Stellarator Impurity STRAHL Code Development in NIFS

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The new Stellarator Impurity Transport (SIT) code is an extended version of STRAHL code [1], which can be used for non-axisymmertic magnetic configurations to evaluate impurity behavior in the frame of the stellarator-specific neoclassical transport, which is strongly dependent on magnetic topology and the radial electric field. The code solves the system of 1D continuity equations (averaged over the magnetic flux surfaces) for impurity ions of each charge state, coupled due to the ionization and recombination. It calculates the time and space evolution of density and emission of impurity ions coming from the wall or deposited within the plasma during the pellet ablation. An analytical description of the neoclassical transport coefficient for the background plasmas was generalized to impurity ions of arbitrary mass and charge state and used in the code as a neoclassical transport model for impurities. Calculations of the electric field and transport coefficients are included within the time dependent iterative loop. Various models of anomalous drift velocities and diffusion coefficients were incorporated. The code can be used as an interpretative and predictive tool for simulation of impurity behavior in arbitrary non-axisymmetric configurations.

Keywords: impurity code, impurity transport, stellarator impurity simulation, electric field in stellarator plasma, impurity confinement, impurity screening

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1. Introduction

The Stellarator Impurity Transport STRAHL code (SIT STRAHL) is an extended and upgraded version of the STRAHL impurity code [1]. It aims to calculate the evolution of impurity ions coming into a bulk stellarator plasma from the wall or due to pellet ablation. The code solves the system of continuity equations (averaged over the magnetic flux surfaces) for impurity ions of each charge state, coupled due to the ionization, charge-exchange and recombination. The code evaluates impurity behavior in the frame of the stellarator-specific neoclassical transport, which unlike the tokamak configuration is strongly dependent on magnetic topology and the radial electric field. In the case of a test impurity approximation, considered here, the radial electric field is evaluated from the ambipolarity condition in the background plasma and depends on neoclassical transport coefficients for electrons and ions. An analytical description of the neoclassical transport coefficient for the background plasmas (based on numerical results from the DKES code [2] and monoenergetic Monte Carlo simulations) was generalized to impurity ions of arbitrary mass and charge state and used in the code as a neoclassical transport model for impurities. The reduction of Pfirsch-Schlüter convection due to the radial electric field and its impact on impurity dynamics has been included. Calculations were performed for given plasma density and temperature profiles. However, the time variation of the background plasma can also be taken into account by incorporating the experimentally measured profiles into the ongoing calculation.

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2. Impurity Equations, Transport Coefficients and Boundary Conditions

The SIT STRAHL code solves the set of coupled, time dependent, one-dimensional continuity equations for the impurity density n_j^I for each ionization state j of a given impurity species I, averaged over the magnetic surfaces, ψ:

$$\frac{\partial n_j^I}{\partial t} + \frac{1}{\sqrt{g}}\frac{\partial}{\partial x}(\sqrt{g}\Gamma_j^I) = S_j^I \quad ; \quad j = 1, 2, ..., Z_I \qquad (1)$$

Here $g = \det|g_{ik}|$, $g_{ik}(\psi)$ are the metric coefficients, calculated from the equilibrium, the impurity flux Γ_j^I can be written as $\Gamma_j^I = -D_j^I \nabla n_j^I + n_j^I V_j^I$. In general, the radial diffusion coefficient $D_j^I = D_{1,j}^I + D_{an}^I$, and the convective velocity $V_j^I = V_{Ware}^I + V_{an}^I$ consist of a neoclassical and an anomalous term. Since in stellarators the Ware pinch can be neglected, the neoclassical impurity flux can be written as

$$\begin{aligned}\Gamma_j &= -D\nabla n_j + n_j V_j \\ &= -D^I_{1j} n_j \left\{ \frac{n'_j}{n_j} - Z_j \frac{E_r}{T_j} + \left(\frac{D^I_{2j}}{D^I_{1j}} - \frac{3}{2} \right) \frac{T'_j}{T_j} \right\} \\ &= -D^I_{1j} \nabla n_j \\ &\quad + n_j \left\{ D^I_{1j} Z_j \frac{E_r}{T_j} - D^I_{1j} \left(\frac{D^I_{2j}}{D^I_{1j}} - \frac{3}{2} \right) \frac{T'_j}{T_j} \right\} \\ &= \Gamma^{diff}_j + \Gamma^{conv}_j \end{aligned} \tag{2}$$

The first term in equation (2) describes the impurity diffusion flux, whereas the remaining terms constitute the convective flux. Here and further we assume that all impurity ions have the same temperature, $T_I \approx T_i \equiv T$ and the prime denotes the radial derivative. The sign and the value of the neoclassical convective flux (two second terms in (2)) depend on the radial electric field and the thermal force. The functional dependence of the neoclassical transport coefficients $D^I_{n,j}$ for impurity species on plasma parameters is taken the same as that for the background plasma coefficients and the only difference arises in the collisionality due to the mass and charge of the impurity.

