Derivation of the friction and thermal force for SOLPS-ITER multicomponent plasma modelling

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SOLPS-ITER is a code package for tokamak plasma boundary modelling comprising the B2.5 plasma fluid code and the EIRENE neutral kinetic code. The form of the momentum balance equation, used in the SOLPS-ITER code before version 3.0.6 (and in all previous versions of SOLPS codes), was simplified due to numerical reasons – the electric field term was replaced with the electron gradient pressure term, friction and thermal force terms were derived using the trace impurity assumption. It has now been decided to switch back to the general Braginskii version of this equation. Derivation of the new form of the parallel friction and thermal force terms has been required to allow the use of the general form of the equation and allow more accurate modelling of multicomponent plasmas. The new form is based on the theoretical description of multicomponent plasma derived by V. Zhdanov [V M Zhdanov. "Transport Processes in Multicomponent Plasma". In: Plasma Physics and Controlled Fusion 44.10 (2002), pp. 2283–2283]. In the present paper, a detailed derivation of these terms is presented and their implementation into the SOLPS-ITER code package is discussed.

1. Introduction

Future tokamak reactors, of which the ITER machine will be prototypical, require that very high levels of plasma power be exhausted from the device [2]. This requires high levels of radiative power dissipation which, in the case of high atomic number target materials like tungsten, can only be achieved with the injection of extrinsic seed impurities such as nitrogen (N), neon (Ne), argon, etc. In the case of ITER, where plasma power entering the scrape-off layer (SOL) is expected to be in the range of P_{SOL} ~100 MW, the medium atomic number (Z) radiators, N and Ne, are expected to be sufficient, with the majority of the radiation occurring in the divertor

plasma region [3]. The required impurity density will be at the level of a few percent of the local electron density in the divertor plasma and hence far above trace concentrations.

The ITER divertor required intense numerical studies [3 and references therein]. These simulations have been largely performed with the SOLPS-4.3 [4] code package which comprises a fluid plasma code describing plasma transport in the SOL and divertor region (the B2 code in the case of SOLPS-4.3) coupled to a Monte Carlo kinetic code (the EIRENE code [5]) for the neutral dynamics. The very first version of the fluid part of the code was developed by B. Braams in 1987 [6], and consisted of a Braginskii solver for multifluid plasma dynamics parallel to the tokamak magnetic field. Since then, the fluid code has been coupled to EIRENE and has been developed notably to include solution of the current continuity equation and addition of drift terms [7].

The most modern version of the code, SOLPS-ITER [8] was launched in 2015 by the ITER Organization and is being continuously updated. It comprises the most up-to-date versions of the fluid code (B2.5). The most recent update in 2016 [9] includes a generalization of the parallel momentum balance equation for ions (PMBE) used in the fluid component [10]. This generalization required a change of the treatment of friction and thermal force terms, the detailed physics description of which is the subject of the present paper.

The SOLPS-ITER equations are given in toroidal geometry, with the assumption of toroidal symmetry, and do not include any variation of the variables in the toroidal (z) direction. Coordinates are denoted as follows: x - for poloidal direction, y - for radial direction, z - toroidal coordinate (absent in the equations and used only in the geometry description). The coordinate system is orthogonal and for its description in the code gathering equations metric coefficients are used. These coefficients (Lame coefficients) are defined as follows: $h_x = \frac{1}{|\nabla x|}$; $h_y = \frac{1}{|\nabla y|}$; $h_z = \frac{1}{|\nabla z|}$. The notations $\sqrt{g} = h_x h_y h_z$, $b_x = B_x / |B|$ are used.

It is important to note, that in all discussed SOLPS equations, each of the impurity ion charged states is treated as a separate ion species - for instance, there are momentum equations for each of these charged states and also the friction forces between the different charged states of the same impurity are taken into account.

The previous version of the PMBE for ion species α, used in the code, was simplified for numerical reasons - excluding the electric potential from the system helped to improve the convergence. So instead of using the general Braginskii form of the equation, the modified version was used, in which the potential gradient was replaced by the electron pressure gradient term:

$$m_\alpha \frac{\partial n_\alpha V_{\alpha\parallel}}{\partial t} + \frac{1}{h_z\sqrt{g}}\frac{\partial}{\partial x}\left(\frac{h_z\sqrt{g}}{h_x}\Gamma^m_{\alpha x}\right) + \frac{1}{h_z\sqrt{g}}\frac{\partial}{\partial y}\left(\frac{h_z\sqrt{g}}{h_y}\Gamma^m_{\alpha y}\right) + \frac{b_x}{h_x}\frac{\partial n_\alpha T_i}{\partial x} + \frac{b_x}{h_x}\frac{z_\alpha n_\alpha \partial n_e T_e}{n_e \partial x} \quad (1)$$
$$= S^m_{\alpha\parallel} + S^m_{CF_\alpha} + S^{m\_OLD}_{fr_\alpha} + S^{m\_OLD}_{Therm_\alpha} + S^m_{I_\alpha} + S^m_{R_\alpha} + S^m_{CX_\alpha}$$

Here m_α, n_α, $V_{\alpha\parallel}$ are respectively the mass, density, and the parallel velocity of the ion species α, n_e is the electron density, z_a is the charge number of the species α. The term $m_\alpha \frac{\partial n_\alpha V_{\alpha\parallel}}{\partial t}$ is the time derivative of the

momentum flux; $\frac{1}{h_z\sqrt{g}}\frac{\partial}{\partial x}\left(\frac{h_z\sqrt{g}}{h_{x,y}}\Gamma^m_{\alpha x,y}\right)$ - terms of the divergence of the parallel momentum flux Γ^m_α;

$\frac{b_x}{h_x}\frac{\partial n_\alpha T_i}{\partial x}$ is the parallel projection of the ion pressure gradient term.

The term $\frac{b_x}{h_x}\frac{z_\alpha n_\alpha \partial n_e T_e}{n_e \partial x}$ is the parallel projection of the electron pressure gradient term multiplied by the factor $\frac{z_\alpha n_\alpha}{n_e}$. This term, in combination with the $S^{m\_OLD}_{fr_\alpha} + S^{m\_OLD}_{Therm_\alpha}$ from the l. h. s. provides the replacement for the electric gradient term, which is supposed to be present in this equation [11].

