Transport of neutrals in turbulent scrape-off layer plasmas

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Abstract. The effect of turbulence on the transport of neutral species (atom, molecules) in plasmas is investigated. A stochastic model relying on a multivariate Gamma distribution is introduced to describe turbulent fluctuations, and implemented in EIRENE. The effect of fluctuations on the neutral density, ionization source and radial profiles are investigated. Two important control parameters are identified, namely the ratio of the neutral mean free path to the size of turbulent structures, and the ratio of recycling time scales to the turbulent times. First calculations with ITER scrape-off layer parameters are presented, and two distinct regimes are identified depending on the far SOL electron temperature.

1. Introduction

Edge plasmas of fusion devices are known to exhibit strong intermittent turbulence, which governs perpendicular transport of particles and heat. Up to now, the role of these fluctuations on the transport of neutrals in edge plasmas has not been addressed quantitatively. It could play a major role in the far scrape-off layer (SOL), a region which was poorly described in edge codes up to very recently [1], and where fluctuations are large. In addition, the latter might affect the penetration depth of neutral particles into the edge transport barrier, and the resulting source terms there. This problem is of interest both for spectroscopic diagnostic purposes and for edge modelling. In fact, when coupling plasma fluid codes to neutral transport codes (e.g. the current ITER edge transport code B2-EIRENE), the effect of turbulence on neutral particle transport is neglected in the sense that neutrals evolve on an average plasma background. This would remain the case even if in the future the cross-field plasma fluxes would be obtained from a direct coupling of turbulence simulations into the plasma fluid solver of current edge transport code suites. We show in sec. 2 that consistent accounting for turbulence in neutral particle transport amounts to introduce terms of the same nature as the turbulent fluxes in the plasma equations. Obtaining explicit expressions for these terms requires solving the turbulence and neutral transport problems in a consistent way, which could be done by coupling EIRENE to a turbulence code. Here, in a preparatory step to guide this quite demanding extension we try to gain understanding on how neutrals behave in turbulent plasmas [2]. To this end, we treat neutrals as passive species, in a simplified 2D slab geometry for the SOL, in which plasma parameters are assumed to be constant in the direction of the magnetic field (flute approximation). Turbulence is described by a stochastic model introduced in Sec. 3 to 5, which is flexible enough to investigate the physics of the problem, but the parameters of which can also be fitted to experiments. A tentative application of our model to the ITER SOL is presented in Sec. 6.

2. Stochastic Boltzmann equation

Neutral particles in fusion plasmas are best described in terms of a Boltzmann equation for the particle distribution function f [3],

$$\left(\frac{\partial}{\partial t} + \mathrm{v}\Omega\cdot\nabla\right) f(\mathbf{r},\mathrm{v},\Omega,t) = \left(\frac{\partial f}{\partial t}\right)_c + s(\mathbf{r},\mathrm{v},\Omega,t), \tag{1}$$

where **r** is the position vector, v the modulus of the velocity, and **Ω** the unit vector such that **v**=v**Ω**. The first term on the r.h.s. is the collision operator, which is given by

$$\left(\frac{\partial f}{\partial t}\right)_c = -\nu_{io}\left(N_e(\mathbf{r},t),T_e(\mathbf{r},t)\right)\ f(\mathbf{r},\mathrm{v},\Omega,t), \tag{2}$$

where ν_{io} is the ionization rate, provided scattering (*e.g.*, charge exchange) is neglected. The second term, s(**r**,v,Ω,t) is a source term, which in our case is located at the wall. For simplicity, we will assume in the following that the time derivative in Eq. (1) is negligible, *i.e.* that the response of the neutral particle distribution function to changes in plasma density or temperature is instantaneous. This approximation is valid provided the typical relaxation time ν_{io}^{-1} is short compared to the time scales over which the plasma field evolve (~ μs for drift wave turbulence), a condition that is not always fulfilled in our applications. However, this adiabatic assumption is very useful to understand the physics of the problem. If Eq. (1) is now time-averaged, over a duration long compared to the turbulent times but short compared to the macroscopic time scales of the discharge, we obtain

