B2.5-Eunomia simulations of Pilot-PSI plasmas

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Abstract

The B2.5-Eunomia code is used to simulate the plasma and neutral species in and around a Pilot-PSI plasma beam. B2.5, part of the SOLPS5.0 code package, is a multi-fluid plasma code for the scrape-off layer. Eunomia is a newly developed non-linear Monte Carlo transport code that solves the neutral equilibrium, given a background plasma. Eunomia is developed to simulate the relevant neutral species in Pilot-PSI and Magnum-PSI, linear devices that study plasma surface interactions in conditions expected in the ITER divertor. Results show the influence of the neutral species on the Pilot-PSI plasma beam. We show that a fluid description for the neutrals is not sufficient and Eunomia is needed to describe Pilot-PSI. The treatment of individual vibrational states of molecular hydrogen as separate species is crucial to match the experiment.

Keywords: Divertor modelling, Molecular effects, Neutral modelling, Edge modelling

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1. Introduction

A newly developed parallel non-linear three dimensional Monte Carlo code, called Eunomia [1] has been coupled to B2.5 [2] to investigate the role of neutral species in the linear plasma generator Pilot-PSI [3]. The plasma conditions in Pilot-PSI and its successor Magnum-PSI [4], with plasma densities of $\approx 5 \cdot 10^{20}$ m^{-3} and plasma temperatures below 5 eV, are similar to those expected in the ITER divertor. The plasma described here differs significantly from that in other linear machines such as PISCES [5], PSI-2 [6], and NAGDIS-II [7]. Those experiments typically have plasma densities of around 10^{19} m^{-3} and a plasma temperature around 10 eV. The design of the source and the plasma conditions in Pilot-PSI and Magnum-PSI result in a much higher production of neutrals. This implies that Pilot-PSI enters a different, interesting regime, where the mean free path of neutrals is short enough to strongly influence the plasma. On the other hand, the neutral mean free path is so long that neutrals will face changing plasma conditions in between their collisions. This requires a kinetic description for the neutral species.

Previous simulations with the coupled B2-Eirene code [2] addressed plasma conditions expected in Magnum-PSI, assuming higher temperatures than observed in Pilot-PSI [8]. The simulations performed with B2.5-Eunomia are in a high density, low temperature regime that is more challenging, both in the complexity of the physics and the statistical demands.

Eunomia is developed to model the behaviour of neutral species under these high density, low temperature conditions in detail. The code can be applied to both linear machines and tokamaks. Where for tokamak simulations the symmetry in the toroidal direction is used, the axisymmetry around the z-axis is used to model the geometry of linear machines. Eunomia calculates the particle density, temperature and flow of the relevant neutral species by simulating collisions with ions, electrons, neutrals and the surrounding walls. The physics included in Eunomia is similar to other neutral transport codes such as Eirene and DEGAS 2 [9; 10]. In Eunomia special attention is paid to

improving the work load balance for parallelisation and to reduce statistical noise, in particular near the symmetry axis, by applying cell based adaptive particle weights.

In this paper we report on the importance and behaviour of atomic and molecular hydrogen in and around a Pilot-PSI plasma beam. Figure 1 shows a schematic drawing of Pilot-PSI. The B2.5-Eunomia simulations are compared to experimental results. The inlet plasma boundary conditions are taken from Thomson scattering measurements near the source. Simulation results are compared to Thomson scattering profiles near the floating target. To draw an ion current we applied a bias voltage to the target. The potential at which the ion saturation current is reached is compared to measurements in Pilot-PSI.

2. B2.5

B2.5, part of the SOLPS5.0 code package, is a multi-fluid two temperature plasma code for simulation of the scrape-off layer and divertor of a tokamak. B2.5 solves five equations: The electron and ion heat equations, the continuity, parallel momentum and potential equations. The drift velocities and electric currents are included. For the cylindrically symmetric geometry of Pilot-PSI extensions are made to the inlet and target boundary conditions. At the inlet we implemented an option to apply radial profiles for the ion and electron temperatures, the potential and the density or particle flux density as boundary conditions. At the target we implemented a floating target boundary condition. To obtain a given total current, the target potential is adjusted during the simulation.

3. Eunomia

Eunomia solves the equilibrium state of each neutral species. The plasma and neutral background is specified as cell averaged values on a tetrahedral grid. Eunomia calculates a new neutral background characterised by the density, flow velocity and temperature of each neutral species. Eunomia converges by iteratively updating the neutral background.

Eunomia simulates collisions between test-particles and particles drawn from the local background. The rates of neutral-electron collisions are a function of the local electron

density and temperature. The neutral-neutral and neutral-ion collisions are simulated in the center of mass frame. For those heavy particle collisions we use cross sections and apply the null collision method. Rates and cross sections for collisions with charged particles and volume recombination are taken from the same databases as used by Eirene and BIT [9; 11; 12; 13]. For collisions between neutral species the BGK approximation is used [14].