Terms $S^m_{\alpha\|}$, $S^m_{CF_\alpha}$, $S^m_{I_\alpha}$, $S^m_{R_\alpha}$, $S^m_{CX_\alpha}$ are the parallel momentum sources caused correspondingly by viscosity, centrifugal force, ionization, recombination and charge exchange.

Formulation of the OLD friction and thermal force terms acting in the ion species α has the following form [11]:

$$S^{m\_OLD}_{Therm,\alpha} = n_\alpha\left(\frac{z_\alpha}{n_e} - \frac{z_\alpha^2}{\sum_{a=0}^{n_s-1} z_a^2 n_a}\right) n_e \frac{b_x}{h_x}\left[\frac{1}{n_e}\frac{\partial n_e T_e}{\partial x} - e\frac{\partial \varphi}{\partial x} - 2.65\frac{\partial T_i}{\partial x}\right] \quad (2)$$

$$S^{m\_OLD}_{fr,\alpha} = \sum_{\substack{\beta=0 \\ \beta\neq\alpha, Z_\alpha\neq 0, Z_\beta\neq 0}}^{n_s-1} \frac{1}{\xi_p} m_p \sqrt{\mu_{\alpha\beta}} z_\alpha^2 z_\beta^2 n_\alpha n_\beta (V_{\beta\|} - V_{\alpha\|}) \quad (3)$$

Here $z_{a,\beta}$ is the charge number of the species α and β, $\frac{b_x}{h_x}$ is the coefficient for the parallel projection of the following terms: $\frac{\partial n_e T_e}{\partial x}$ - electron pressure gradient; $\frac{\partial \varphi}{\partial x}$ - electric potential gradient; $\frac{\partial T_i}{\partial x}$ - ion temperature gradient; $\mu_{\alpha\beta}$ is the reduced mass for species pair α, β, $\zeta_p = \frac{3}{4\sqrt{2\pi}}\frac{\sqrt{m_p}T_i^{\frac{3}{2}}}{\Lambda}\left(\frac{4\pi\varepsilon_0}{e^2}\right)^2$ - normalized to the density collision time for protons; m_p is the proton mass, Λ is the Coulomb logarithm, and ε_0 is the vacuum permittivity.

This form of the friction and thermal force terms is the modified form of the classical expression for these terms in [12], the modification was made in order to match equation (1).

In the SOLPS-ITER code, the full Braginskii form [12] of the parallel momentum balance equation (PMBE) is solved:

$$m_\alpha \frac{\partial n_\alpha V_{\alpha\parallel}}{\partial t} + \frac{1}{h_z\sqrt{g}}\frac{\partial}{\partial x}\left(\frac{h_z\sqrt{g}}{h_x}\Gamma^m_{\alpha x}\right) + \frac{1}{h_z\sqrt{g}}\frac{\partial}{\partial y}\left(\frac{h_z\sqrt{g}}{h_y}\Gamma^m_{\alpha y}\right) + \frac{b_x}{h_x}\frac{\partial n_\alpha T_i}{\partial x} + z_\alpha e n_\alpha \frac{b_x}{h_x}\frac{\partial \varphi}{\partial x} = \quad (4)$$
$$= S^m_{\alpha\parallel} + S^m_{CF_\alpha} + S^m_{fr_\alpha} + S^m_{Therm_\alpha} + S^m_{I_\alpha} + S^m_{R_\alpha} + S^m_{CX_\alpha}$$

This equation is written in the form in which it is implemented in the code. Here $S^m_{Therm_\alpha}$, $S^m_{fr_\alpha}$ are the thermal and friction force terms which will be derived and discussed below; $z_\alpha e n_\alpha \frac{b_x}{h_x}\frac{\partial \varphi}{\partial x}$ - electric field term; all the other terms are the same as in equation (1).

For a full description of other variables and of the specific formulation used in the SOLPS code suite, see [7]. Note that all ion species in eq (2) and in all following equations are assumed to share a common temperature T_i, which is the fundamental assumption in the SOLPS-ITER physics model. The importance of the implementation of the Braginskii form of the PMBE is discussed in [10]. This implementation requires the derivation of the general form for the friction and thermal force terms for a multi-component plasma: $S^m_{Therm_\alpha}$ and $S^m_{fr_\alpha}$, because the terms $S^{m\_OLD}_{fr_\alpha}$ and $S^{m\_OLD}_{Therm_\alpha}$ could not be used anymore. The present paper focuses on the detailed derivation of these terms.

The starting point for this derivation is the general description of friction and thermal forces, which is valid for arbitrary plasma composition. This description is taken from [13] and is based on the following simplifying assumptions:

- A single main ion species;
- Impurity ions assumed to have much larger mass than the main ions.

These assumptions limit the applicability of the derived terms, but they are fulfilled for the modeling of most of the key exhaust scenarios of interest in the case, for example, of impurity seeding for divertor power flux control in present tokamaks. The lightest impurity discussed as a divertor radiator is nitrogen with its atomic mass 7 times bigger than that of deuterium. The main ion here is one of the hydrogen isotopes (D, T, or H), the density of which is assumed to be at least one order of magnitude higher than the sum of all other ion species densities. In the equations below, the main ion species will be denoted by the subscript MAIN. All species other than main ions and electrons are impurity ions with subscript IMP.

The paper is organized as follows: the form of the terms and the procedure for the definition of the numerical coefficients appearing in front of the force terms are presented in Section 2, collision times and averaged collision frequencies used in the formulation are given in Section 3, with the final form of the terms presented in Section 4. A comparison of the modeling results with the old and new forms of the parallel momentum balance equation for the ASDEX Upgrade model case is presented in Section 5. Section 6 discusses the reformulation of the terms for implementation in SOLPS-ITER.

