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A coarse-grained kinetic equation for neutral particles in turbulent fusion plasmas

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A coarse-grained kinetic equation for neutral particles (atoms, molecules) in magnetized fusion plasmas, valid on time scales large compared to the turbulence correlation time, is presented. This equation includes the effects of plasma density fluctuations, described by gamma statistics, on the transport of neutral particles. These effects have so far been neglected in plasma edge modeling, in spite of the fact that the amplitude of fluctuations can be of order unity. Density fluctuations are shown to have a marked effect on the screening of neutrals and on the spatial localization of the ionization source, in particular at high density. The coarse-grained equations obtained in this work are readily implemented in edge code suites currently used for fusion plasma analysis and future divertor design (ITER, DEMO).
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Predicting the plasma flow (heat and particles) as well as density and temperature profiles near strongly plasma exposed surfaces is of essential importance to quantitative understanding of current magnetic fusion experiments, as well as for the ITER design process.[1] In the latter case, predictions currently rely on the 2D SOLPS transport code, which is a plasma fluid code (B2) coupled to a Monte Carlo solver for the neutral particles (EIRENE).[2] A specific feature of edge plasmas of fusion devices is to exhibit intermittent turbulence,[3] which governs perpendicular transport of particles and heat. The equations solved in current edge transport code suites are time averages of those describing turbulence, i.e., coarse-grained equations. For example, the averaged continuity equation reads

$$\partial_t\langle n_e\rangle + \mathbf{\nabla}\cdot(\langle n_e\rangle\langle\mathbf{V}\rangle + \langle\tilde{n}_e\tilde{\mathbf{V}}\rangle) = \langle S_p\rangle, \tag{1}$$

where $\mathbf{V}$ is the fluid velocity, $\tilde{n}_e$ and $\tilde{\mathbf{V}}$ are the fluctuating parts of the density and the velocity fields, and the brackets $\langle\cdot\rangle$ stand for the time average. This average introduces a turbulent contribution to the particle flux $\mathbf{\Gamma}_{\rm turb} = \langle\tilde{n}_e\tilde{\mathbf{V}}\rangle$, often modeled in transport approximations by a sum of a diffusive and a convective flux, the latter describing coherent structures traveling ballistically through the scrape-off layer (SOL).[3] Recent efforts have been made to improve this model, by including the dynamics of these structures ("blobs") in a transport code, properly accounting for their 3D filamentary nature.[4] In this work, we use plasma equations averaged over fluctuations, including filaments, and obtain a consistent formulation for neutrals at this level of coarse graining. In other words, we focus on the averaged particle source $\langle S_p\rangle$, defined by $\langle S_p\rangle = \int d\mathbf{v}\langle\nu f(\mathbf{v},\mathbf{r},t)\rangle$, where f is the neutral particle distribution function, $\mathbf{v}$ their velocity, and ν their absorption (e.g., ionization or molecular dissociative ionization) rate. The equation governing the time average of $f(\mathbf{r},\mathrm{v},\mathbf{\Omega},t)$ is

$$(\partial_t + \mathbf{\Omega}\mathrm{v}\cdot\mathbf{\nabla})\langle f\rangle = -\langle\nu f\rangle + \langle Q[f]\rangle, \tag{2}$$

where $\mathbf{\Omega} = \mathbf{v}/\mathrm{v}$, and $Q[f]$ is an integral term describing scattering processes (charge exchange, elastic collisions). Neglecting fluctuations on neutral particle transport, i.e., using $\nu(\langle n_e\rangle)\langle f\rangle$ (resp. $Q[\langle f\rangle]$) instead of $\langle\nu f\rangle$ (resp. $\langle Q[f]\rangle$) in Eq. (2), is especially questionable in the far SOL, where the amplitude of fluctuations can be of order unity (up to $R\sim 95\%$ in Ref. 5), as first pointed out by Prinja[6] (the situation is similar for parallel transport coefficients[7,8]). The statistical properties of fluctuations in SOL plasmas show remarkable similarities between various devices.[9] Recent studies have made use of the observed parabolic scaling relation between the skewness $S = \langle\tilde{n}_e^3\rangle/\sigma^3$ and the kurtosis $K = \langle\tilde{n}_e^4\rangle/\sigma^4 - 3$ of density fluctuations (σ^2 being their variance), namely, $K = 1.502\,S^2 - 0.226$, to show that all the experimental PDFs (probability density functions) are closely related to the gamma PDF.[5]