$$\mathrm{v}\Omega\cdot\nabla\langle f\rangle = \langle \nu_{io} f\rangle + \langle s\rangle, \tag{3}$$

so that a statistical closure is required to express $<\nu_{io}\ f>$ in terms of $<f>$. As a result, the average ionization source $<S_p>=<\nu_{io}N_0>$, where $N_0 = \int dv f$ is the neutral particle density, has an extra term of the form $<\delta\nu_{io}\ \delta N_0>$ (δ stands for fluctuations around the mean), similar to turbulent fluxes. Therefore, for consistency, ionization sources in edge plasma fluid codes should account for these contributions, whenever anomalous transport coefficients are introduced in the transverse direction. Moreover, the average density $<N_0>$ at the separatrix is related to the neutral influx into the confined plasma, so that $<N_0>$ allows to estimate the SOL screening efficiency.

3. Multivariate Gamma model for plasma turbulence in the SOL

The density field is discretized on a 2D $n \times n$ spatial grid, in slab geometry (in the following, we set $N=n^2$). Its statistics is assumed to follow a multivariate Gamma distribution [4], a choice which has three major advantages. First, the one point marginal is a Gamma distribution, in accordance with turbulence measurements [5]. Next, analytical results can be obtained for various quantities, including the turbulent ionization source, provided scattering is neglected (*e.g.*, charge exchange for atoms). This approximation is valid for molecules and neutral impurities, except in high density and low temperature plasmas (typically close to divertor plates), when elastic scattering starts to play a role. Finally, random sampling from the multivariate Gamma distribution with m degrees of freedom and a given $N \times N$ correlation matrix **C** (such that $C_{ij}=<<N_e(\mathbf{r}_i)N_e(\mathbf{r}_j)>>$ in cumulant notation), amounts to sample from a multivariate Gaussian distribution P(**X**) such that $<X_i>=0$ and

$$\langle X_i X_j\rangle = G_{ij} = \pm\sqrt{\frac{C_{ij}}{2m}}, \tag{4}$$

so that it lends itself to a convenient Monte Carlo treatment. In practice, the Gaussian correlation matrix is symmetric positive-definite and can be Cholesky factorized as $\mathbf{G}=\mathbf{L}\mathbf{L}^T$, where the superscript ^{T} denotes matrix transpose. m vectors $\mathbf{Y}_j = (Y_{1j},\ldots Y_{Nj})^T$ of N independent Gaussian numbers Y_{ij} are first sampled, then the $\mathbf{X}_j=\mathbf{L}\mathbf{Y}_j$ are m sets of N Gaussian random numbers with correlation matrix **G**, and the density field obtained from

$$\left(N_e\right)_i = \sum_{j=1}^{m} X_{ij}^{\ 2} \tag{5}$$

has multivariate Gamma statistics with m degrees of freedom. In this model, the fluctuation rate, defined by $R(\mathbf{r})=\sigma(\mathbf{r})/\langle N_e(\mathbf{r})\rangle$, where $\sigma^2(\mathbf{r})$ is the density variance at point **r**, is constant in space, and its value is given by $R=\sqrt{2/m}$. The model can be extended to space dependent fluctuation rates upon replacing m by m_i in Eq. (5) [6], but care has to be taken to ensure that both **C** and **G** are positive-definite. Here, we impose the following autocorrelation function

$$\rho\left(\left|\mathbf{r}-\mathbf{r}'\right|\right) = \frac{C(\mathbf{r},\mathbf{r}')}{\sigma(\mathbf{r})\sigma(\mathbf{r}')} = \exp -\frac{\left|\mathbf{r}-\mathbf{r}'\right|}{\lambda}, \tag{6}$$

where λ is the integral scale or correlation length, which determines the typical size of the turbulent structures. Two density maps calculated for two different values of λ, namely $\lambda=0.025L$ and $\lambda=0.15L$ where L is the size of the simulation domain, and assuming spatially homogeneous statistics, are shown on FIG. 1a) and 1b). The size of the structures clearly

