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Modelling of turbulent impurity transport in fusion edge plasmas using measured and calculated ionization cross sections

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ABSTRACT

Turbulent transport of trace impurities in the edge and scrape-off-layer of tokamak fusion plasmas is modelled by three dimensional electromagnetic gyrofluid computations including evolution of plasma profile gradients. The source function of impurity ions is dynamically computed from pre-determined measured and calculated electron impact ionization cross section data. The simulations describe the generation and further passive turbulent $E \times B$ advection of the impurities by intermittent fluctuations and coherent filamentary structures (blobs) across the scrape-off-layer.

1. Introduction

Magnetically confined plasmas for fusion research would ideally be composed of electrons and only the main hydrogen ion species, which usually are either simply protons or deuterium ions for most present experiments, or consist of a deuterium and tritium ion fuel mixture and helium ions as their fusion product in burning plasmas. The electron-hydrogen plasma unavoidably gets into contact with wall materials, both (preferentially) in designated strike areas in the divertor region, and also (strongly undesired) on the first wall surrounding the bulk plasmas.

Plasma–wall interaction processes in tokamak fusion experiments [1–4] can generate various neutral and ionized atoms and molecules, which may penetrate into and profoundly disturb the main plasma, and also can lead to unfavourable co-deposition of materials and composites (e.g. of tritiated hydrocarbons) in other areas of the vessel. Detailed knowledge of atomic and molecular interactions in the edge of tokamaks and of the transport of impurities is therefore of considerable interest for understanding and modelling of fusion plasmas.

The major cross-field transport mechanism of particles and energy in magnetized fusion plasmas is turbulent fluid-like convection by wave-like fluctuating electric fields $\mathbf{E}(\mathbf{x}, t)$ acting on the plasma through the $\mathbf{E} \times \mathbf{B}$ drift velocity in a background magnetic field [5–12]. The relevant drift wave turbulence micro-scales in tokamak edge plasmas are in the order of sub-mm spatial vortex structures in the MHz frequency range, but are further closely coupled to macro-scale zonal flow structures [13] and meso-scale instabilities like edge-localized modes [14] and magnetic islands.

Once impurities, which are born at the outer edge of the plasma region, are ionized by electron impact or other processes, they are also subjected to the turbulent $\mathbf{E} \times \mathbf{B}$ advection and may as a consequence be efficiently transported further across the field and radially inwards.

In this work we study the passive transport of fusion relevant trace impurity ions by means of multi-species edge turbulence computations, which include dynamical electron-impact ionization in fluctuating filamentary plasma structures as a source for impurity ions in the scrape-off-layer region of a tokamak.

2. Gyrofluid turbulence model including impurities

The present flux-driven 3-d multi-species isothermal gyrofluid turbulence model includes evolution of density profile gradients

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and dynamically couples the edge pedestal region with a limiter bounded scrape-off layer (SOL).

The model is based on the local gyrofluid electromagnetic model "GEM3" by Scott [10,15] and the SOL (limiter) model by Ribeiro and Scott [16,17], applying globally consistent geometry [18] with a shifted metric treatment of the coordinates [19]. An Arakawa–Karniadakis numerical scheme [21,20,22] is used for the computations. The present multi-species code ("TOEFL") has been cross-verified in the local cold-ion limit with the tokamak edge turbulence standard benchmark case of Falchetto et al. [23], and with the results of finite Larmor radius (warm ion) SOL blob simulations of Madsen [24].

In the local (delta-f) isothermal multi-species gyrofluid model [15] the normalised equations for the fluctuating gyrocenter densities n_s, including evolution of the profile gradients, are

$$\partial_t n_s + [\phi_s, n_s] = \nabla_{||} v_{s||} + \kappa(\phi_s + \tau_s n_s) + S_{ns} \tag{1}$$

where the index s denotes the species with $s \in (e, i)$ for the main plasma components (electrons and here main deuterium ions) plus one or more additional ion species ($s \equiv z$). The parallel velocities $v_{s||}$ and the vector potential $A_{||}$ evolve according to

$$\hat{\beta} \quad \partial_t A_{||} + \hat{\mu}_s(\partial_t v_{s||} + [\phi_s, v_{s||}]) = -\nabla_{||}(\phi_s + \tau_s n_s) - \hat{C} J_{||} + 2\hat{\mu}_s \tau_s \kappa(v_{s||}). \tag{2}$$

The gyrocenter densities are coupled to the electrostatic potential ϕ by the local gyrofluid polarisation equation

$$\sum_s a_s[\Gamma_{1s} n_s + \left(\frac{1}{\tau_s}\right)(\Gamma_{0s} - 1)\phi] = 0 \tag{3}$$

and the velocities and current to the parallel component of the fluctuating vector potential by Ampere's equation

$$\nabla_\perp^2 A_{||} = J_{||} = \sum_s a_s v_{s||}. \tag{4}$$

where the gyro-averaging operators in Padé approximation are defined by $\Gamma_{0s} = (1 + b_s)^{-1}$ and $\Gamma_{1s} = (1 + (1/2) b_s)^{-1}$ with $b_s = \tau_s \mu_s \nabla_\perp^2$. Spatial scales are normalised by the drift scale $\rho_0 = \sqrt{T_e m_i}/(eB)$, where T_e is a reference electron temperature, m_i is the ion mass, and B is the magnetic field strength. Time scales are normalized by $c_s/L_\perp$, where $c_s = \sqrt{T_e/m_i}$, and $L_\perp$ is the generalized profile gradient scale length.