2. General form of the thermal and friction terms and procedure for determining numerical force term coefficients

The present derivation of the new form for the friction and thermal force terms is based on the multicomponent plasma description introduced by V. Zhdanov [13]. The key equation for the derivation is Eq. (5) below, taken from paragraph 8.4 of [13]. This equation describes the sum of the friction and thermal forces, acting on ion species α. These forces include the friction and thermal forces with all the other ion species and with the electrons.

$$S^m_{Therm_\alpha} + S^m_{Fr_\alpha} = -n_\alpha \left(\sum_\beta \left[c^{(1)}_{\alpha\beta} \mu_{\alpha\beta} \tau^{-1}_{\alpha\beta} \left(V_{\alpha\parallel} - V_{\beta\parallel} \right) - \frac{c^{(2)}_{\alpha\beta} \tau^{-1}_{\alpha\beta}}{\tilde{\tau}^{-1}_\beta} \frac{\mu_{\alpha\beta}}{m_\alpha} \nabla_\parallel T_\beta \right] + c^{(5)}_\alpha \nabla_\parallel T_\alpha \right) \tag{5}$$

where m_α and n_α are the mass and density of species α, $\tilde{\tau}^{-1}_\alpha = \sum_\beta \frac{\mu_{\alpha\beta}}{m_\alpha} \tau^{-1}_{\alpha\beta}$ the averaged collision frequency, $\mu_{\alpha\beta} = \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}$ is the reduced mass for species pair α, β, $\tau^{-1}_{\alpha\beta}$ the collision frequency between species α and β (the exact form of the collision frequency is discussed below), $V_{\alpha\parallel}$, $V_{\beta\parallel}$ the projections of the velocities for species α and β on the direction parallel to the magnetic field and $\nabla_\parallel T_\alpha$ the projection of the gradient of the temperature of species α on the parallel direction. Coefficients $c^{(1)}_{\alpha\beta}$ are assumed to be symmetric against the permutation of α, β indices.

The first term in the sum in Eq. (5) corresponds to the friction force interaction between plasma species α and β. The second term in the sum and the last term correspond to the thermal forces. In [13] the different ion species are assumed to have different temperatures, so there are separate terms with parallel temperature gradients in Eq. (5): the term associated with other species' temperature gradients is part of the sum normalized by the collision frequency (the ratio $\frac{\tau^{-1}_{\alpha\beta}}{\tilde{\tau}^{-1}_\beta}$ originates from the kinetic derivation of (5)); the last term on the RHS of Eq. (5) is associated with the temperature gradient of the species under consideration.

The most complicated aspect of the implementation of Eq. (5) is the calculation of the numerical coefficients $c^{(1)}_{\alpha\beta}$, $c^{(2)}_{\alpha\beta}$, and $c^{(5)}_\alpha$. In general, this should be performed for each simulated plasma composition (set of the types of ions chosen for modeling, e.g. pure deuterium plasma, D-T mixture, D plasma with N impurity, etc.).

Depending on the masses of the ions present in the composition, coefficients can be calculated by integration of the system of kinetic equations using generalized Laguerre polynomials.

As shown in [13], for relatively light plasma particles *k*, with low mass in comparison to that of other species in the same plasma, the calculation of these coefficients can be simplified as:

$$c_{k\alpha}^{(1)} = c_{\alpha k}^{(1)} = \frac{(1+0.24\tilde{z}_k)(1+0.93\tilde{z}_k)}{(1+2.56\tilde{z}_k)(1+0.29\tilde{z}_k)},\ c_{k\alpha}^{(2)} = 0,\ c_{\alpha k}^{(2)} = 1.56\frac{(1+1.4\tilde{z}_k)(1+0.52\tilde{z}_k)}{(1+2.56\tilde{z}_k)(1+0.29\tilde{z}_k)} \quad (6)$$

Where $\tilde{z}_k = \sum_{a,m_a>>m_k} \frac{n_a z_a^2}{n_k z_k^2}$ is an averaged charge of the heavy particles with respect to the lighter species. In case of the mass separation of electrons from all the ion species $\tilde{z}_e = \sum_{a,m_a>>m_e} \frac{n_a z_a^2}{n_e} = z_{eff}$.

In the implementation discussed here, the same mass separation is performed between the main and impurity ions, with the latter assumed to be heavy particles, $m_{IMP} >> m_{MAIN}$. This assumption limits the applicability of the suggested thermal and friction force model for the cases with helium impurity, since this impurity ion is not much heavier than D or T.

With these separations, the coefficients $c_{\alpha k}^{(1)}$, $c_{\alpha k}^{(2)}$ and $c_{k\alpha}^{(2)}$ in the implementation of Eq (5) are computed in the SOLPS-ITER code as follows:

- for electrons separated as light particles from all ion species:

$$c_{e\_MAIN}^{(1)} = c_{e\_IMP}^{(1)} = \frac{(1+0.24z_{eff})(1+0.93z_{eff})}{(1+2.56z_{eff})(1+0.29z_{eff})} = c_e^{(1)};\ c_{e\_MAIN;IMP}^{(2)} = 0 \quad (7)$$

$$c_{MAIN\_e}^{(2)} = c_{IMP\_e}^{(2)} = 1.56\frac{(1+1.4z_{eff})(1+0.52z_{eff})}{(1+2.56z_{eff})(1+0.29z_{eff})} = c_e^{(2)} \quad (8),$$

where $z_{eff} = \sum_{a\in ion\_species} n_a z_a^2 \Big/ n_e$

- for heavy impurity ions separated as light particles from main ions:

- $$c_{MAIN\_IMP}^{(1)} = c_{IMP\_MAIN}^{(1)} = \frac{(1+0.24z_{eff\_imp})(1+0.93z_{eff\_imp})}{(1+2.56z_{eff\_imp})(1+0.29z_{eff\_imp})} \equiv c_{IMP}^{(1)} \quad (9)$$

- $$c_{MAIN\_IMP}^{(2)} = 1.56\frac{(1+1.4z_{eff\_imp})(1+0.52z_{eff\_imp})}{(1+2.56z_{eff\_imp})(1+0.29z_{eff\_imp})} \equiv c_{IMP}^{(2)};\ c_{IMP\_MAIN}^{(2)} = 0 \quad (10)$$

where $z_{eff\_imp} = \sum_{a \in IMP} n_a z_a^2 \Big/ n_{MAIN} z_{MAIN}^2$.

In the improved thermal and friction force description presented here, the definition of the coefficients $c_{\alpha\alpha}^{(2)}$ and $c_{\alpha}^{(5)}$ is performed in two steps (for α going through all plasma species).