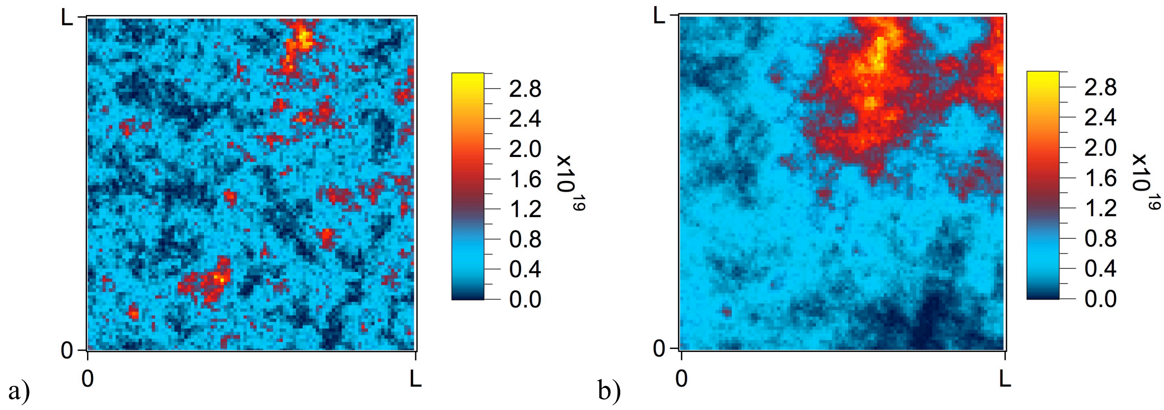


FIG. 1. Examples of 2D density maps sampled from the multivariate Gamma distribution, for an exponential correlation function with correlation length a) $\lambda/L=0.025$ and b) $\lambda/L=0.15$. Here, m=3 (R=82%) and the average density is $\langle N_e\rangle=5\times10^{18}\ m^{-3}$.

increases with λ. This sampling scheme has been implemented in the EIRENE Monte Carlo code. In practice, a background plasma density is sampled, then the Boltzmann equation for neutrals is solved for the statistical quantities of interest. These steps are repeated until statistical noise is reduced to a negligible level (typically after up to 10^4 realizations).

4. Source of neutral particles

The main source of neutral particles in a Tokamak discharge is recycling, and is therefore essentially located at places where most of the plasma-wall interaction takes place (limiters or strike points in a divertor configuration). In our 2D slab geometry, where the x axis represents the radial direction and the y axis the poloidal direction, we assume that the main source of neutral particles is located on the first wall at x=0. This assumption is not realistic if the slab position is close to the divertor, but should be sensible around the equatorial plane. In the following, we investigate two limiting cases, respectively called slow and fast recycling. In the first case, turbulent time scales are assumed to be very fast compared to those of recycling processes, and the neutral source at the wall is taken to be uniform and non stochastic. In the opposite case, the recycling flux response to the plasma flux is instantaneous, and the neutral source has the same "blobby" character as turbulence. Physically, fast recycling occurs through backscattering, while thermalization in a non-saturated wall followed by molecule release is likely to be much slower [7]. Technically, the fast recycling case is implemented numerically by using the poloidal plasma flux profile at the wall Γ(x=0,y) as a probability density to sample to the neutral particle birth location.

