Sensitivity of scrape-off layer codes to modelling approaches

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The study of plasma exhaust remains a core focus of current efforts towards viable DEMO-class magnetically confined fusion devices. The scrape-off layer (SOL) features complex physics. This is especially true for detachment, a mechanism where a cloud of neutrals forms at the divertor target and becomes a sink of plasma energy, momentum and particles through atomic and molecular processes. Edge plasma physics inherently necessitates modelling assumptions, and is often investigated using complex, computationally intensive 2D and 3D codes.

1D SOL models offer a powerful platform to investigate fundamental model aspects thanks to their high interpretability and low computational cost. In this work, we compare two 1D codes: SD1D [1], a highly flexible fluid code and part of the BOUT++ framework [2], and SOL-KiT [3], a kinetic electron / fluid ion code with a self-consistent fluid electron option. SOL-KiT's ability to switch between fluid and kinetic descriptions of electrons makes it an ideal test platform for validating reduced-kinetic heat transfer models implemented in SD1D [4], which could eventually lead to their implementation in 2D and 3D codes. Realising this objective demands SD1D to replicate SOL-KiT's performance in fluid mode so that kinetic electron effects can be isolated. The present work represents the first stage of this benchmark and features abridged physics reflective of the original version of SOL-KiT: molecular processes, flux expansion, impurity radiation, neutral pressure and neutral temperature evolution are neglected.

Both codes solve the Braginskii fluid equations, with SD1D featuring a bulk plasma energy and momentum equation [1], assuming equal electron and ion velocity, density and temperature. SOL-KiT solves for ion and electron velocities, from which an SD1D-equivalent equation can be derived assuming the velocities are equal, with the only difference being in the way the momentum loss terms are calculated. SOL-KiT neglects ion temperature and solves only for electron temperature, while SD1D considers both species through solving a bulk plasma energy equation. Since neither code considers ion conduction, this difference only manifests itself in SD1D having double the plasma pressure for the same electron temperature, as shown in eq. 1 where the SD1D plasma equation was rearranged in terms of electron pressure only assuming

$p_e = p_i$:

$$2\left[\frac{\partial}{\partial t}\left(\frac{3}{2}p_e\right)\right] = 2\left[-\frac{5}{2}\frac{\partial(p_e u)}{\partial x} + u\frac{\partial p_e}{\partial x}\right] + \frac{\partial}{\partial x}\left(\kappa_{\|e}\frac{\partial T_e}{\partial x}\right) + Q_{ext} - R - E \quad (1)$$

Where the RHS terms include convective heat transfer, compression heating, conduction, external heating, radiative losses and heavy particle energy exchange (set to zero under the isothermal neutral assumption in the present work). The factors of 2 represent the contribution of the ion pressure (assumed equal to electron pressure) in SD1D. One can eliminate this contribution by doubling the remaining terms (Q_{ext}, R, $\kappa_{\|e}$) as well as the sheath heat transmission coefficient. This allows SD1D to solve an electron energy equation with $\gamma_{sheath} = \gamma_e = 4.8$, matching the SOL-KiT approach without requiring changes to the code. The codes also differ in sheath BC implementation: SOL-KiT features a zero-gradient T_e and free (exponentially extrapolated) n_e, while SD1D defaults to linearly extrapolated n_e and p_e. The exact SOL-KiT approach was implemented in SD1D code and found to have negligible impact on results.

The primary difference between the codes lies in the treatment of the atomic processes. SD1D uses curve-fit reaction rates, allowing the prediction of particle source, energy and momentum transfer based on local plasma conditions. The rates come from the 1D code SOLF1D [7], and partially originate from the AMJUEL and HYDHEL databases compiled for the code EIRENE [8], a part of the SOLPS-ITER [5] edge code. The databases feature semi-analytical data in [6] as well as collisional-radiative model (CRM) extensions to this data (e.g. [9]). They contain several rates for each process and come in the form of one or two-parameter polynomials in terms of temperature, density, or collision energy. SOL-KiT features its own built-in CRM and uses no rate fits, explicitly tracking the evolution and interactions of over 20 excited neutral states at runtime. While CRM codes are highly complex and the SOL-KiT implementation is distinct from that in [9], they share use of the fundamental cross-sections from Janev [6].

SD1D rates are compared to those used in EIRENE. The recombination rate is the same (AMJ H.4 2.1.8), but ionisation is different, with SD1D opting for the rate HYD H.2 2.1.5 which features no density dependence, unlike the EIRENE rate AMJ H.4 2.1.5. SOL-KiT also includes density dependence, since it arises through the lower ionisation threshold present in excited neutral states which are explictly tracked in SOL-KiT. Evaluating the SD1D rate revealed it to closely match the EIRENE rate in the coronal approximation, but predict a nearly 50% lower ionisation rate at densities of interest ($1 \times 10^{20} m^{-3}$). SD1D also includes an excitation energy-weighted rate, representing the total net energy losses from excitation, de-excitation and ionisation. The SOLF1D rate featured in SD1D was found to be similar to the EIRENE rate

H.10 2.1.5, but once again without a density dependence.

A density scan was performed with a power input of 16MW/m^2, 100% recycling and a domain length of 12m, and repeated for each modification made to SD1D to assess the match with SOL-KiT. The resulting target mass fluxes and temperatures are shown in figs. 1A) and 1B).