Importantly, we note that Eq (5) for each plasma species effectively contains these coefficients only in the specific combination $\left(c_{\alpha}^{(5)} - \frac{1}{2} c_{\alpha\alpha}^{(2)} \tau_{\alpha\alpha}^{-1} \widetilde{\tau}_{\alpha} \right)$. This requires manipulations of equation (5), which are demonstrated below. Once this combination is obtained in the equation, there will be no need to define the coefficients $c_{\alpha\alpha}^{(2)}$ and $c_{\alpha}^{(5)}$ separately – only the combination will need to be defined.

To show that only the mentioned combination is necessary, here we separate the part of the thermal force driven by $\nabla_{\parallel} T_{\alpha}$ in Eq. (5) as:

$$S_{Therm_\alpha}^{m} + S_{Fr_\alpha}^{m} = -n_\alpha \left(\sum_{\beta \neq \alpha} \left[c_{\alpha\beta}^{(1)} \mu_{\alpha\beta} \tau_{\alpha\beta}^{-1} \left(V_{\alpha\parallel} - V_{\beta\parallel} \right) - \frac{c_{\alpha\beta}^{(2)} \tau_{\alpha\beta}^{-1}}{\widetilde{\tau}_{\beta}^{-1}} \frac{\mu_{\alpha\beta}}{m_\alpha} \nabla_{\parallel} T_\beta \right] + \left[c_{\alpha}^{(5)} - \frac{c_{\alpha\alpha}^{(2)} \tau_{\alpha\alpha}^{-1}}{\widetilde{\tau}_{\beta}^{-1}} \frac{\mu_{\alpha\alpha}}{m_\alpha} \right] \nabla_{\parallel} T_\alpha \right) \qquad (11)$$

By the definition of the reduced mass, $\frac{\mu_{\alpha\alpha}}{m_\alpha} = \frac{1}{2}$, so the last term would be $\left[c_{\alpha}^{(5)} - \frac{1}{2} \frac{c_{\alpha\alpha}^{(2)} \tau_{\alpha\alpha}^{-1}}{\widetilde{\tau}_{\beta}^{-1}} \right] \nabla_{\parallel} T_\alpha$.

Now, according to Newton's third law, the sum of all thermal force and friction terms from all species should be 0. This means that after summing up the separate momentum balance equations for all plasma species all terms should cancel out:

$$\begin{aligned} &\sum_{\alpha} \left(S_{Fr_\alpha}^{m} + S_{Therm_\alpha}^{m} \right) = 0 = \\ &= -\sum_{\alpha} n_\alpha \left(\sum_{\beta \neq \alpha} \left[c_{\alpha\beta}^{(1)} \mu_{\alpha\beta} \tau_{\alpha\beta}^{-1} \left(V_{\alpha\parallel} - V_{\beta\parallel} \right) - \frac{c_{\alpha\beta}^{(2)} \tau_{\alpha\beta}^{-1}}{\widetilde{\tau}_{\beta}^{-1}} \frac{\mu_{\alpha\beta}}{m_\alpha} \nabla_{\parallel} T_\beta \right] + \left[c_{\alpha}^{(5)} - \frac{1}{2} \frac{c_{\alpha\alpha}^{(2)} \tau_{\alpha\alpha}^{-1}}{\widetilde{\tau}_{\beta}^{-1}} \right] \nabla_{\parallel} T_\alpha \right) \end{aligned} \qquad (12)$$

The first term on the RHS of Eq (12) gives the condition $c_{\alpha\beta}^{(1)} = c_{\beta\alpha}^{(1)}$ (to eliminate velocity terms in the total sum), which was mentioned above (symmetry of the $c_{\alpha\beta}^{(1)}$ coefficient). The remaining terms correspond to the thermal force:

$$0 = -\sum_{\alpha} n_\alpha \left(\sum_{\beta \neq \alpha} \left[-\frac{c_{\alpha\beta}^{(2)} \tau_{\alpha\beta}^{-1}}{\widetilde{\tau}_{\beta}^{-1}} \frac{\mu_{\alpha\beta}}{m_\alpha} \nabla_{\parallel} T_\beta \right] + \left[c_{\alpha}^{(5)} - \frac{1}{2} \frac{c_{\alpha\alpha}^{(2)} \tau_{\alpha\alpha}^{-1}}{\widetilde{\tau}_{\beta}^{-1}} \right] \nabla_{\parallel} T_\alpha \right) \qquad (13)$$

It is convenient to define the coefficients in Eq (12) by putting α equal to each type of plasma particle separately. Here the procedure will be demonstrated for coefficients corresponding to electron temperature gradients.

In this case $\frac{\mu_{e\beta}}{m_e} \approx \frac{m_e}{m_e} = 1$ for β denoting any sort of ion species.

$$c^{(2)}_{e\_MAIN}\frac{\tau^{-1}_{e\_MAIN}}{\tilde{\tau}^{-1}_{e}}\nabla_{\parallel}T_{MAIN} + c^{(2)}_{e\_IMP}\frac{\tau^{-1}_{e\_IMP}}{\tilde{\tau}^{-1}_{e}}\nabla_{\parallel}T_{IMP} + c^{(2)}_{MAIN\_e}\frac{\tau^{-1}_{MAIN\_e}}{\tilde{\tau}^{-1}_{e}}\nabla_{\parallel}T_{e} + c^{(2)}_{IMP\_e}\frac{\tau^{-1}_{IMP\_e}}{\tilde{\tau}^{-1}_{e}}\nabla_{\parallel}T_{e} + \left(c^{(5)}_{e} - c^{(2)}_{ee}\frac{1}{2}\frac{\tau^{-1}_{ee}}{\tilde{\tau}^{-1}_{e}}\right)\nabla_{\parallel}T_{e} = 0 \tag{14}$$

Substituting the values of $c^{(2)}_{e\_MAIN}$, $c^{(2)}_{e\_IMP}$, $c^{(2)}_{MAIN\_e}$, $c^{(2)}_{IMP\_e}$ from (7), (8) we obtain:

$$\left(c^{(5)}_{e} - c^{(2)}_{ee}\frac{1}{2}\frac{\tau^{-1}_{ee}}{\tilde{\tau}^{-1}_{e}}\right) = c^{(2)}_{e}\left(\frac{\tau^{-1}_{e\_MAIN}}{\tilde{\tau}^{-1}_{e}} + \frac{\tau^{-1}_{IMP\_e}}{\tilde{\tau}^{-1}_{e}}\right) \tag{15}$$

which yields the combination $\left(c^{(5)}_{e} - c^{(2)}_{ee}\frac{1}{2}\frac{\tau^{-1}_{ee}}{\tilde{\tau}^{-1}_{e}}\right)$ mentioned above. With these, the implementation of Eq (5) for electrons in the mass separation assumption is complete.