5. Analytical results and validation of the EIRENE calculations

The implementation of the model in EIRENE has been validated against analytical results obtained in the case where charge exchange is neglected, the geometry is 1D with spatially homogeneous statistics, and in the one speed transport (*i.e.* monokinetic) approximation. Furthermore, the ionization rate coefficient is assumed to be independent on the density. In the slow recycling case, the average density is then given by [2]:

$$\langle N_0(x_k)\rangle_{\mathrm{slow}} = \frac{\Gamma_0}{\mathrm{v}_0}\frac{1}{\det\left(\mathbf{I}+2\mathbf{G}\mathbf{U}_k\right)^{m/2}}, \tag{7}$$

where Γ_0 is the non stochastic flux density (unit $m^{-2}.s^{-1}$) at the wall, v_0 the initial neutral particle velocity, **I** the n × n identity matrix (N=n in the 1D case), **G** the Gaussian correlation matrix defined by Eq. (4), and $\left(\mathbf{U}_k\right)_{ij} = \varepsilon/\mathrm{v}_0 \;\; \delta_{i\le k}\delta_{ij}$ (ε is the spatial grid step, $x_k = (k-1)\varepsilon$). The average density, given by Eq. (7), is plotted on FIG. 2a) in log scale as a function of distance from the wall for m=3 (R=82%), and different values of the ratio a=l/λ of the neutrals mean free path (denoted by l) to the turbulence correlation length (i.e. the size of blobs). The agreement with EIRENE calculations (circles) is excellent, showing that the numerical implementation is correct. It should be noted that for this very simplified (1D, one speed, no charge exchange) problem, the so-called "conditional expectation estimator" in EIRENE provides the exact result tracking only one particle (*i.e.*, there is no Monte Carlo

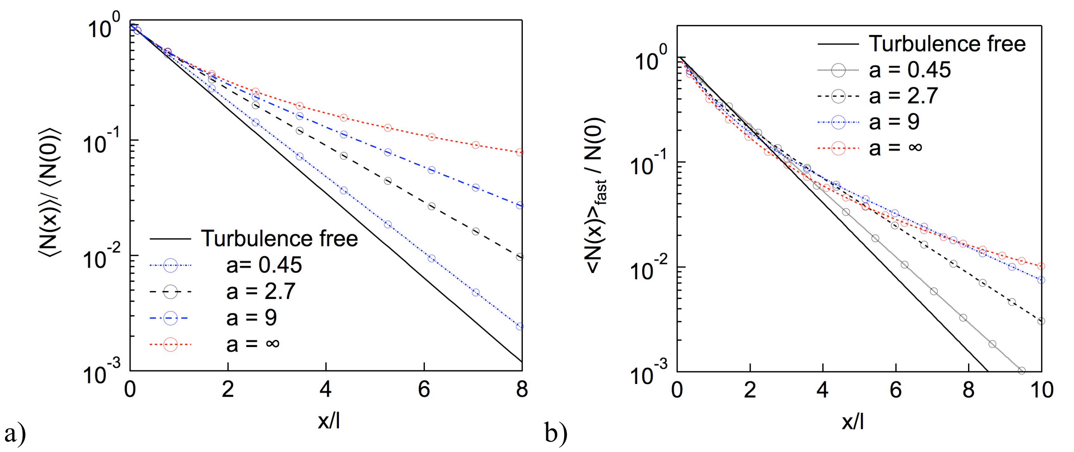


FIG. 2. a) Average density $<N_0>_{slow}$ in the slow recycling case as a function of x/l in semi-logarithmic scale, for m=3 and a=0.45, 2.7, 9 and ∞. In the fluctuation free case, $<N_0>$ has an exponential decay with e-folding length v_0/ν_{io}, where ν_{io} is the ionization rate. b) Same plot, but in the fast recycling case. The effect of fluctuations is markedly different in the latter case (see text). In both figures, circles correspond to EIRENE calculations and lines to Eqs. (7) and (8).