Atomic and molecular hydrogen have elastic collisions with atomic and molecular hydrogen, and with protons. For atomic hydrogen we also consider charge exchange ($H^+ + H \rightarrow H + H^+$), excitation ($e + H \rightarrow e + H^*_{n=2}$) and ionization ($e + H \rightarrow 2e + H^+$).

Charge exchange with molecular hydrogen (ion conversion) produces a molecular ion, which is assumed to recombine instantaneously ($H^+ + H_2(v) \rightarrow H + H_2^+(v)$; $e + H_2^+(v) \rightarrow H^*_{n\geq 2} + H$). At the low plasma temperature of Pilot-PSI this process, called molecule activated recombination (MAR) [15], recombines the plasma efficiently. Dissociative attachment produces a negative ion, which is assumed to recombine instantaneously ($e + H_2(v) \rightarrow H + H^-$; $H^- + H^+ \rightarrow H + H^*_{n=3}$). In case vibrational states are treated as separate species, electron impact vibrational excitation and de-excitation are also considered.

Excited hydrogen atoms are not simulated in Eunomia. They are assumed to ionize or de-excite to the ground state instantaneously. The probability to ionize the excited atom is obtained from a table generated by a separate stand-alone collisional-radiative model that is based on the excitation and ionization rates from [11]. Neutral particles reflecting from surfaces will return thermalised to the wall temperature with a cosine velocity distribution. Atoms associate to molecules with a probability of 1%.

4. Coupling of B2.5 and Eunomia

The coupling of B2.5 and Eunomia is done by linking the codes into one executable. B2.5 can access Eunomia data internally. The modifications to both codes are limited and in such a way that the codes can still be used independently.

Based on the plasma background from B2.5, Eunomia calculates sources of plasma particles, ion parallel momentum and ion and electron heat. Collisions between neutrals and the plasma contribute to these sources. For instance, an ionization event is a source of one ion and one electron, and an electron energy sink equal to the ionization potential. In practice, ionization is a multi-step process, including radiative losses. However, due to the high density in Pilot-PSI, ionization is dominated by electron processes and radiative losses are small. The velocity vector of the neutral particle is used to determine the ion heat and ion momentum source. The sources in a certain cell are given by

$$\begin{aligned} S_P &= \textstyle\sum_i \Delta P_i, \\ \mathbf{S}_M &= \textstyle\sum_i m\left(\mathbf{v}-\mathbf{u}\right), \\ S_H &= \textstyle\sum_i \frac{1}{2}m\|\mathbf{v}-\bar{\mathbf{v}}\|^2 - \frac{1}{2}m\|\mathbf{u}-\bar{\mathbf{v}}\|^2, \\ S_E &= \textstyle\sum_i \Delta E_i, \end{aligned} \tag{1}$$

where i is the collision event. Here $\bar{\mathbf{v}}$ is the ion background velocity and $\mathbf{u}$ and $\mathbf{v}$ are the velocity vectors of the ion before and after the collision event. ΔP_i = -1, 0 or 1 and ΔE_i equals the electron energy gain or loss for the collision event. For example, ΔP_i equals minus one for charge exchange of a proton and a hydrogen molecule, zero for charge exchange with a hydrogen atom and one for ionization.

B2.5 also provides Eunomia with ion fluxes to surfaces. Surface recombination is simulated by a neutral source in Eunomia. B2.5, like most fluid codes, does not resolve the sheath, but simulates up to the sheath entrance. Eunomia requires the ion temperature T_i, the sheath potential V_{sh} and the parallel ion velocity $v_\parallel$ from B2.5 to determine the average energy of neutral particles leaving the target:

$$E_n = \alpha\left(\frac{3}{2}T_i + eV_{sh} + \frac{1}{2}m_i v_\parallel^2\right), \tag{2}$$

where α is the energy reflection coefficient and is set to 0.3 for this paper. Also a fraction of 30% of the ions will return thermalised to the wall temperature as atomic hydrogen. The current implementation allows to study sensitivities of the wall reflection by modifying a few parameters. However, more complex reflection models are required

in the future [16; 17]

Typically every ten iterations B2.5 calls Eunomia. On the updated plasma background Eunomia calculates a new neutral background and updates the source terms for the B2.5 equations. Recursively this will converge to the B2.5-Eunomia steady state solution.

5. Results and discussion

We compare B2.5-Eunomia simulation results to Pilot-PSI experiments at a magnetic field of 0.8 T. Figure 2 shows the two dimensional representation of the simulated domain. Under the same conditions Thomson scattering measurements near the source and near the target are made. The radial electron density and electron temperature profiles obtained from the Thomson scattering measurements near the source are used as inlet boundary conditions for B2.5. At this boundary a potential profile derived from rotation measurements is applied. At the target B2.5 sheath conditions are applied.