The same procedure is followed for the main ion temperature gradient, resulting in:

$$\left(c^{(5)}_{MAIN} - \frac{1}{2}c^{(2)}_{MAIN\_MAIN}\frac{\tau^{-1}_{MAIN\_MAIN}}{\tilde{\tau}^{-1}_{MAIN}}\right) = -\sum_{IMP}\frac{c^{(2)}_{IMP}}{2}\frac{\tau^{-1}_{MAIN\_IMP}}{\tilde{\tau}^{-1}_{MAIN}}\frac{\mu_{MAIN\_IMP}}{m_{IMP}} \tag{16}$$

Terms due to different temperature gradients between impurity and main ions are neglected in this implementation of the PMBE, as mentioned above. The derivation of the coefficients in front of such terms cannot be performed by the same procedure and would require future effort. These terms are second order with respect to impurity density and at the moment they are not included in the code.

3. Collision times.

The definition of the collision times is essential when dealing with processes of particle interactions in plasmas. Here we follow the formulation from [13], which matches the approach of Braginskii [12]. Before presenting the collision times it is convenient to define the following quantities:

$$\zeta_p = \frac{3}{4\sqrt{2\pi}}\frac{\sqrt{m_p}T_i^{\frac{3}{2}}}{\Lambda}\left(\frac{4\pi\varepsilon_0}{e^2}\right)^2; \tag{17a}$$

$$\zeta_e = \frac{3}{4\sqrt{2\pi}}\frac{\sqrt{m_e}T_e^{\frac{3}{2}}}{\Lambda}\left(\frac{4\pi\varepsilon_0}{e^2}\right)^2 \tag{17b}$$

Here m_p, m_e are respectively the proton and electron masses, Λ is the Coulomb logarithm, and ε_0 is the vacuum permittivity. These are normalized collision times for protons and electrons respectively. Definitions of (17a) and (17b) simplify the symmetry-checking procedure of the final equations.

The collision times can then be written as follows:

$$\tau_{\alpha\beta}^{-1} = \frac{4\sqrt{2\pi}\sqrt{2}n_\beta}{3}\frac{z_\alpha^2 z_\beta^2 \Lambda}{T_i^{3/2}\mu_{\alpha\beta}^{1/2}}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 = \sqrt{2}\zeta_p^{-1} n_\beta z_\alpha^2 z_\beta^2 \frac{\sqrt{m_p}}{\sqrt{\mu_{\alpha\beta}}} \tag{18a}$$

$$\tau_{e\beta}^{-1} = \frac{4\sqrt{2\pi}n_\beta}{3}\frac{z_\beta^2 \Lambda}{T_e^{3/2} m_e^{1/2}}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 = \zeta_e^{-1} n_\beta z_\beta^2 \tag{18b}$$

$$\tau_{\beta e}^{-1} = \zeta_e^{-1} n_e z_\beta^2 \tag{18c}$$

$$\tau_{ee}^{-1} = \frac{4\sqrt{2\pi}\sqrt{2}n_e}{3}\frac{\Lambda}{T_e^{3/2} m_e^{1/2}}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 = \sqrt{2}\zeta_e^{-1} n_e \tag{18d}$$

To use equation (5) it is also necessary to compute the average collision frequency for species α,

$$\tilde{\tau}_\alpha^{-1} = \sum_\beta \frac{\mu_{\alpha\beta}}{m_\alpha}\tau_{\alpha\beta}^{-1}\,.$$

For electrons we then have (neglecting terms proportional to the electron mass):

$$\begin{aligned}\tilde{\tau}_e^{-1} &= \sum_\gamma \frac{\mu_{\gamma e}}{m_e}\tau_{e\gamma}^{-1} = \sum_{IMP}\tau_{e\_IMP}^{-1} + \tau_{e\_MAIN}^{-1} + \frac{1}{2}\tau_{ee}^{-1} = \\ &\zeta_e^{-1}\sum_{IMP} n_{IMP} z_{IMP}^2 + n_{MAIN} z_{MAIN}^2 \zeta_e^{-1} + \frac{\sqrt{2}}{2}\zeta_e^{-1} n_e = n_e z_{eff}\zeta_e^{-1}\left(z_{eff} + \frac{\sqrt{2}}{2}\right)\end{aligned} \tag{19}$$

and for the main ions:

$$\begin{aligned}\tilde{\tau}_{MAIN}^{-1} &= \sum_\gamma \frac{\mu_{MAIN\_\gamma}}{m_{MAIN}}\tau_{MAIN\_\gamma}^{-1} = \sum_{IMP}\frac{\mu_{IMP\_MAIN}}{m_{MAIN}}\tau_{MAIN\_IMP}^{-1} + \frac{1}{2}\tau_{MAIN\_MAIN}^{-1} + \frac{m_e}{m_{MAIN}}\tau_{MAIN\_e}^{-1} = \\ &= \sum_{IMP}\sqrt{2}\,\frac{\mu_{IMP\_MAIN}}{m_{MAIN}}\frac{\sqrt{m_p}}{\sqrt{\mu_{IMP\_MAIN}}} n_{IMP} z_{IMP}^2 z_{MAIN}^2 \zeta_p^{-1} \\ &+ \frac{1}{2}\frac{\sqrt{m_p}}{\sqrt{\frac{m_{MAIN}}{2}}}\sqrt{2} n_{MAIN} z_{MAIN}^4 \zeta_p^{-1} + \frac{m_e}{m_{MAIN}} z_{MAIN}^2 \zeta_e^{-1} n_e \\ &\cong \sqrt{2}\zeta_p^{-1} z_{MAIN}^2 \frac{\sqrt{m_p}}{m_{MAIN}}\sum_{IMP}\sqrt{\mu_{IMP\_MAIN}}\, n_{IMP} z_{IMP}^2 + \sqrt{\frac{m_p}{m_{MAIN}}} n_{MAIN} z_{MAIN}^4 \zeta_p^{-1}\end{aligned} \tag{20}$$

In deducing the final form of equations (19) and (20), the term proportional to the electron mass is neglected to simplify the result.