For background plasma the radial transport coefficients D^I_n (with $n = 1$, 2 and $I = e$, i), are obtained by energy convolution of the monoenergetic transport coefficients with a normal distribution. For various magnetic field configurations, the databases of these coefficients calculated by the DKES code are fitted, then, with traditional analytic theory, taking into account the axisymmetric contribution. Finally, the functional dependence of these coefficients on the plasma parameters is expressed analytically, whereas the radial dependence for a given magnetic field configuration is calculated by using the least-squares fitting of numerical results [3, 4]. This semi-analytic description makes possible a rapid numerical simulation of the impurity transport. The explicit dependence of the neoclassical transport coefficients on the ambipolar radial electric field is a distinctive feature in the case of non-axisymmetric configurations. In the collisional case this dependence appears, since even modest values of the radial electric field result in a poloidal rotation and suppression of charge separation thus reducing diffusion coefficients to the classical level [5]. Calculations show, that the dependence on electric field is important particularly for high Z impurity ions. The radial electric field can be found from the ambipolarity condition,

$$\Gamma^i(E_r) + \sum \Gamma_z(E_r) \approx \Gamma^e(E_r). \tag{3}$$

The variation of the electric field in the poloidal direction could have a noticeable impact on heavy impurity transport and will be included later. The impurity transport coefficients are strongly dependent on the radial electric field. Even in the case of strong collisional plasma the Pfirsch-Schlüter convection can be reduced due to the additional poloidal rotation, caused by the radial electric field. Beyond a critical collisionality of the background plasma, $\nu^{eff} > \iota V/3R_0\Omega_E$, the poloidal rotation due to the radial electric field is sufficient to suppress the charge separation responsible for Pfirsch-Schlüter diffusion, and the losses are then reduced to the classical level. So, as the collisionality increases, D^I_{PS} drops to its classical value and then becomes independent on the electric field. The decrease in D^I_{PS} value causes the lowering of the electric field. This effect has been taken into account [6].

Introducing the pitch angle cosine $\varsigma = \mathrm{v}_{\|}/\mathrm{v}$, one can write the pitch angle scattering part of the Coulomb collision differential operator for particles of type I as

$$\mathcal{P}^I = \frac{\nu^I}{2} \frac{\partial}{\partial\varsigma} \left(1 - \varsigma^2\right) \frac{\partial}{\partial\varsigma}, \tag{4}$$

where the dimensional factor $\nu^I\big/2$ [s^{-1}] is given by

$$\frac{\nu^I}{2} = \frac{\pi e^4 \Lambda}{\sqrt{2}} \left(\frac{Z_I}{m_I} \right)^2 \sum_\beta n_\beta Z^2_\beta \left(\frac{m_\beta}{T_\beta} \right)^{3/2} P(\upsilon). \tag{5}$$

The summation index β is over all the charged plasma species. In formula (5) and those below we omit the ionization state index j. Λ is the Coulomb logarithm. The dimensionless velocity argument υ is equal to

$$\upsilon = \sqrt{\frac{T_I}{T_\beta} \frac{m_\beta}{m_I}} \sqrt{x}, \text{ where } x = \frac{m_I \mathrm{v}^2}{2T_I} \tag{6}$$

in turn is the dimensionless kinetic energy. The dimensionless special function $P(\upsilon)$ is defined as

$$P(\upsilon) = \frac{\Phi(\upsilon) - G(\upsilon)}{\upsilon^3}, \tag{7}$$

where $\Phi(\upsilon) = \frac{2}{\sqrt{\pi}} \int_0^\upsilon e^{-t^2} dt$ is the error function and

$$G(\upsilon) = \frac{1}{2\upsilon^2} \Phi(\upsilon) - \frac{1}{\sqrt{\pi}\upsilon} e^{-\upsilon^2} \tag{8}$$

is the Chandrasekhar function.