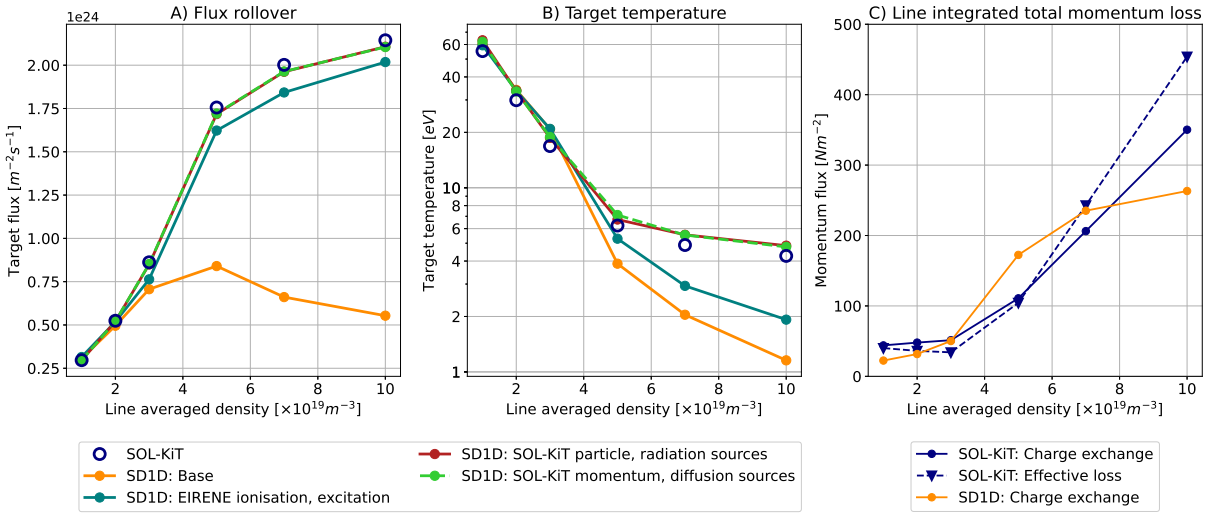

Figure 1: *Code agreement in target mass flux in temperature for each stage of match*

The comparison is done over four steps. The "base" version of SD1D includes the SOL-KiT-like sheath boundary condition and energy equation approach. It results in a poor match, with SD1D featuring lower fluxes. This is substantially improved upon implementing the EIRENE ionisation and excitation rates, which improve upon SD1D rates by including a density dependence. The faster ionisation depletes the neutral population, reducing its ability to radiate energy and reduce plasma momentum and significantly delaying detachment. Most of the remaining discrepancy is due to the SOL-KiT CRM predicting different ionisation and energy loss rates to the EIRENE rates, as evidenced by the match becoming near-exact once SOL-KiT sources are explicitly imposed on the SD1D domain. However, the change in fluxes is small, suggesting SOL-KiT CRM's performance is comparable.

The final step in figs. 1A) and 1B) consists of imposing SOL-KiT momentum losses and neutral diffusion coefficient profiles in SD1D. While they have been found to have negligible impact on the results within the studied density range, the codes differ in approach. With neutral momentum evolution being disabled for the initial stage of the benchmark, SD1D momentum losses are dominated by charge exchange, evaluated from the EIRENE rate H.3 3.1.8 using the plasma temperature and a fixed collision energy. The SOL-KiT model is also dominated by charge exchange, but features a cold ion and neutral assumption leading to no temperature dependency. Instead, the rate is driven by the excited state population through the charge exchange cross-section having a strong dependency on the quantum number: $\sigma_{cx,n} \propto n^4$ [6]. This

effectively gives SOL-KiT only a density dependence, in contrast to the approach in AMJUEL. This fundamental difference is still being investigated. Some previous studies [10] found the density dependence to be much weaker than the cross-sections would suggest.

The charge exchange momentum loss integral in both codes across the studied cases is shown in fig. 1C), revealing very similar rates despite the differences in approach. This is true for all but the highest density even after computing the overall effective SOL-KiT momentum loss, which features an additional term from recombination as well as a correction due to the numerical treatment of the boundary. It is suspected that the disagreement may be more significant at higher densities, which are currently being studied. The codes have similar neutral diffusion models and rely on a neutral diffusion coefficient, which is dominated by charge exchange in both codes. SOL-KiT also considers the impact of elastic electron-neutral collisions (which is negligible) while SD1D considers the impact of ionisation (which is small) and the impact of neutral-neutral ideal gas collisions, which is minimal at the low temperatures present near detachment. The codes were found to predict values of D_n within 20% of each other at densities above $5 \times 10^{19} \mathrm{m}^{-3}$.

In conclusion, the codes SD1D and SOL-KiT were compared against each other in the first stage of a benchmark study, with SD1D being made to reflect SOL-KiT's energy equation and sheath boundary condition approach. The differences in performance were evaluated through a rollover density scan, with the major discrepancy arising through SD1D's lack of density dependence in the ionisation and excitation curve-fit rates. The inclusion of density dependence through the implementation of EIRENE ionisation and excitation rates results in a close match to SOL-KiT. This was further enhanced through imposing SOL-KiT particle and radiation sources on the SD1D domain, revealing that the SOL-KiT CRM predicts similar, but lower rates of energy loss compared to when EIRENE ionisation and excitation rates are used. The codes feature fundamental differences in the charge exchange approach, but these were found to not have a significant impact on the results within the studied density range.

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