4. Final form of the friction and thermal force terms.

Now that the collision frequencies have been defined, Eq (5) can be rewritten in more detail.

The friction and thermal forces acting on the electrons are given by:

$$S^m_{Fr_e} + S^m_{Therm_e} = -c_e^{(1)} m_e \zeta_e^{-1} Z^2_{MAIN} n_{MAIN} n_e \left(V_{e\|} - V_{MAIN\|}\right) - c_e^{(1)} m_e \zeta_e^{-1} \sum_{IMP} n_{IMP} Z^2_{IMP} n_e \left(V_{e\|} - V_{IMP\|}\right)$$
$$- c_e^{(2)} \left(\tau^{-1}_{MAIN\_e} \tilde{\tau}_e + \sum_{IMP} \tau^{-1}_{IMP\_e} \tilde{\tau}_e \right) n_e \nabla_\| T_e \qquad (21)$$

Using (17)

$\tau^{-1}_{MAIN\_e} \tilde{\tau}_e = \dfrac{z^2_{MAIN}}{z_{eff} + \dfrac{\sqrt{2}}{2}}$; $\tau^{-1}_{IMP\_e} \tilde{\tau}_e = \dfrac{z^2_{IMP}}{z_{eff} + \dfrac{\sqrt{2}}{2}}$, so that the final form of the electron equation will be:

$$S^m_{Fr_e} + S^m_{Therm_e} = -c_e^{(1)} m_e \zeta_e^{-1} z^2_{MAIN} n_{MAIN} n_e \left(V_{e\|} - V_{MAIN\|}\right) - c_e^{(1)} m_e \zeta_e^{-1} \sum_{IMP} n_{IMP} z^2_{IMP} n_e \left(V_{e\|} - V_{IMP\|}\right)$$
$$- c_e^{(2)} \left(\frac{z^2_{MAIN}}{z_{eff} + \frac{\sqrt{2}}{2}} + \sum_{IMP} \frac{z^2_{IMP}}{z_{eff} + \frac{\sqrt{2}}{2}_e} \right) n_e \nabla_\| T_e \qquad (22)$$

This form, in the pure plasma limit ($n_{IMP} = 0$), matches the Braginskii friction and thermal force expression:

$$S^m_{Fr_e} + S^m_{Therm_e} = -0.51 \frac{1}{\tau_e} \left(V_{i\|} - V_{e\|}\right) m_e n_e - 0.71 n_e \nabla_\| T_e \qquad (23)$$

To write Eq (5) for the case of ion-ion interactions Eq (20) is used:

$$\tau^{-1}_{IMP\_MAIN} \tilde{\tau}_{MAIN} \frac{\mu_{IMP\_MAIN}}{m_{MAIN}} = \frac{n_{MAIN} z^2_{IMP} \sqrt{\dfrac{\mu_{IMP\_MAIN}}{m_{MAIN}}}}{\displaystyle\sum_{IMP} \sqrt{\frac{\mu_{IMP\_MAIN}}{m_{MAIN}}} n_{IMP} z^2_{IMP} + \frac{\sqrt{2}}{2} n_{MAIN} z^2_{MAIN}},$$

so the thermal force term for each impurity charge state will be

$$c^{(2)}_{IMP} \frac{n_{MAIN} z^2_{IMP} \sqrt{\dfrac{\mu_{IMP\_MAIN}}{m_{MAIN}}}}{\displaystyle\sum_{IMP} \sqrt{\frac{\mu_{IMP\_MAIN}}{m_{MAIN}}} n_{IMP} z^2_{IMP} + \frac{\sqrt{2}}{2} n_{MAIN} z^2_{MAIN}} n_{IMP} \nabla T_{MAIN}.$$

The final form of Eq (5) for ions – including the sum of all the friction and thermal forces acting on the main ions and on each impurity ion species - becomes correspondingly:

$$
\begin{aligned}
&S^m_{Therm_{MAIN}} + S^m_{Fr_{MAIN}} = -c_e^{(1)} m_e \zeta_e^{-1} n_e n_{MAIN} z^2_{MAIN} \left(V_{MAIN\|} - V_{e\|}\right) \\
&- \sum_{IMP} c^{(1)}_{IMP} \zeta_p^{-1} \sqrt{2} \sqrt{\mu_{MAIN\_IMP} m_p}\, n_{MAIN} z^2_{MAIN} n_{IMP} Z^2_{IMP} \left(V_{MAIN\|} - V_{IMP\|}\right) + \\
&+ c_e^{(2)} \frac{n_{MAIN} z^2_{MAIN}}{z_{eff} + \frac{\sqrt{2}}{2}} \nabla_{\|} T_e - \frac{\sum_{IMP} c^{(2)}_{IMP} n_{MAIN} n_{IMP} z^2_{IMP} \sqrt{\frac{\mu_{IMP\_MAIN}}{m_{MAIN}}}}{\sum_{IMP} \sqrt{\frac{\mu_{IMP\_MAIN}}{m_{MAIN}}} n_{IMP} z^2_{IMP} + \frac{\sqrt{2}}{2} n_{MAIN} z^2_{MAIN}} \nabla_{\|} T_{MAIN}
\end{aligned}
\tag{24}
$$

$$
\begin{aligned}
&S^m_{Therm_{IMP}} + S^m_{Fr_{IMP}} = -c_e^{(1)} m_e \zeta_e^{-1} n_e n_{IMP} z^2_{IMP} \left(V_{IMP\|} - V_{e\|}\right) \\
&- c^{(1)}_{IMP} \zeta_p^{-1} \sqrt{2} \sqrt{\mu_{MAIN\_IMP} m_p}\, n_{MAIN} z^2_{MAIN} n_{IMP} z^2_{IMP} \left(V_{IMP\|} - V_{MAIN\|}\right) - \\
&- \sum_{IMP*} \zeta_p^{-1} \sqrt{2} \sqrt{\mu_{IMP*\_IMP} m_p}\, n_{IMP*} z^2_{IMP*} n_{IMP} z^2_{IMP} \left(V_{IMP\|} - V_{IMP*\|}\right) + \\
&+ c_e^{(2)} \frac{n_{IMP} z^2_{IMP}}{z_{eff} + \frac{\sqrt{2}}{2}} \nabla_{\|} T_e + c^{(2)}_{IMP} \frac{n_{MAIN} n_{IMP} z^2_{IMP} \sqrt{\frac{\mu_{IMP\_MAIN}}{m_{MAIN}}}}{\sum_{IMP*} \sqrt{\frac{\mu_{IMP*\_MAIN}}{m_{MAIN}}} n_{IMP*} z^2_{IMP} + \frac{\sqrt{2}}{2} n_{MAIN} z^2_{MAIN}} \nabla_{\|} T_{MAIN}
\end{aligned}
\tag{25}
$$

Here in Eq. (24) IMP in the sum index going through all the impurity species in the system.