One of the sources in Eunomia is volume recombination by two and three body recombination. Another neutral source is the surface recombination of the ion flux to the target. The cascaded arc source gas flow is 1.5 standard liters per minute and reaches an ionization efficiency of 10–15%. The neutral particles released by the source are accounted for by a gas puff near the inlet of the computational domain. As indicated in figure 2, at a segment of the vessel wall a small fraction of test-particles is absorbed, simulating pumping. The absorption probability is automatically adjusted to obtain the measured background gas pressure of 2.4 Pa.

When impinging on walls, atoms reflect as atoms or associate to molecules. Due to dissociation and MAR two or three atoms per molecule are produced. The balance of the sources and sinks due to pumping, volume recombination, wall interactions and collisions lead to an equilibrium density, temperature and flow profile for each neutral species.

Figures 3 and 4 compare the radial profiles of the electron density and temperature obtained from B2.5-Eunomia with the Thomson scattering measurements near the tar-

get. For the B2.5 standalone case atomic hydrogen is simulated as a fluid. This model cannot describe all the important physics in Pilot-PSI conditions correctly. We were not able to apply it to a reasonably high neutral pressure of a few Pascal. The low neutral background pressure of < 1 Pa, where simulations were possible, explains the high electron temperature and density for this case.

In the case of B2.5-Eunomia with atomic hydrogen only, the simulated temperature fits the Thomson measurements very well. The plasma is effectively cooled by the efficient and frequent charge exchange collisions with atomic hydrogen. However, the peak density is clearly too high, and the density profile is much broader than in the experiment. Plasma only recombines weakly due to two and three body recombination, leading to a higher density than in the experiment.

When molecular hydrogen is included as single species in the Eunomia calculations, while keeping the neutral pressure at the same value, the density of atomic hydrogen drops. Figure 3 shows that molecular hydrogen, formed by association of atomic hydrogen at the vessel wall, will decrease the plasma density via the MAR process.

The best fit with the experiment is obtained when simulating all vibrational states of the hydrogen molecule as separate species. The density profile is almost identical to the case with H_2 simulated as one species. The width of the density profile is slightly decreased by dissociative recombination processes, which become more efficient at the edge of the plasma beam. The temperature is reduced when treating H_2 as 15 separate species, again improving the match with the experiment. The error bars of the Thomson scattering data only includes the statistical noise of the measurement. Uncertainties originating from for instance alignment and calibration are not included. The shot to shot variance is around 15%. We ensured the statistical noise in B2.5-Eunomia is much less than this value. Especially for the density, the width of the plasma profile is best reproduced by B2.5-Eunomia simulations including vibrational states of molecular hydrogen as separate species. Charge exchange with molecular hydrogen is very efficient around the vibrational states 3 and 4. The distribution over the vibrational states of

molecular hydrogen produced at the wall is according to [18]. Combined with the vibrational excitation by electron impact collisions, the vibrational levels 3 and 4 of hydrogen molecules at the edge of the beam are well populated. Therefore, more plasma at the edge of the beam will recombine, resulting in a reduced width of the plasma beam. The simulated density profile is still broader than the Thomson scattering profile. One explanation for this could be that recombination via vibrational excited hydrogen molecules is still underestimated in these simulations. Another explanation is that recombining ions probably partly return as molecules, recombining more plasma at the edge of the plasma beam near the target.

Figure 5 shows the integrated current, calculated by B2.5-Eunomia, as function of the radius for different target potentials. The integrated current $I_{ic}(r)$ is given by

$$I_{ic}(r) = 2\pi \int_0^r j(r')r'dr' \tag{3}$$

with $j(r)$ the current density at radius r. The non-zero gradient at $r < 0.015$ m shows that there are currents in the plasma beam. In the simulations we found a floating potential of around -9 V. When biasing the target negatively, at some potential one should reach the ion saturation current. Figure 5 shows that at a target potential of -40 V the ion saturation current has almost been reached. In the experiment, the floating potential was around -27 V and we reached the saturation current at -60 V. There is a clear mismatch between the simulations and the experiments. However, the difference between the floating potential and target potential at saturation is just over 30 V in both the experiment and the B2.5-Eunomia simulations.

In the experiment, the saturation current was around 30 A. The total current through the target at the ion saturation current as calculated by B2.5-Eunomia is a factor 2 too high. This can partially be explained by the broader beam in the simulations. The influence of the prescribed inlet profiles can also be an effect. In the simulation we kept all settings the same, except for the target potential. However, in the experiment some inlet profiles, such as the density profile, are influenced by the target biasing. Moreover,

the potential profile is based on rotation measurements of neutrals. The $\mathbf{E} \times \mathbf{B}$ rotation, and therefore also the electric field and potential, might be underestimated, since the neutrals do not rotate as fast as the ions. The influence of the beam width and the changes to the inlet profiles on the target potential and current through the target has to be studied in more detail.