The neoclassical transport coefficients are calculated as mentioned above via the energy integral convolution with the Maxwellian probability density function

$$D^I_n = \frac{2}{\sqrt{\pi}} \int_0^{+\infty} D^I(x) x^{n-1/2} e^{-x} dx \tag{9}$$

using the following expression for the monoenergetic diffusion coefficient analogous to the one discussed in [3]

$$\begin{aligned} D^I = &\left({D^I_{PS}}^{3/2} + \frac{1}{\left(1\big/D^I_b + 1\big/D^I_p\right)^{3/2}} \right)^{2/3} \\ &+ \frac{1}{1\big/D^I_{1/\nu} + 1\big/D^I_{\sqrt{\nu}} + 1\big/D^I_\nu} \end{aligned}$$

For the calculation of the components of this expression one requires radial profiles of the toroidal modulation $\varepsilon(r)$, helical modulation $\varepsilon_h(r)$ and the component $b_{0,0}(r)$ of the magnetic field strength taken as described in [7]. The magnetic surface label r is related to the toroidal magnetic flux as $\psi = B_0 r^2 / 2$. Moreover, the inverse aspect ratio $\varepsilon_t(r) = r/R_0$, the rotational transform angle $\iota(r)$ and the effective helical modulation [3] for $1/\nu$ regime transport calculation $\varepsilon_h^{eff}(r)$ are required. R_0 is the major radius and B_0 is the average B value at $r = 0$.

The explicit formula for the banana partial diffusion coefficient [3] used in (9) is

$$D_b^I = \frac{\sqrt{\varepsilon}}{\varepsilon_t^2} \frac{\mathrm{v_d} R_0 \nu^I}{\Omega \iota^2}, \tag{10}$$

where $\mathrm{v_d} = \frac{c m_I \mathrm{V}^2}{2 Z_I e B_0 R_0}$ and $\Omega = \frac{Z_I e B_0}{c m_I}$. The plateau partial diffusion coefficient is taken in the form

$$D_p^I = \frac{\pi}{16} \left(\frac{\varepsilon}{\varepsilon_t} \right)^2 \frac{\mathrm{v_d v}}{\Omega \iota} \tag{11}$$

and the Pfirsch-Schlüter component is

$$D_{PS}^I = \frac{4}{3} \frac{\mathrm{v_d} R_0 \nu^I}{\Omega} \left(1 + \frac{(\varepsilon / \iota \varepsilon_t)^2}{1 + \left(3 \nu^I \Omega_E \left(R_0 / \iota \mathrm{v} \right)^2 \right)^2} \right) \tag{12}$$

with $\Omega_E = \frac{c E_r}{r B_0}$.

The formulas for the $1/\nu$, $\sqrt{\nu}$ and ν regime diffusion coefficients used in the code are

$$D_{1/\nu}^I = \frac{4}{9\pi} \frac{(2\varepsilon_h^{eff})^{3/2} \mathrm{v_d^2}}{\nu^I}, \tag{13}$$

$$D_{\sqrt{\nu}}^I = \frac{4\sqrt{2}}{9\pi} \left(\frac{\mathrm{v_d} \varepsilon}{\varepsilon_t} \right)^2 \sqrt{\frac{\nu^I}{|\Omega_t|^3}}, \tag{14}$$

$$D_\nu^I = \frac{1}{2} \frac{\nu^I}{\mathcal{F}_b} \left(\frac{\mathrm{v_d} \varepsilon}{\Omega_t \varepsilon_t} \right)^2, \tag{15}$$

where $\mathcal{F}_b = \sqrt{\varepsilon + 2\varepsilon_h} - \sqrt{2\varepsilon_h}$ and

$$\Omega_t = \Omega_E - \frac{\mathrm{v_d}}{\varepsilon_t} \frac{d b_{0,0}}{dr}. \tag{16}$$

The impurity density equations (1) are integrated from the plasma center ($\rho = 0$, $\rho \equiv r/a$) to the edge ($\rho = 1$). The boundary conditions at the edge depend on the thermal velocity of impurity ions, V_T^I, and the recycling coefficient, R_I

$$\Gamma_j^I = 0.25 R_I n_j^I V_T^I \tag{17}$$

The boundary conditions at $r = 0$ are $\Gamma_j^I(0,t) = 0$. The density of neutral atoms entering at the plasma edge, $r = a$ decays inside the plasma as [1],

$$n_0(r) = n_0(a) \frac{a}{r} \exp\left(- \int_r^a \frac{n_e s_0}{\mathrm{v}_0} dr \right), \tag{18}$$

where v_0 is the thermal velocity and s_0 is the ionization rate of the injected impurity atoms. The impurity influx can last during the entire operation time or can be terminated after some short time, simulating the case of pellet injection at any radial position.

The metric coefficients in density equation are calculated from the magnetohydrodynamic Variational Moments Equilibrium Code (VMEC). The equilibrium data which matches the best fit to the electron temperature profile measured by Thomson scattering is selected from the equilibrium database of various beta values and their profiles.

