in the flux tube that gives the largest discrepancy of the three considered flux tubes. It can be seen that for this flux tube, S_{n_i} and S_{E_e} are off by a factor 2 and the momentum source even by a factor of 3. This was of course to be expected since the mean-free path of neutrals in this low recycling case does not justify a fluid assumption, thus taking this fluid neutral model outside its area of applicability.

² Note that this is an approximation, since the regime itself can also deviate from what is found using a kinetic neutral model.

Fig. 3 Comparison of the continuity, momentum, and electron energy sources from plasma-neutral interactions evaluated with the new fluid neutral model in B2.5 (solid) and the Monte Carlo evaluation of the kinetic model in EIRENE (dashed). The sources are shown as a function of their poloidal cell number x for a specific flux tube. The flux tube numbers correspond to those indicated in figure 1. Because of the symmetry in the case set-up, only half of the flux tube is shown.

Indeed, looking at the comparison in the detached regime, much better comparison is found. For all three flux surfaces, the fluid neutral model is able to match the sources S_{ni} , $S_{mu_{||}}$, and S_{E_e} of the kinetic simulation nearly exactly. The largest discrepancies of the particle and electron heat source are found at the ionization peak, where the error is about 10%. The peak sources are locally smoothed in the fluid model results, an effect most probably induced by the discretization error, as it was shown to be a dominant error contribution in fluid neutral models in Ref. [3]. In the comparison of the parallel momentum sources, the largest discrepancies are found directly at the target with a relative error going as high as 28%. Also here, the discretization error is a likely cause, possibly together with so-called *first-flight effects*, not included in the fluid model.

Finally, let us examine the assumption of temperature equilibration between ions and neutrals in the fluid neutral model. We have verified that for the high density case, the difference between the combined ion-neutral temperature (obtained with the fluid model) and the kinetic neutral temperature (from Eirene) differ by less than 10% close to the target where the sources are strongest. For the lower density case, these differences are much larger (up to 70%).

4 Discussion and outlook

A novel fluid model, derived directly from the kinetic equations, has been introduced into the SOLPS-ITER code suite. On a purely orthogonal slab case, the fully-fluid coupled plasma-neutral model is then converged and sources are compared to those of the EIRENE Monte Carlo code. While the comparison is relatively poor for a low recycling case, the results match nearly excellently for a detached case, for which its use is truly intended. Given these promising results, further progress can now be made towards computationally-affordable simulations of reactor-relevant plasmas. Concerning numerics, the first step should be the introduction of a 9-point stencil

to accurately capture the isotropic neutral transport in non-orthogonal grid geometries [11]. Secondly, a grid extending up to the vessel wall [12] is necessary to model the neutrals in realistic test cases. Additionally, the model should be extended to incorporate molecules. Finally, this work forms a first step towards hybrid fluid-kinetic neutral models, which reduce statistical noise and computational time w.r.t. kinetic neutral models without loss of accuracy.

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