In previous works,[10,11] we have used the multivariate generalization of the gamma distribution proposed by Krishnamoorthy and Parthasarathy[12] to describe density fluctuations on a discrete spatial grid (electron temperature fluctuations are neglected, their amplitude being typically markedly smaller than density fluctuations). Its moment generating function is given by $Z(\mathbf{u}) = \langle\exp-\mathbf{u}\cdot n_e\rangle = |\mathbf{I}+2\mathbf{GU}|^{\beta}$, where $\boldsymbol{I}$ is the identity matrix, $U_{ij} = u_i\delta_{ij}$ and $\beta = M/2$, M being the number of degrees of freedom. The matrix $\boldsymbol{G}$ is related to the correlation matrix $\boldsymbol{C}$ of density fluctuations by $G_{ij}^2 = C_{ij}/(4\beta)$. Therefore, the main input to the model is the spatial two point correlation of the density field ρ, which can be chosen to match experimental or numerical results (e.g., Ref. 3). Time correlations did not enter our model, because fluctuations were assumed to be frozen in time during the neutral particles

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lifespan, of the order of $\tau_i = \langle\nu\rangle^{-1}$ (adiabatic approximation). Our approach, based on solving Eq. (2) for several thousand realizations of the density field, was computationally too heavy to be applied to coupled neutrals/plasma calculations, especially if the adiabatic approximation were to be relaxed (the size of the correlation matrix would become prohibitive). In this letter, we show that for fluctuations following a multivariate gamma distribution (MGD), an exact coarse-grained kinetic equation can be obtained for $\langle f\rangle$. This result turns our model into a practical tool, and at the same time allows relaxing the adiabatic approximation. In addition, in this formulation β is no longer constrained to be half integer, provided the correlation function is exponential,[13] so that our model is now able to cover the whole range of fluctuation amplitudes measured in Ref. 5 (for the MGD, $R^2 = \langle(n_e - \langle n_e\rangle)^2\rangle/\langle n_e\rangle^2 = 1/\beta$).

We focus on molecules and impurity atoms, which have typically much shorter mean free paths than fuel atoms. Indeed, the effects of fluctuations on the transport of neutral particles increase sharply with the ratio of the turbulence correlation length to the average mean free path.[10] In other words, if the mean free path is large compared to the size of turbulent structures, fluctuations average out over the neutral particle trajectories. As a result, we consider only the scattering free case (that is $Q[f]=0$ in Eq. (2)), since resonant charge exchange is weak for impurities, and elastic scattering of molecules is important only in very cold and dense regions close from the neutralizer plates where the amplitude of fluctuations is thought to be small.[7] We focus instead on the main chamber SOL, which has become an important investigation topic. In fact, the clearance between the plasma and the wall is not large enough so as to ensure that plasma wall interactions are negligible, because of long range blob transport.[14] The solution of Eq. (2), after relaxation of the initial condition, is given by

$$\langle f(\mathbf{r},t)\rangle = \left\langle \Gamma\left(\mathbf{r}_w, t - \frac{|\mathbf{r}-\mathbf{r}_w|}{\mathrm{v}}\right) \times \exp\left(-\frac{1}{\mathrm{v}}\int_0^{|\mathbf{r}-\mathbf{r}_w|} ds\,\nu(\mathbf{r}-s\boldsymbol{\Omega}, t - s/\mathrm{v})\right)\right\rangle, \tag{3}$$

where $\mathbf{r}_w$ locates the point where the neutral particle left the wall, and Γ is the particle in-flux from the wall. In general, one expects a linear relationship between the latter and the instantaneous plasma out-flux Γ_p, namely,

$$\Gamma(\mathbf{r}_w, t) = \int_{-\infty}^{t} h(t-t')\Gamma_p(\mathbf{r}_w, t'), \tag{4}$$

where $h(t-t')$ is the response function of the wall. In the case of the desorption of molecules, for a saturated wall (the typical situation for steady state discharges), the response of the wall is expected to be slow compared to turbulence. In this case (slow wall response), $\Gamma \simeq \langle\Gamma_p\rangle$ is constant (i.e., non-stochastic). Assuming ν to be linear in n_e and using the properties of the moment generating function(-al), we get the following result for the term $\langle\nu f\rangle$ in Eq. (2):