noise). The average neutral density $<N_0>_{\mathrm{slow}}$ has a slower decay than its turbulent free counterpart [2], that is neutral screening is reduced by density fluctuations as shown in FIG. 2a). This is consistent with previous studies dealing with either a stochastic mixture of two fluids [8], or fluctuations with Gaussian statistics [9]. This effect is all the more pronounced than $a=\lambda/l$ is large, that is in the small mean free path limit. If the typical blob size is of the order of 1 cm [10], $N_e=10^{19}$ m^{-3} and $T_e=20$ eV, we obtain $a_D \sim 2\times10^{-2}$ for deuterium atoms with $E_D=100$ eV. For the same conditions, but for D_2 molecules such that $E_{D2}=0.03$ eV, we have $a_{D2} \sim 2$. As a result, the effect of fluctuations on the average molecule density profiles should be much stronger than for atoms, provided temperature fluctuations are neglected. The picture is quite different in the fast recycling case, for which the analytical solution is given by [1]

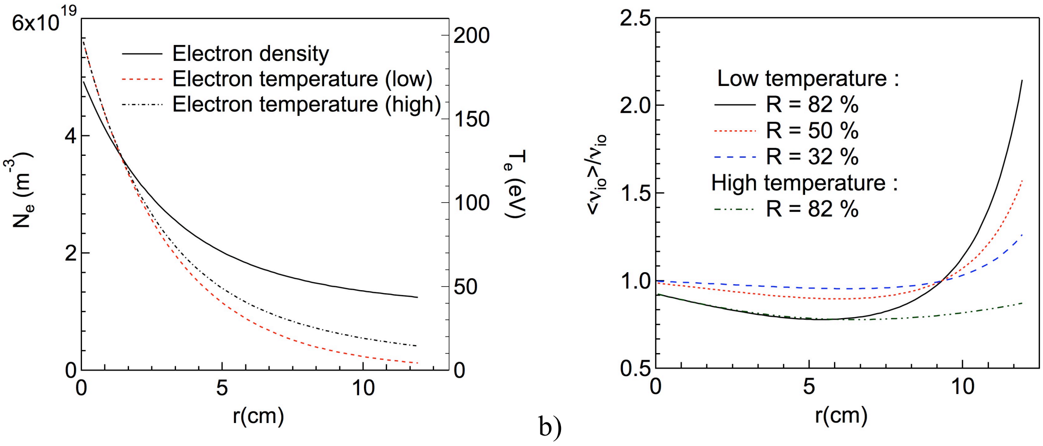
$$\langle N_0(x_k)\rangle_{\text{fast}} = \frac{\varpi(x_k)}{\langle \nu_{io}\rangle}\langle N_0(x_k)\rangle_{\text{slow}}, \quad \text{with} \quad \varpi(x_k) = \frac{\text{m}}{2}\frac{1-\left(\mathbf{A}_k^{-1}\right)_{kk}}{\varepsilon}\text{v}_0 \ , \tag{8}$$

where ν_{io} is the ionization rate, and $\mathbf{A}_k=\mathbf{I}+2\mathbf{GU}_k$. The quantity $\varpi(x_k)$ is a space dependent effective ionization rate, monotonously decreasing with increasing x_k. For $x_k/l>>a$, $\varpi(x_k)$ tends towards an asymptotic value $\varpi_\infty(\lambda,m)$ that can be calculated from Szegö's theorem [2]. The corresponding density profiles are plotted in FIG. 2.b), and the strong reduction of neutral screening obtained in the slow recycling case is no longer observed for moderate values of x/l, but reappears for x/l>>a. The physical reason for these different behaviours is easily understood. In the slow recycling case, the magnitude of the local neutral particles source does not depend on the local plasma flux on the wall, so that many neutrals penetrate deeply into the plasma through regions of low density. Conversely, in the fast recycling case the magnitude of the source is large only where the flux (*i.e.* the plasma density) is large, and neutral particles are therefore more likely to be ionized close to the wall. For x/l>>a, the plasma density at x is almost independent on its value at the wall, and the neutral particle density profiles given by Eq. (7) are recovered, up to a factor $\varpi_\infty/\langle\nu\rangle < 1$ which results from the increased average optical depth of the plasma layer between x=0 and $x=x_k$, compared to the slow recycling case. Furthermore, it is clear that for $a=\lambda/l << 1$, the two recycling models should yield the same density profiles, a tendency which is observed on FIG. 2. In the latter case, turbulence still has an effect on neutral particle transport provided $\langle\nu_{io}(N_e,T_e)\rangle$ and $\nu_{io}(\langle N_e\rangle,\langle T_e\rangle)$ are different, *i.e.* provided ν_{io} is a non linear function of the plasma parameters. Obviously, temperature fluctuations will have a stronger effect than density fluctuations in this regime, especially around the ionization threshold (see below).