In Eq. (25) $IMP*$ is the index in the sum which also goes through all the impurity species in the system, including the impurity, for which the equation (25) is written (IMP).

Since the expressions for electron-ion friction and thermal force are now modified, the expression for parallel current should be modified accordingly. The starting point is the electron parallel momentum balance equation in its stationary form:

$$0 = -\nabla_{\parallel} p_e + en_e \nabla_{\parallel}\varphi + c_e^{(1)} m_e \zeta_e^{-1} n_e \sum_{\substack{ions \\ (MAIN,IMP)}} n_\alpha z_\alpha^2 \left(V_{\alpha\parallel} - V_{e\parallel}\right) - c_e^{(2)} \frac{z_{eff}}{z_{eff} + \frac{\sqrt{2}}{2}} \nabla_{\parallel} T_e \tag{26}$$

from which it is possible to construct an expression for the parallel current. By definition, the latter is $j_{\parallel} \equiv e \sum_{\substack{ions \\ (MAIN,IMP)}} n_\alpha V_{\alpha\parallel} z_\alpha - en_e V_{e\parallel}$. To extract such an expression from (26) the term $c_e^{(1)} m_e \zeta_e^{-1} n_e \sum_{\substack{ions \\ (MAIN,IMP)}} n_\alpha V_{\alpha\parallel} z_\alpha$ can be added and subtracted, leading to:

$$\begin{aligned} &0 = -\nabla_{\parallel} p_e + en_e \nabla_{\parallel}\varphi + \\ &\frac{c_e^{(1)} m_e}{e\zeta_e} \left(n_e e \sum_{\substack{ions \\ (MAIN,IMP)}} n_\alpha z_\alpha^2 V_{\alpha\parallel} + \sum_{\substack{ions \\ (MAIN,IMP)}} \left(en_\alpha z_\alpha^2 \sum_{\substack{ions \\ (MAIN,IMP)}} n_\beta z_\beta V_{\beta\parallel} - n_\alpha z_\alpha^2 n_e e V_{e\parallel} - en_\alpha z_\alpha^2 \sum_{\substack{ions \\ (MAIN,IMP)}} n_\beta z_\beta V_{\beta\parallel} \right) \right) \\ &- c_e^{(2)} \frac{z_{eff}}{z_{eff} + \frac{\sqrt{2}}{2}} \nabla_{\parallel} T_e \end{aligned} \tag{27}$$

Now we are able to construct $j_{\parallel}$ by combining $\sum_{\substack{ions \\ (MAIN,IMP)}} \left(en_\alpha z_\alpha^2 \sum_{\substack{ions \\ (MAIN,IMP)}} n_\beta z_\beta V_{\beta\parallel} - n_\alpha z_\alpha^2 n_e e V_{e\parallel} \right)$ and taking $j_{\parallel} \equiv e \sum_{\substack{ions \\ (MAIN,IMP)}} n_\beta V_{\beta\parallel} z_\beta - en_e V_{e\parallel}$ out from the sum operator. The equation (27) will then take the following form:

$$\begin{aligned} &0 = -\nabla_{\parallel} p_e + en_e \nabla_{\parallel}\varphi + \\ &\frac{c_e^{(1)} m_e}{e\zeta_e} \left(e \sum_{\substack{ions \\ (MAIN,IMP)}} n_\alpha z_\alpha^2 \left(n_e V_{\alpha\parallel} - \sum_{\substack{ions \\ (MAIN,IMP)}} n_\beta z_\beta V_{\beta\parallel} \right) + j_{\parallel} \sum_{\substack{ions \\ (MAIN,IMP)}} n_\alpha z_\alpha^2 \right) \\ &- c_e^{(2)} \frac{z_{eff}}{z_{eff} + \frac{\sqrt{2}}{2}} \nabla_{\parallel} T_e \end{aligned} \tag{28}$$

Using $\sum_{\substack{ions \\ (MAIN,IMP)}} n_\alpha z_\alpha^2 = n_e z_{eff}$ and regrouping the terms then leads to:

$$\begin{aligned} &0 = -\nabla_{\parallel} p_e + en_e \nabla_{\parallel}\varphi + \\ &\frac{c_e^{(1)} m_e}{e\zeta_e} \left(e \sum_{\substack{ions \\ (MAIN,IMP)}} n_\alpha z_\alpha^2 \left(n_e V_{\alpha\parallel} - \sum_{\substack{ions \\ (MAIN,IMP)}} n_\beta z_\beta V_{\beta\parallel} \right) \right) + \frac{n_e z_{eff} c_e^{(1)} m_e}{e\zeta_e} j_{\parallel} - c_e^{(2)} \frac{z_{eff}}{z_{eff} + \frac{\sqrt{2}}{2}} \nabla_{\parallel} T_e \end{aligned} \tag{29}$$

From which $j_{\parallel}$ can be extracted to yield the following expression:

$$j_\parallel = \frac{e^2\zeta_e}{c_e^{(1)} m_e z_{eff}}\left(\frac{1}{en_e}\nabla_\parallel p_e - \nabla_\parallel \varphi\right) - \frac{1}{z_{eff}}\left(e\sum_{\substack{ions\\(MAIN,IMP)}} n_\alpha z_\alpha^2\left(n_e V_{\alpha\parallel} - \sum_{\substack{ions\\(MAIN,IMP)}} n_\beta z_\beta V_{\beta\parallel}\right)\right) + c_e^{(2)}\frac{z_{eff}}{z_{eff}+\frac{\sqrt{2}}{2}}\nabla_\parallel T_e \quad (30)$$

