Journal of Physics: Conference Series **490** (2014) 012210 doi:10.1088/1742-6596/490/1/012210

“Shell” approach to modeling of impurity spreading from localized sources in plasma

Mikhail Z. Tokar and Mikhail Koltunov

Institute for Energy and Climate Research - Plasma Physics (IEK-4), Research Center Jülich, 52428, Jülich, Germany

E-mail: m.tokar@fz-juelich.de

Abstract. In fusion devices strongly localized intensive sources of impurities may arise unexpectedly or can be created deliberately through impurity injection. The spreading of impurities from such sources is essentially three-dimensional and non-stationary phenomenon involving physical processes of extremely different time scales. Numerical modeling of such events is still a very challenging task even by using most modern computers. To diminish drastically the calculation time a ”shell” model has been elaborated that allows to reduce equations for particle, parallel momentum and energy balances of various ion species to one-dimensional equations describing the time evolution of radial profiles for several most characteristic parameters. The assumptions of the ”shell” approach are verified by comparing its predictions with a numerical solution of one-dimensional time dependent diffusion equation.

1. Introduction

In fusion devices impurities may intrude unexpectedly or can be deliberately injected for various purposes into the plasmas of hydrogen isotopes. Normally spots through which impurity particles enter into machines are much smaller than the total surface of the walls bounding the plasma. The spreading of impurity from such sources is essentially a three-dimensional and non-stationary, at least at the beginning, process. It includes the mutual transformation of impurity ions in different charge states by ionization with electrons, their friction and heating by coulomb collisions with the background ions, etc. Moreover, already at a very moderate injection rate the local impurity density can be comparable with that of the plasma before the injection and therefore the impurity ionization can lead to a significant increase of the electron density here. This affects the ionization process and makes the impurity spreading process nonlinear. Therefore, a proper numerical modeling of this phenomenon, being of very importance for the understanding of impurity transport mechanisms and impacts on plasma behavior, is cumbersome. By keeping in mind that options for parallelization of impurity transport computations are limited, a straightforward approach to modeling may be extremely time consuming, even by using the most modern computers.

Difficulties outlined above motivate to develop reduced models and approaches which require a significantly less calculations but allow, nonetheless, to extract the most important information about the spreading process. Such an information could be the time evolution of dimensions along and across the magnetic field of plasma regions occupied predominantly with impurity ions of a given charge Z, characteristic values of their density, flux and temperature. For low enough Z the regions in question are nested clouds, expanding in time but remaining small

Journal of Physics: Conference Series **490** (2014) 012210 doi:10.1088/1742-6596/490/1/012210

compared with the whole plasma volume. For such species the line of thinking outlined above is realized in the so called "shell model", see Refs. [1, 2], where instead of searching for detailed spatial profiles of impurity parameters their shape are parameterized by analytical expressions. The latter are approximate solutions of underlying equations and take into account that the cloud dimensions are controlled by the competition between the spreading of impurity species in question from their source, where these are generated by the ionization of lower charged ones, and the ionization into the higher charge state. By integrating three-dimensional fluid transport equations over some sub-regions of the shells, being the cross-sections by magnetic surfaces of the regions occupied with impurity ions of the given charge, one can get equations for the time evolution of key characteristics mentioned above. In Refs. [1, 2] also the shape of impurity parameter profiles in the radial direction r, perpendicular to the magnetic surfaces, has been analytically prescribed. Such a prescription is, however, very unsure since the radial profiles of impurity characteristics are essentially determined by the density and temperature of the background plasma. The latter are always inhomogeneous in the radial direction because the particle source is localized predominantly at the edge and heat source - in the core of the plasma. In the present paper the "shell" approach is elaborated further to describe the radial structure of impurity ion shells and is verified by comparing with a direct numerical solution of a diffusion equation. We use an orthogonal reference system (r, y, l) with the coordinate y aligned on the magnetic surface perpendicular to the magnetic field that is oriented in the direction l.