It should be emphasized that the average ionization source $\langle S_p\rangle=\langle\nu_{io}N_0\rangle$, which is perhaps the most relevant quantity for integrated edge modelling, is in general *not* related in a simple way to the average density. In the slow recycling case, we have $\langle S_p\rangle_{slow}=\varpi(x)\langle N_0\rangle_{slow}$, so that $\langle S_p\rangle_{slow}$ has the same behaviour as $\langle N_0\rangle_{fast}$, which is plotted in FIG. 2b). The effect of fluctuations is smaller on $\langle S_p\rangle_{slow}$ than on the average density, because of a subtle compensation mechanism: schematically, neutrals that penetrate deeply in the plasma do so in realizations where the ionization rate (*i.e.* density) is low. The weight of these realizations in $\langle S_p\rangle_{slow}$ is therefore smaller than for $\langle N_0\rangle_{slow}$. With fast recycling, a similar compensation mechanism exists for the average density, but the ionization source $\langle S_p\rangle_{fast}$ then becomes more peaked towards the wall, as already guessed. To summarize, two main control parameters have been identified for the transport of neutral particles in turbulent plasmas, namely the ratio of the typical turbulent structures size to the neutral mean free path $a=\lambda/l$, and the ordering between recycling and turbulence time scales.

6. Tentative application to the ITER scrape-off layer

We finally present the first detailed EIRENE Monte Carlo calculations relying on the model presented in sec. 3., in 2D and including charge exchange with ITER relevant plasma profiles. The average plasma profiles are taken from ref. [11], and are plotted in FIG. 3a). We consider two different temperature profiles, for which the temperature at the wall is respectively of the order of 5 and 15 eV, for reasons that will be clear below. The parameters of our stochastic model are chosen so as to reproduce these average profiles, and the fluctuation rate is taken



a) b)

FIG. 3 a) Radial profiles in the ITER SOL for the electron density and temperature, taken from Ref. [11]. The separatrix is at r=0, and the wall (i.e., the local recycling source) is assumed to be located at r=12 cm. The ion temperature is given by $T_i=2T_e$. b) Ratio of the average ionization rate to the ionization rate calculated for the average plasma parameters as a function of the position in the SOL, for different fluctuation rates (corresponding to m=3, 8 and 20) in the low temperature case. In the high temperature case, the ratio is almost constant in space even for m=3.