The sum $\sum_{\substack{ions\\(MAIN,IMP)}} n_\alpha z_\alpha^2\left(n_e V_{\alpha\parallel} - \sum_{\substack{ions\\(MAIN,IMP)}} n_\beta z_\beta V_{\beta\parallel}\right)$ can be significantly simplified. Defining the electron density through z_{eff} the following way $n_e = \sum_{\substack{ions\\(MAIN,IMP)}} n_\alpha z_\alpha^2 \Big/ z_{eff}$ this sum can be rewritten as:

$$\frac{1}{z_{eff}}\sum_{\substack{ions\\(MAIN,IMP)}} n_\alpha z_\alpha^2 V_{\alpha\parallel} \sum_{\substack{ions\\(MAIN,IMP)}} n_\beta z_\beta^2 - \sum_{\substack{ions\\(MAIN,IMP)}} n_\alpha z_\alpha^2 \sum_{\substack{ions\\(MAIN,IMP)}} n_\beta z_\beta V_{\beta\parallel} \quad (31)$$

Since both indices α and β in the sums run over the same values, in the second sum one can intervert the indices ($\alpha \leftrightarrow \beta$), after which the terms in (31) can be regrouped the following way:

$$\sum_{\substack{ions\\(MAIN,IMP)}} n_\beta z_\beta^2 \sum_{\substack{ions\\(MAIN,IMP)}} \left(\frac{1}{z_{eff}} n_\alpha z_\alpha^2 V_{\alpha\parallel} - n_\alpha z_\alpha V_{\alpha\parallel}\right) \quad (32)$$

Finally, gathering $\sum_{\substack{ions\\(MAIN,IMP)}} n_\beta z_\beta^2$ in (32) back into $z_{eff} n_e$ and substituting it into (30) results in the following expression for $j_\parallel$

$$j_\parallel = \frac{e^2\zeta_e}{c_e^{(1)} m_e z_{eff}}\left(\frac{1}{en_e}\nabla_\parallel p_e - \nabla_\parallel \varphi\right) + \frac{c_e^{(2)} e\zeta_e}{c_e^{(1)} m_e\left(z_{eff}+\frac{\sqrt{2}}{2}\right)}\nabla_\parallel T_e - \frac{e}{z_{eff}}\sum_{ions} n_\alpha V_{\alpha\parallel}\left(z_\alpha^2 - z_\alpha z_{eff}\right) \quad (33)$$

5. Implementation in modeling

Comparisons of the modeling results with the new and old versions of the PMBE were first published in [10]. More figures from this comparison are presented below to demonstrate the effect of the new form of the equation in terms of the impurity transport.

Here the modeling results are presented for the ASDEX Upgrade geometry. No attempt to match the data for a specific experimental shot was made. Instead, typical H mode parameters were chosen. The input parameters were inspired by [15]: 5 MW heating power; D fueling was set to 2e22 atoms/s, two N seeding values were considered: 8e18 atoms/s (trace impurity case) and 8e19 atoms/s. All drifts and currents were included in the SOLPS-ITER modeling and the transport barrier was imposed through the transport coefficients profiles [10].

In Figs. 1 – 4, electron density and temperature profiles are presented at the outer midplane and at the outer target. Outer target profiles change with the increase of the impurity seeding - the temperature peak at the outer target is significantly decreased with the higher impurity seeding. The main point of these graphs in the context of this paper is to demonstrate that the influence of the new form of PMBE on the main ions is minor for the chosen modeling parameters.

In Figs. 5 and 6, the total nitrogen ion density, summed over all charged states, is plotted at the midplane and at the outer target. As it can be expected, the effect of new equations is more significant for higher impurity density. Here, a rather strong effect of the new form of the parallel momentum balance equation can be seen for the 8e19 atoms/s nitrogen seeding case. The new form of the equation results in the redistribution of the impurity ions: more impurity ions are dragged from the divertor target towards upstream and the impurity density in the core region grows significantly. This difference can be crucial when modeling impurity seeding discharges and therefore the new form of the equation was made the default in SOLPS-ITER. starting from the 3.0.6 version [9].

More results with the new version of the equation for ITER input parameters can also be found in Ref, [16].

6. Summary.

New forms of the friction and thermal force terms are derived for the Braginskii form of the parallel momentum balance equation in the SOLPS-ITER physics model. The derivation is based on the kinetic description from V. Zhdanov [13], simplified with the mass separation procedure, which allows for the uncoupling of the equations for different sorts of ion species and obtaining an analytical form for the final coefficients. Corresponding changes are also made in the expression for the parallel current. The obtained friction and thermal force formulations are implemented in the master version of SOLPS-ITER code. The derivation allows to obtain a simple and yet accurate form of the terms when given assumptions (mass of impurity ions is much bigger than the mass of main ions; density of impurity ions is much smaller than that of main ions) are fulfilled. The present work aims to serve as the basis for future improvements of the model equations for friction and thermal forces interactions between particles for SOLPS-ITER and other tokamak edge plasma codes. Such improvements in the SOLPS-ITER model could be the modification of the friction and thermal force model to be able to describe several isotopes for the main ions, which is important to model ITER DT plasmas.

Disclaimer.

ITER is the Nuclear Facility INB no. 174. The views and opinions expressed herein do not necessarily reflect those of the ITER Organization.

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Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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Figure captions

Figure 1: Electron density profiles at the outer midplane. Solid lines represent modeling results obtained with the new form of PMBE, dashed lines represent the modeling results obtained with the old form of PMBE. Blue lines represent modeling results with the 8e18 atoms/s nitrogen seeding, red lines represent modeling results with the 8e19 atoms/s nitrogen seeding.

Figure 2: Electron temperature profiles at the outer midplane. Curves are color-coded as in Fig. 1.

Figure 3: Electron density profiles at the outer target. Curves are color-coded as in Fig. 1. Abbreviation PFR means private flow region.

Figure 4: Electron temperature profiles at the outer target. Curves are color-coded as in Fig. 1.

Figure 5: Nitrogen density profiles at the outer midplane. Curves are color-coded as in Fig. 1.

Figure 6: Nitrogen density profiles at the outer target. Curves are color-coded as in Fig. 1.