2. Basic equations

We consider a jet of impurity neutrals injected into the tokamak confined region through the outlet of a valve with a square cross-section in the (y, l)-plane, $|y|, |z| \leq b$. The outlet is situated at the last closed flux surface (LCFS), $r = a$, and is tangential to the LCFS. Neutrals are assumed moving with the speed V_0 in the radial direction r across magnetic surfaces towards the plasma axis, $r = 0$. The neutral density n_0 is homogeneous inside the jet cross-section and vanishes outside it. The variation of the n_0 radial profile in time t is described by the continuity equation:

$$\frac{\partial n_0}{\partial t} - V_0 \frac{\partial n_0}{\partial r} = -\nu_0 n_0 \tag{1}$$

where $\nu_Z \equiv k_{ion}^Z n_e$ is the ionization frequency of impurity particles of the charge Z, with k_{ion}^Z being the ionization rate coefficient and n_e the electron density; the latter is computed according to the plasma quasi-neutrality condition $n_e = n_i + \sum_{Z=1}^{Z_{\max}} Z n_Z$, with n_i being the density of the background ions of hydrogen isotopes.

The three-dimensional profile of the density n_Z of impurity ions with the charge Z is governed by the continuity equation [3]:

$$\partial_t n_Z + \partial_r \left(r \Gamma_{Zr} \right) / r + \partial_y \Gamma_{Zy} + \partial_l \Gamma_{Zl} = \nu_{Z-1} n_{Z-1} - \nu_Z n_Z \tag{2}$$

Here the impurity ion transport in all directions is assumed as diffusion and for the flux density components we assume $\Gamma_{Zr} = -D_r \partial_r n_Z$, $\Gamma_{Zy} = -D_y \partial_y n_Z$ and $\Gamma_{Zl} = -D_l \partial_l n_Z$ with prescribed diffusivity components D_r, D_y and D_l.

In the "shell model" we take into account that the cross-sections by magnetic surfaces of regions occupied by impurity ions of different charges Z are nested shells. The $(Z-1)$-shell with the dimensions l_{Z-1} along the magnetic field and δ_{Z-1} across that in the y-direction is the source region for the Z-ions. Beyond the $(Z-1)$-shell the density of Z-ions vanishes at some characteristic distances l_{Zd} and δ_{Zd} due to ionization into the $Z+1$ state. Since the Z-shell is the source for the $Z+1$-ions, the following recurrent relationships can be applied:

$$l_Z \approx l_{Z-1} + l_{Zd}, \;\; \delta_Z \approx \delta_{Z-1} + \delta_{Zd},$$

Journal of Physics: Conference Series **490** (2014) 012210 doi:10.1088/1742-6596/490/1/012210

with $l_0 = \delta_0 = b$ in the case of neutrals, $Z = 0$. Consider three regions in the Z-shell: the total shell $0 \le |y|, |l|$, y-subregion $\delta_{Z-1} \le |y|, 0 \le |l|$ and the l-subregion $0 \le |y|, l_{Z-1} \le |l|$. The total, per unit length in the r-direction, numbers of Z-ions in these regions, $N_Z(t,r) = \int\limits_0^\infty dy \int\limits_0^\infty n_Z dl$, $N_{Zy}(t,r) = \int\limits_{\delta_{Z-1}}^\infty dy \int\limits_0^\infty n_Z dl$ and $N_{Zl}(t,r) = \int\limits_0^\infty dy \int\limits_{l_{Z-1}}^\infty n_Z dl$, are governed by the integrals of equation (2) over the regions:

$$\partial_t N_Z - \partial_r \left(r D_r \partial_r \frac{N_Z}{r} \right) = \nu_{Z-1} N_{Z-1} - \nu_Z N_Z \tag{3}$$

$$\partial_t N_{Zy} - \partial_r \left(r D_r \partial_r \frac{N_{Zy}}{r} \right) = G_{Zy} - \nu_Z N_{Zy} \tag{4}$$

$$\partial_t N_{Zl} - \partial_r \left(r D_r \partial_r \frac{N_{Zl}}{r} \right) = G_{Zl} - \nu_Z N_{Zl} \tag{5}$$

with $G_{Zy} = -\int\limits_0^\infty D_y \partial_y n_Z(t,r,\delta_{Z-1},l)\, dl$ and $G_{Zl} = -\int\limits_0^\infty D_l \partial_l n_Z(t,r,y,l_{Z-1})\, dy$.