constant in space for simplicity. To investigate the effect of temperature fluctuations, we assume in the course of the random sampling process that N_e and T_e are related by $T_e(x,y)=g(x)N_e(x,y)$, where $g(x)=\langle T_e(x)\rangle/\langle N_e(x)\rangle$, and that $T_i(x,y)=2T_e(x,y)$. This *ansatz* means that when the local density is above average, so is the temperature. Physically, this amounts to envision "blobs" as over-dense and hot plasma filaments propagating through the SOL, from the separatrix to the wall. The fluctuation rates for the density and temperature are taken to be equal to R=82% (m=3), so that the latter is overestimated for electron temperature. The correlation length, which gives the typical size of the turbulent structures, is set to λ=2.4 cm (the latter is typically of the order of the centimetre in current devices [10]). All the calculations presented here have been carried out in the slow recycling regime, with a source of D^+ ions impinging on the Beryllium wall. These somewhat extreme assumptions will allow us to get a feeling about the maximum effects that can be expected from fluctuations. For both high and low temperature cases, when temperature fluctuations are neglected, the effects of turbulence on either the average atom density or ionization source from atoms are very weak, as expected because $a_D=\lambda/l_D \ll 1$. The molecular density and ionization source radial profiles are plotted on FIG. 4 a) and b) together with the turbulent free case. The effect of fluctuations is indeed much larger for molecules than for atoms, owing to the much smaller initial velocity of the former. The average molecule density and ionization source extend farther from the wall when density fluctuations are included. This effect is reinforced when temperature fluctuations are retained, for the obvious reason that the ionization rate is an increasing function of N_e and T_e for T_e< 100 eV.

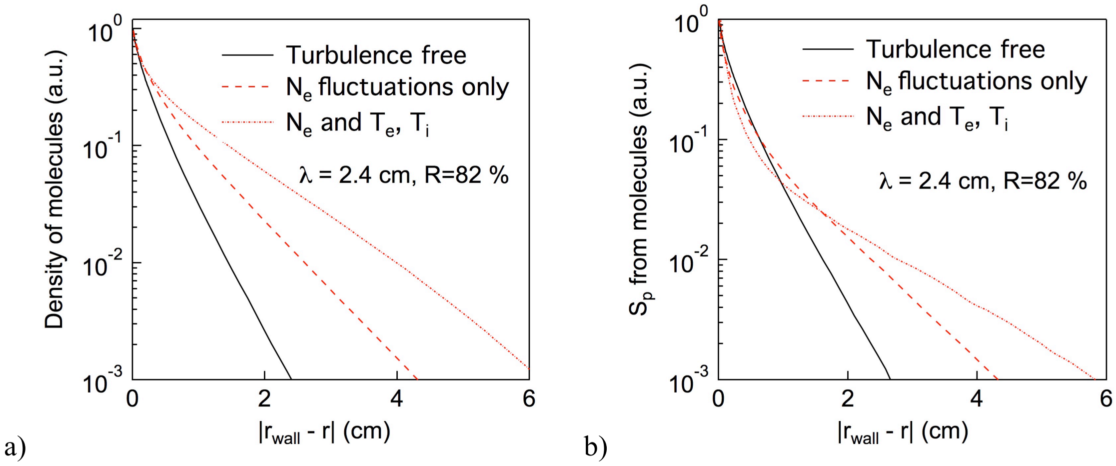


FIG. 4 a) Average density of D_2 molecules as a function of radial distance from the wall (the radial direction is reversed compared to FIG. 3), for the high temperature case. b) Particle source resulting from the ionization of molecules, as a function of radial distance. On both figures, the average profiles (with or without temperature fluctuations) are compared to those obtained in the turbulent free case.

In the low temperature case, the effects of fluctuations of N_e on the radial profile of molecule density is comparable to that observed in the high temperature case (FIG. 5 a)). However, the particle source associated to ionization of D atoms, plotted on FIG. 5 b), turns out to be very sensitive to temperature fluctuations, in contrast with what happens in the high temperature case. In fact, as pointed out in Sec. 5, in the regime where $a=\lambda/l \ll 1$, fluctuations can still have an effect on neutral particle transport, because the ionization rate is a non-linear function of T_e (and to a lesser extent of N_e because of the multi-step effects of the collisional radiative ionization cascade). In fact, for the low temperature case the average temperature close to the wall is well below