$$\langle\nu(\mathbf{r},t)f\rangle = -\frac{\Gamma}{\mathrm{v}\langle\nu\rangle}\frac{\delta Z[u]}{\delta u(|\mathbf{r}-\mathbf{r}_w|)}\bigg|_{u=u_c} = \varpi^S(|\mathbf{r}-\mathbf{r}_w|)\langle f\rangle, \tag{5}$$

where $u_c = -\langle\nu\rangle/(\mathrm{v}\langle n_e\rangle)$. The superscript ϖ^S stands for "slow," and ϖ^S is a coarse-grained ionization rate, given by

$$\varpi^S(|\mathbf{r}-\mathbf{r}_w|) = \lim_{N\to+\infty}\frac{\mathrm{v}N}{R^2|\mathbf{r}-\mathbf{r}_w|}[1-(A^{-1})_{NN}], \tag{6}$$

with $A_{ij} = \delta_{ij} + \langle\nu\rangle R^2|\mathbf{r}-\mathbf{r}_w|G_{ij}/(N\mathrm{v})$, and

$$G_{ij} = \frac{\langle\nu\rangle R^2}{2}[\rho(|i-j|s\boldsymbol{\Omega}/N, |i-j|s/(N\mathrm{v}))]^{1/2}. \tag{7}$$

N is the number of points used to discretize the integral in Eq. (3), and $s = |\mathbf{r}-\mathbf{r}_w|$. In other words, we obtain a closed coarse-grained kinetic equation for $\langle f\rangle$,

$$(\partial_t + \boldsymbol{\Omega}\mathrm{v}\cdot\boldsymbol{\nabla})\langle f\rangle = -\varpi^S(\mathbf{r})\langle f\rangle. \tag{8}$$

This equation is of the Boltzmann type, and can thus be solved with the same tools as Eq. (2). A similar result is obtained in the case where the wall responds instantaneously to the impinging plasma flux, namely, $h(t-t') = \delta(t-t')$ ("fast response," denoted by the superscript ^{F}), provided $\Gamma(\mathbf{r}_w,t) \propto n_e(\mathbf{r}_w,t)$. Differentiating $Z[u]$ twice (in order to get $\langle n_e(\mathbf{r}_w, t-|\mathbf{r}-\mathbf{r}_w|/\mathrm{v})n_e(\mathbf{r},t)f(\mathbf{r},t)\rangle$) leads to

$$\varpi^F = \varpi^S + \frac{\mathrm{v}}{|\mathbf{r}-\mathbf{r}_w|}\lim_{N\to+\infty}N(A^{-1})_{NN}\frac{(A^{-1})_{NN}-(B^{-1})_{pp}}{1-(A^{-1})_{NN}}, \tag{9}$$

where $p=N-1$ and B is a $p\times p$ matrix such that $B_{ij} = A_{ij}$ for $i,j\le p$. In this model, the flux of neutrals originating from the plasma surface increases locally when the turbulent flux increases, as it is the case for back-scattering or sputtering processes, given the distances and velocities at play. Therefore, in both "slow" and "fast" response cases, properly accounting for density fluctuations amounts to replace ν by a coarse-grained rate in the Boltzmann equation. This provides a simple and computationally efficient way to retain the effects of density fluctuations in edge code suites. The coarse-grained particle source $\langle S_p\rangle$ is obtained by integrating $\varpi^{S,F}\langle f\rangle$ over velocities. We now examine the behavior of $\varpi^{S,F}$ with $|\mathbf{r}-\mathbf{r}_w|$, for the correlation function given by

$$\rho(|\mathbf{r}-\mathbf{r}'|, |t-t'|) = \exp-\frac{|\mathbf{r}-\mathbf{r}'|}{\lambda}\exp-\frac{|t-t'|}{\tau}, \tag{10}$$

where λ and τ are, respectively, the turbulence correlation length and time. Typically, one has $\lambda\sim 1$ cm and $\tau\sim 10\,\mu$s.[3] Statistical homogeneity and separability (in time and space) of ρ are assumed here only to make the discussion of the physics clearer. It should be noted that ballistic propagation of coherent structures can be accounted for using non-separable