3. Atomic Processes and Atomic Data

We are considering here essentially non-stationary processes distinguished from the coronal equilibrium, such as when ionization and recombination are unbalanced respectively. The source term in equation (2) describes the atomic processes of recombination and ionization between the different charge states:

$$S_j^I = n_e \left\{ s_{j-1} n_{j-1}^I - (s_j + \alpha_j) n_j^I + \alpha_{j+1} n_{j+1}^I \right\}. \tag{19}$$

Here the ionization s_j and recombination α_j rates for impurity ions as well as the emissivity coefficients of the considered impurity ions are taken from the files in ADAS. In case of high Z impurities we will use instead of (19) a moment approach for the description of the impurity population [8]. In the case of a Titanium (Ti) tracer, TiKα emission has been measured by a soft x-ray pulse height analyzer in the energy range of ~4.7 keV, and the decay time of the TiKα emission lines is measured under different plasma conditions. To estimate the emissivity signal, measured in the TESPEL experiment, several lines in the range of 0.239-0.296 nm have been summed up in evaluation. Most of these data are stored according to ADAS conventions. However some lines for the Ti tracer are still missing in the ADAS data , so a stand alone approach has been applied for the calculation of the Ti line emissivity. Apart from emission in the spectral range of soft x-ray diagnostics, the code gives also the following data: bremsstrahlung due to electron scattering by the main ions and the spectral emissivity for one wavelength, charge exchange with thermal neutral hydrogen and the line emission of special lines. Line-of-sight integrals of specific impurity lines, are calculated by a Van-Regemorter-type formula. The radiation of each sort of impurity is determined by the expression $I_z = n_e \sum n_z^j L_z^j$, where L_z^j is The cooling rate, which accounts for bremsstrahlung, linear and recombination radiation.

4. Calculation of Sightline-Integrated SXR Signals

A line-integrated SXR signal $I(t)$ along a certain observation chord can be calculated in the code and compared with experimental data. The chord integral calculation approach is similar to that described in [9]. The measurements are usually made along a particular direction in the LHD experiment. Assuming the existence of nested magnetic surfaces, the integration along the viewing chord gives:

$$I(t) = \frac{\Omega S_a}{4\pi} \int_{\rho_{min}}^{1} g(\rho, t) \{Q^{+}(\rho) - Q^{-}(\rho)\} d\rho, \qquad (20)$$

where $g(\rho$, t) [erg/cm^{3}s] is the local SXR source function, $\Omega S_a/4\pi$ is the diagnostic étendue, and ρ is the effective minor radius defined as a square root of the normalized magnetic flux $(\Psi/\Psi_{LCMS})^{1/2}$. The sight line Λ enters the plasma at $\rho = 1$, crosses the deepest region $\rho = \rho_{\min}$ and exits the plasma at the contour line $\rho = 1$ again. The two corresponding branches of the integral kernel are expressed as the functions $Q^{-}(\rho) = \mathrm{d}\Lambda/\mathrm{d}\rho < 0$ on the interval from $\rho = 1$ to the point $\rho = \rho_{\min}$ and $Q^{+}(\rho) = \mathrm{d}\Lambda/\mathrm{d}\rho > 0$ on the interval from the point $\rho = \rho_{\min}$ to $\rho = 1$. The magnetic surface structure is known from VMEC calculations. This allows one to determine the functions $Q^{-}(\rho)$ and $Q^{+}(\rho)$ in explicit form and to evaluate the integral.

5. Conclusion

The Stellarator Impurity Transport code described here can be used for diagnostic data analysis purposes, particularly as an interpretative tool in TESPEL experiments in LHD. In this paper the first description of the code is presented. The code solves the system of continuity equations (averaged over the magnetic flux surfaces) for impurity ions in each charge stage, coupled due to the ionization and recombination. It calculates the evolution of density and emission in time and space of impurity ions coming from the wall or originating within the plasma due to pellet ablation. Under this condition the transport equations become stiff, which has required a considerable change in the numerical scheme. The radial electric field is evaluated from the ambipolarity condition and depends on neoclassical transport coefficients. An analytical description of the neoclassical transport coefficient for the background plasmas (based on numerical results from the DKES code and monoenergetic Monte Carlo simulations) was generalized to impurity ions of arbitrary mass and charge state and used in the code as a neoclassical transport model for impurities. The reduction of Pfirsch-Schlüter convection due to the radial electric field and its impact on impurity dynamics has been included. Calculations of the electric field and transport coefficients were included within the time dependent iterative loop. Various models of anomalous drift velocities and the diffusion coefficient were also included. The calculation examples are discussed in [10]. Currently the calculations are performed for the given plasma density and temperature profiles. In the future this calculation will be also done in a self consistent manner. Because of its modular structure, the SIT STRAHL code can be easily incorporated into 1-D plasma transport codes like ASTRA or PROCTR.

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