The parameter $a_s = Z_s n_{s0}/n_{e0}$ describes the ratio of species normalising background densities n_{s0} to the reference density n_{e0} (here usually taken at mid-pedestal value) for species with charge state Z_s. The mass ratio is given by $\mu_s = m_s/(Z_s m_i)$, and the (constant) temperature ratio by $\tau_s = T_s/(Z_s T_e)$.

For electrons $a_e = \tau_e = -1$, $\mu_e \approx 0$, and finite Larmor radius (FLR) effects are neglected so that $b_e \equiv 0$. The gyro-screened potentials acting on the ions are given by $\phi_s = \Gamma_s \phi$.

Defining $\hat{\epsilon} = (qR/L_\perp)^2$ as the squared ratio between parallel length scale $L_{||} = qR$ (for given safety factor q and torus radius R) and perpendicular scale $L_\perp$, the main parameters are $\hat{\mu}_s = \mu_s \hat{\epsilon}$, $\hat{\beta} = (n_{e0} T_e / B_0^2)\hat{\epsilon}$, and $\hat{C} = 0.51(m_e \nu_e L_\perp / c_{s0})\hat{\epsilon}$. Quasi-neutrality implies $a_i = 1 - a_z$. If gradients were to be fixed with $g_s \equiv \partial_x n_{s0}$ (alternatively to the present fixed source flux computations) then also $g_i = (1 - a_z g_z)/(1 - a_z)$ needs to be satisfied. For flux-driven computations the sources have to obey quasi-neutrality and ensure vorticity free injection.

The nonlinear advection terms in Eqs. (1) and (2) are expressed through Poisson brackets using the notation $[a, b] = (\partial_x a)(\partial_y b) - (\partial_y a)(\partial_x b)$. Normal and geodesic components of the magnetic curvature enter the compressional effect on vortices due to magnetic field inhomogeneity by $\kappa = \kappa_y \partial_y + \kappa_x \partial_x$ where the curvature components in toroidal geometry are a function of the poloidal angle θ mapped onto the parallel coordinate z. For a circular torus $\kappa_y \equiv \kappa_0 \cos(\theta)$ and $\kappa_x \equiv \kappa_0 \sin(\theta)$ when $\theta = 0$ is defined at the outboard midplane.

The term S_{ns} on the right hand side of the density Eq. (1) describes particle sources and sinks. For electrons a constant core flux driven density source is applied, which is localized around the inside (left) radial computational boundary at r_0 following a narrow Gaussian profile $S_{ne} \sim s_e(r - r_0)$. The corresponding vorticity free source function for warm ions is FLR corrected by $s_i = s_e - (1/2)\tau_i \nabla^2 s_e$.

The source (and sink) term S_{nz} for impurity ions is here dynamically set by ionization processes of a neutral impurity cloud, as described in the next section. For quasi-neutral non-trace impurities the electron density has to include a corresponding ionization source term. In the following we however will consider only trace impurities ($a_z \ll 1$) which do not enter into polarization or react back on the convecting main plasma turbulence. For the moment we also neglect recombination processes. Vorticity free Dirichlet conditions are applied for all species on the outer (right) computational boundary. In Ref. [34] the necessity of using consistent energy sources has been stressed for cases when temperature fluctuations are dynamically evolved in addition to density fluctuations. Here we presently focus on an isothermal model, so we do not encounter difficulties due to spurious thermal energy sources.

The present "local" model assumes small density fluctuations on a constant background to approximate $\ln n_s \approx n_s/n_{s0} \equiv n_s$, and can not capture spatially localised non-trace impurity effects, like back-reaction of impurity aggregation on the vortex or zonal flow fine structure. A full-f density ("global") model would have to account for nonlinear (nonlocal) polarisation via

$$\sum_s [q_s \Gamma_{1s} n_s + \nabla \cdot (n_s \mu_s \nabla)\phi] = 0. \tag{5}$$

For passively advected trace impurities ($a_z \ll 1$) we can however consistenly solve the global gyrocenter density equation

$$\partial_t n_z + [\phi_z, n_z] = \nabla_{||}(n_z v_{z||}) + n_z \kappa(\phi_z) + \tau_z \kappa(n_z) + S_{nz} \tag{6}$$

and obtain the actual trace impurity particle density including nonlinear polarisation by $N_z = \Gamma_{1z} n_z + (\mu_z/q_z) \nabla \cdot (n_z \nabla)\phi$. In the present simulations the local Eqs. (1)–(4) are used for the main plasma species, and the global model Eq. (6) to evolve the trace impurities.

3. Dynamical source of impurity ions

For simulations of trace impurity ion transport in a turbulent edge plasma, usually either a cloud of impurity ions is initialized at a single point in time with a given spatial distribution on a turbulent background plasma, or a constant source of impurities is applied at each time step. The evolution of impurities by nonlinear $E \times B$ advection is then further followed to study its migration and inward transport, like in fluid computations of edge turbulence of e.g. Refs. [25–28].

Here we extend such previous approaches by applying a edge-SOL coupled model with global profile gradient evolution, and in addition by including a time dependent impurity ion source dynamically computed from ionization processes depending on the local fluctuating electron density and temperature. A localized and (on the turbulent time scale) stationary neutral impurity cloud acts as the background source.

In the following we exemplarily consider electron impact ionization as the main ionization channel. The temperature dependend reaction rates $R(T) = \langle \sigma v \rangle$ of the ionization processes are (pre-)computed from fit functions of measured or calculated ionization cross sections $\sigma(E)$.

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