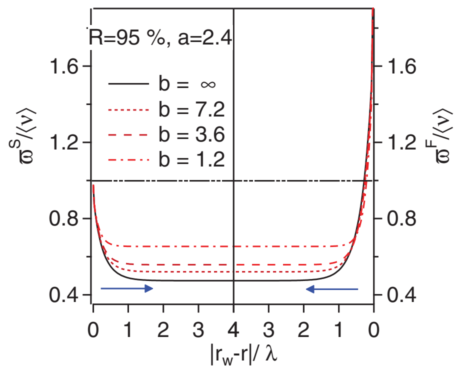

FIG. 1. Plot of the coarse-grained rate in the slow (left) and fast response cases (right, x scale reversed for clarity), normalized to the average rate, as a function of the distance to the wall expressed in units of the turbulence correlation length λ, for $R=95\%$, $a=2.4$ and different values of the ratio $b=\tau/\tau_i$, from $b=1.2$ to $b=\infty$. The latter case corresponds to the adiabatic limit. Both ϖ^S and ϖ^F tend towards the same asymptotic value ϖ_∞ for the same value of R, a and b. The blue arrow represents the direction of the neutral particle velocity.

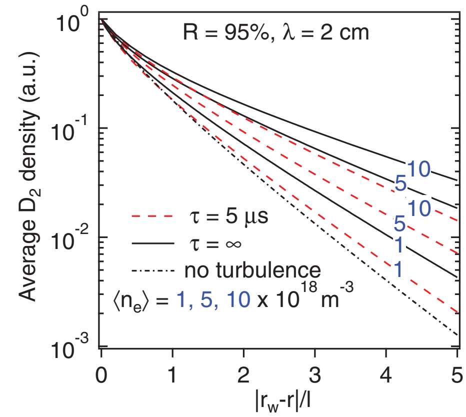

FIG. 2. Average molecular density calculated with EIRENE in a 2D slab geometry, plotted in semi log scale as a function of $|\mathbf{r}-\mathbf{r}_w|/l$ for $\lambda=2\,\mathrm{cm}$, and $\langle n_e\rangle = 1$, 5 and $10\times10^{18}\,\mathrm{m}^{-3}$, $T_e=50\,\mathrm{eV}$ and for $\tau=5\,\mu\mathrm{s}$ (dashed lines), ∞ (solid lines). The dashed dotted line is the turbulent free case. The effect of fluctuations increases both with density and correlation time.

correlation functions. With Eq. (10), we have $G_{ij}=\frac{1}{2}\langle\nu\rangle R^2 \exp[-|i-j|s/(2\lambda_e N)]$, where $\lambda_e=\lambda \mathrm{v}\tau/(\lambda+\mathrm{v}\tau)$, such that $\lambda_e\le\lambda$. This result is related to the finite lifetime of the turbulent structures, possibly shorter than the time needed for the neutral to flight through these structures. We thus introduce the ratio $b=\tau/\tau_i$, which measures whether a neutral particle sees the turbulent field evolve in time before it is ionized (the adiabatic limit corresponds to $b\gg1$). The ratios $\varpi^{S,F}/\langle\nu\rangle$ are plotted on Fig. 1 as a function of $|\mathbf{r}-\mathbf{r}_w|/\lambda$, for $R\simeq95\%$, $a=\lambda/l=1.7$ (l is the mean free path calculated for the average density), and $b=1.2, 3.6, 7.2, \infty$.

The value of N is chosen so that $|\mathbf{r}-\mathbf{r}_w|/N\le\lambda_e/10$. Both ϖ^S and ϖ^F decay monotonously towards an asymptotic value ϖ_∞, reached in practice after a few λ_e. As a result, in these conditions the dissociation rate of molecules is halved after a few cm from the wall when fluctuations are retained. The fact that $\varpi^F=(1+R^2)\langle\nu\rangle>\langle\nu\rangle$ close to the wall is related to our assumption that $\Gamma_p(\mathbf{r}_w,t)\propto n_e(\mathbf{r}_w,t)$. In fact, neutrals enter the plasma preferentially in over-dense regions where they are more likely to be ionized than in a spatially homogenous plasma of density $\langle n_e\rangle$.