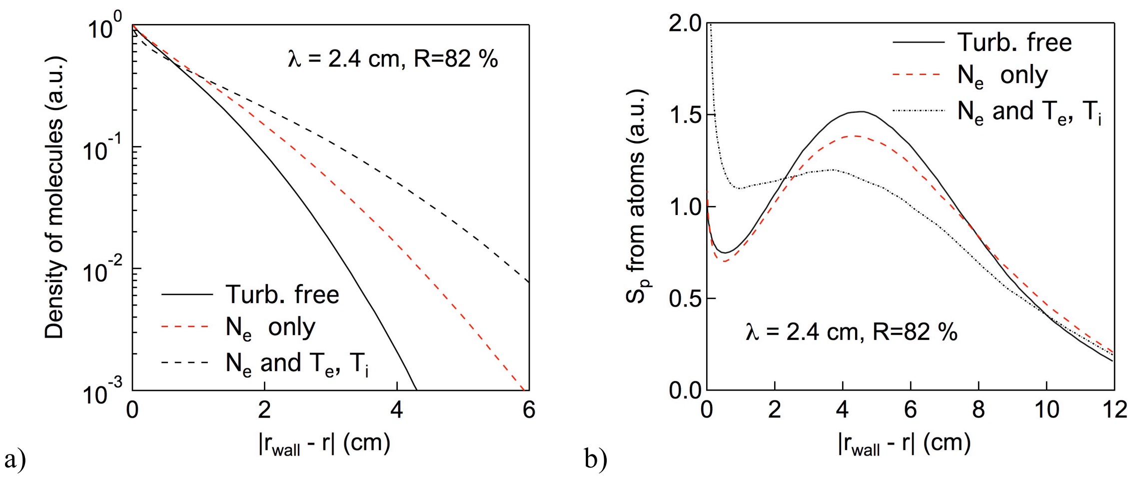


FIG. 5 a) Average density of D_2 molecules as a function of the radial distance from the wall (the radial direction is reversed compared to FIG. 3), for the low temperature case. b) Particle source resulting from the ionization of D atoms, as a function of radial distance. The effect of temperature fluctuations is much stronger than for the high temperature case.

the ionization threshold (13.6 eV for D), in the temperature domain where ν_{io} is a strong function of T_e. This is illustrated on FIG. 3b), where the ratio of the average ionization rate $\langle\nu_{io}\rangle$ to the ionization rate calculated for the average plasma parameters $\nu_{io}(\langle N_e\rangle,\langle T_e\rangle)$ is plotted as a function of space, hence of average temperature, for both high and low temperature cases. In the former case, the ratio remains close to one while it reaches values up to about 2 close to wall for the low density case. In other words, for low average temperature, realizations for which the electron temperature is larger than $<T_e>$ dominate when calculating the average of ν_{io}.

7. Conclusions and perspectives

We have presented a stochastic model for turbulence in the scrape-off layer (SOL), allowing to study the effect of fluctuations on the transport of neutral particles. The model is based on a multivariate Gamma distribution, and can be tailored so as to reproduce basic features of SOL turbulence. This model has been implemented in the EIRENE Monte Carlo code. We show that the strongest deviations from a calculation neglecting turbulence are observed when the turbulence correlation length is large compared to the neutral mean free path. Therefore, in general, the radial profile of molecule density is more affected than its atomic counterpart. The ordering between recycling and turbulence time scales is identified as another important control parameter in the problem. In fact, if the wall response to the plasma flux is instantaneous, re-ionization in the blob responsible for local recycling can be important, so that the ionization source is stronger close to the wall. Finally, the calculations made for plasma parameters foreseen for the ITER SOL confirm that atoms are very weakly affected by density fluctuations, owing to their large velocity compared to molecules. However, temperature fluctuations can change significantly the ionization source associated to atoms, provided the average temperature is below the ionization threshold. In addition, the radial profiles of the average molecule density and ionization source can be very different from their fluctuation free counterpart. Future work will focus on relaxing the adiabatic assumption for the particle distribution function, by coupling EIRENE to the 2D turbulence code TOKAM2D [12], and on devising a computationally efficient way to implement a stochastic model for fluctuations in B2-EIRENE, with focus on the far SOL.

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