In order to relate G_{Zy} and G_{Zl} to N_Z we apply a method for finding of approximate solutions of parabolic partial differential equations, e.g., a diffusion one, outlined in Ref. [4]. This approach is based on the fact that such equations do allow neither periodic sign-changing solutions nor a similar behavior of individual terms in the equation. It presumes that the solution profile in certain direction is mostly controlled by the corresponding transport term in the equation and is not very sensitive to the spatial variation of other terms. Consider, e.g., the variation of n_Z along the coordinate y. In the source region $|y| \le \delta_{Z-1}$, where the dominant process is the generation of the Z-ions, equation (2) is written in the form $-D_y \partial_y^2 n_Z = S$ where the right hand side S combines all other terms, i.e. the source density, time derivative, transport in other directions and so on. For a constant S the solution to this equation is as follows:

$$n_Z(|y| \le \delta_{Z-1}) \approx n_{Z0} \varphi(y) \tag{6}$$

with $n_{Z0} = n_Z(y=0)$ and $\varphi(|y| \le \delta_{Z-1}) = 1 - [1 - n_Z(\delta_{Z-1})/n_{Z0}](y/\delta_{Z-1})^2$. In the region $|y| > \delta_{Z-1}$ the decay of the Z-ions due to ionization is of the most importance and $-D_y \partial_y^2 n_Z = -\nu n_Z$ with some still unknown but assumed constant ν. The solution, vanishing far from the source, is given by the relation (6) with $\varphi(|y| > \delta_{Z-1}) = n_Z(\delta_{Z-1})/n_{Z0} \exp[-(|y| - \delta_{Z-1})/\delta_{Zd}]$ and $\delta_{Zd} = \sqrt{D_y/\nu}$. From the continuity of $\partial_y n_Z$ at $y = \delta_{Z-1}$ we get $n_Z(\delta_{Z-1})/n_{Z0} = 1/[1 + \delta_{Z-1}/(2\delta_{Zd})]$. Similar analytical dependences can be found for the variation of n_Z with l. By using the approximate solutions in the form $n_Z(t,r,y,l) = n_{Z0}(t,r)\varphi(t,y)\varphi(t,l)$, one obtains $N_Z = n_{Z0}\Delta_Z L_Z$, $N_{Zy} = n_{Z0}\Delta_{Zd} L_Z$, $N_{Zl} = n_{Z0}\Delta_Z L_{Zd}$, and

$$\begin{aligned} G_{Zy} &= D_y N_Z / (\delta_{Z-1}/2 + \delta_{Zd}) / \Delta_Z \\ G_{Zl} &= D_l N_Z / (l_{Z-1}/2 + l_{Zd}) / L_Z \end{aligned} \tag{7}$$

where $\Delta_Z = \Delta_{Zs} + \Delta_{Zd}$, $L_Z = L_{Zs} + L_{Zd}$, with $\Delta_{Zs} = \delta_{Z-1}(\delta_{Z-1}/3 + \delta_{Zd})/(\delta_{Z-1}/2 + \delta_{Zd})$, $\Delta_{Zd} = \delta_{Zd}^2/(\delta_{Z-1}/2 + \delta_{Zd})$, $L_{Zs} = l_{Z-1}(l_{Z-1}/3 + l_{Zd})/(l_{Z-1}/2 + l_{Zd})$ and $L_{Zd} = l_{Zd}^2/(l_{Z-1}/2 + l_{Zd})$. These formulas allow to interrelate δ_{Zd} and l_{Zd} with N_Z, N_{Zy} and N_{Zl}:

$$\begin{aligned} \delta_{Zd} &= \delta_{Z-1} \frac{1 + \sqrt{(4N_Z/N_{Zy} - 1)/3}}{2(N_Z/N_{Zy} - 1)} \\ l_{Zd} &= l_{Z-1} \frac{1 + \sqrt{(4N_Z/N_{Zl} - 1)/3}}{2(N_Z/N_{Zl} - 1)} \end{aligned} \tag{8}$$