The implementation of our model in the EIRENE Monte Carlo code[2] is straightforward. The code follows neutral particles trajectories in arbitrary geometry, and the plasma parameters needed to calculate the rates are provided by a plasma fluid code on a mesh. According to Eq. (8), taking fluctuations into account entails calculating the coarse-grained absorption rate every time a neutral particle enters a new cell, since the latter is a function of the distance $|\mathbf{r}-\mathbf{r}_w|$ between the current neutral particle position and the wall. This coarse-grained rate is then also used in the estimator for the particle source. The implementation has been validated against the results obtained by solving the Boltzmann equation for several thousands of realizations, for β half integer and $\tau=\infty$. Calculations in a 2D slab geometry for the average molecule density profile (resp. for the beryllium ion particle source) are presented in Fig. 2 (resp. Fig. 3). The radial distances are in units of the mean free path l. 3D features of SOL turbulence (e.g., filaments aligned with magnetic field lines) are not explored by neutrals having short mean free paths, so that a 2D description where the density field is constant in the z direction is sufficient in our approach. Neutral particles enter the plasma according to a cosine distribution, and are mono-energetic. For molecules we take $E_0=0.08\,\mathrm{eV}$, corresponding to a wall temperature of around 500 K, while for beryllium the maximum of the Thompson distribution is considered, namely, $E_0=1.7\,\mathrm{eV}$. The turbulence correlation length is $\lambda=2\,\mathrm{cm}$ ($a=2.4$ for D_2 molecules), and the correlation time is chosen so that $\tau=5\,\mu\mathrm{s}$ and $\tau=\infty$ (adiabatic limit). The average molecular density profiles, plotted for $\langle n_e\rangle = 1,\ 5,\ 10\times10^{18}\,\mathrm{m}^{-3}$ and $T_e=50\,\mathrm{eV}$, show a large reduction of the SOL screening efficiency at high density when fluctuations are retained. Non-adiabatic effects are important for $\tau=5\,\mu\mathrm{s}$ (i.e., $b=1.2$), a value which is, however, at the lower end of the measured values for τ. The Be^+ particle source is plotted on Fig. 3, for $\langle n_e\rangle=10^{18}\,\mathrm{m}^{-3}$. Fluctuations increase the value of the source by a factor $1+R^2$ in the vicinity of the wall. At a distance of several λ from the wall, the behavior of $\langle S_p\rangle$ is similar to that observed in Fig. 2 for the average density, because $\varpi_\infty\simeq\langle\nu\rangle/2$ (see Fig. 1), and $\langle n_{\mathrm{be}}\rangle$ is much larger that the

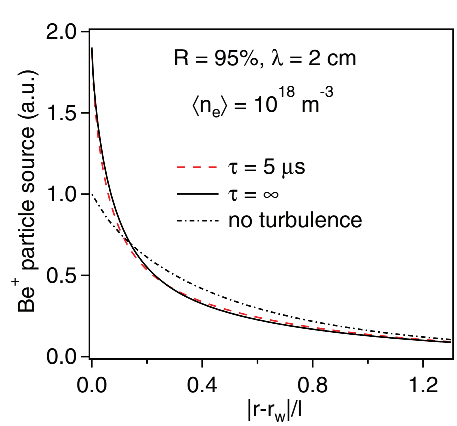

FIG. 3. Average Be^+ particle source calculated with EIRENE assuming fast wall response in a 2D slab geometry, with the same parameters as in Fig. 2. Fluctuations increase the particle source by a factor $(1+R^2)$ close from the wall. The adiabatic approximation is well justified in this case, since the results for τ ranging from $5\,\mu$s to infinity are nearly superimposed.

density calculated neglecting fluctuations. These marked differences in the radial profile of the particle source could have important consequences on the main plasma contamination, especially in the presence of flow reversal.

In summary, coarse-grained kinetic equations are obtained for neutral particles in magnetic fusion plasmas after averaging over SOL turbulence, assuming the latter is described by a multivariate gamma distribution. These equations are straightforward to implement in numerical edge code suites. Fluctuations are found to have large effects on the transport of neutral particles, provided the plasma is dense enough. Our results could also be applied to neutral particle transport during Edge Localized Modes (ELMs).

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