6. Conclusions

The coupled B2.5-Eunomia has successfully been applied to the cylindrically symmetric geometry of Pilot-PSI. The experimentally obtained density and temperature profiles are reproduced when vibrationally excited hydrogen molecules are considered as separate species in Eunomia. The vibrationally excited hydrogen molecules cool the plasma and efficiently recombine the plasma at the edge of the beam. The narrow Thomson scattering profile of the density indicates that the effect of vibrationally excited hydrogen molecules is still underestimated. The potential difference between floating potential and ion saturation current matches the experiments perfectly. However, the simulated floating potential differs 20 V from the experimental value. The sensitivity of the inlet potential and density boundary condition and the beam width have to be studied in detail to solve this.

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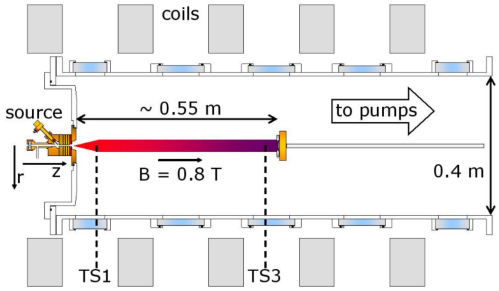

Figure 1: Schematic drawing of Pilot-PSI, with the cascaded arc source on the left and the target on the right of the plasma beam. TS1 and TS3 refer to the Thomson scattering positions at the first and third window.

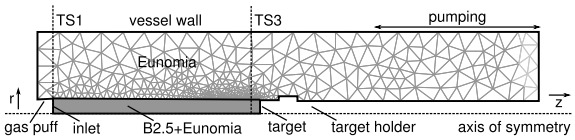

Figure 2: Two dimensional representation of the grid in the (r, z) plane.

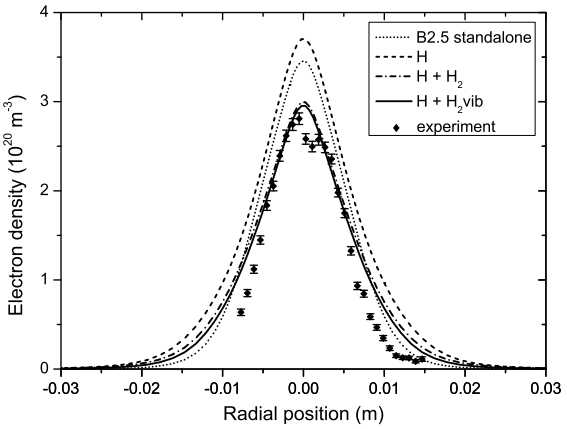

Figure 3: Thomson scattering measurements of the electron density near the target compared with results of B2.5 standalone and three cases of B2.5-Eunomia are shown.

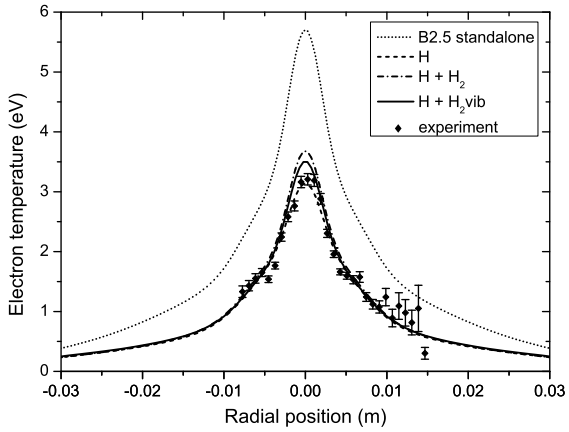

Figure 4: Thomson scattering measurements of the electron temperature near the target compared with results of B2.5 standalone and 3 cases of B2.5-Eunomia are shown.

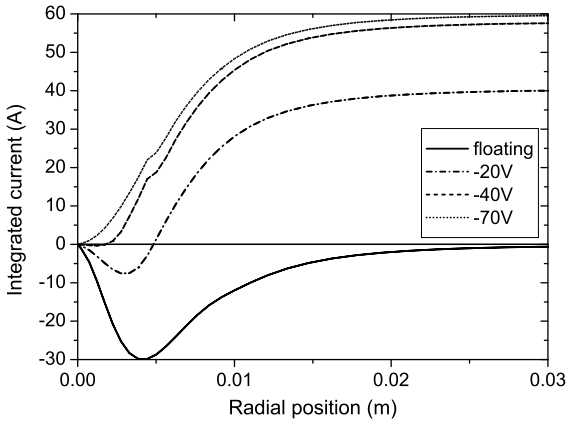

Figure 5: Integrated current for different target potentials.