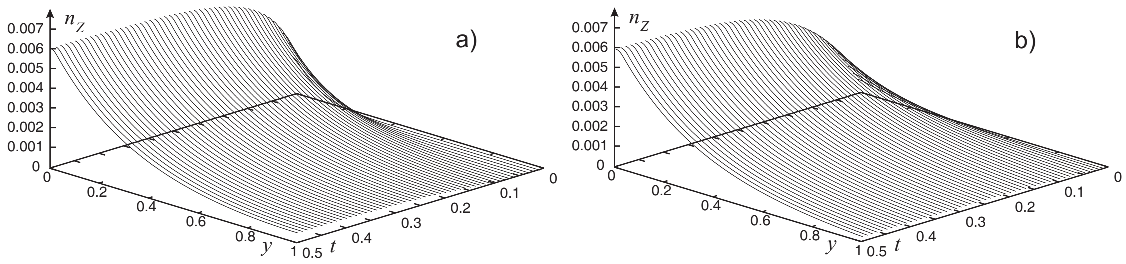

Figure 1. Solution of the diffusion equation (9) found by solving it numerically (a) and by integrating ordinary differential equations (10) deduced in the “shell” approximation (b).

Thus the time evolution of three-dimensional profiles of the impurity ion densities $n_Z\left(t,r,y,l\right)$ can be approximately modeled by solving one-dimensional equations (1) and (3-5) with relations (7), (8). The boundary condition to equation (1) is a prescribed density of neutrals at the injection outlet, $n_0\left(t,a,0,0\right)$; boundary conditions to N_Z, N_{Zy} and N_{Zl} follow from those for n_Z, corresponding to zero derivatives on the plasma axis $r=0$, $\partial_r N_Z=\partial_r N_{Zy}=\partial_r N_{Zl}=0$, and prescribed decay lengths δ_n at the LCFS $r=a$, $\partial_r N_Z/N_Z=\partial_r N_{Zy}/N_{Zy}=\partial_r N_{Zl}/N_{Zl}=-1/\delta_n$. The results for modeling of the penetration process of carbon impurity into a relatively cold edge of Ohmic TEXTOR plasma and of argon into hot H-mode plasma in JET obtained with the ”shell” approach are presented in Ref. [5].

3. Verification of ”shell” approach

To verify equation (6) we compare predictions of shell approximation with the numerical solution for one-dimensional diffusion equation:

$$\partial_t n-\partial_y^2 n=\Theta\left(\delta_0-|y|\right)-\nu n \tag{9}$$

where $\Theta\left(y<0\right)=0,\Theta\left(y\geq 0\right)=1$ is the Heaviside function. In this case the shell variables N and N_y are governed by ordinary differential equations:

$$dN/dt=\delta_0-\nu N,\ dN_y/dt=\frac{4N/N_y-4}{\left[1+\sqrt{\left(4N/N_y-1\right)/3}\right]^2}\frac{N-N_y}{\delta_0^2}-\nu N_y \tag{10}$$

Figure 1a shows $n\left(t,y\right)$ computed by solving numerically equation (9) and figure (1b) - equations (10) for $\delta_0=0.03$, $\nu=10$, initial condition $n\left(0,y\right)=0$ and boundary conditions $\partial n/\partial y\left(t,0\right)=\partial n/\partial y\left(t,1\right)=0$. The difference in the central values $n\left(t,0\right)$ does not exceed 20% and the maximum deviation is approached at $t\approx 0.1$.

References

[1] Koltunov M and Tokar M Z 2012 *Plasma Phys. Control. Fusion* **54** 025003
[2] Tokar M Z and Koltunov M 2012 *Phys. Plasmas* **19** 042502
[3] Stangeby P 2000 *The plasma boundary of magnetic fusion devices*, London, IOP Publishing 94
[4] Kantorowitsch L W and Krylow W I 1958 *Approximate methods of higher analysis*, New York, Interscience Publishers Inc. 304
[5] Tokar M Z and Koltunov M, *Nucl. Fusion*, in press