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

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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 the calculation time drastically 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 transport equations.

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1. Introduction
Impurities may intrude unexpectedly or can be deliberately injected for various purposes into hot plasmas of hydrogen isotopes in fusion devices. 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. Moreover, a significant electric field can be produced. 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 the dimensions along and across the magnetic field of the 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
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, 3], where instead of searching for detailed spatial profiles of impurity parameters their shapes 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 they 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 the shells, being the cross-sections of the regions occupied with impurity ions of a given charge by magnetic surfaces, and some shell sub-regions, one can get equations for the time evolution of key impurity characteristics. In Refs. [1, 2] also the shape of impurity density 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 the heat source - in the core of the plasma. In Ref.[3] the "shell" approach was elaborated further and allows now to describe the detailed radial structure of impurity parameters.

In the present paper we sophisticate the “shell” approach by treating the parallel motion of impurity ions more precisely. In addition, analytical expressions used to describe the profiles of the impurity particle and flux densities on magnetic surfaces are verified by comparing with a direct numerical solution of non-stationary transport equations. It is demonstrated that the “shell” model approximate the “exact” numerical solution with an error not larger 20%. Finally, the results of modeling of argon spreading in H-mode plasma in the tokamak JET are presented and it is shown that the present “shell” approach provides essentially new information being beyond the possibilities of standard one-dimensional numerical codes for impurity transport.

2. Basic equations

Henceforth we use an orthogonal reference system $(r, y, l)$ with the coordinate $y$ aligned on the magnetic surface perpendicular to the magnetic field; the latter is oriented in the direction $l$, see figure 1. 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:

$$\frac{\partial n_0}{\partial t} - V_0 \frac{\partial n_0}{\partial r} = -\nu_Z n_0$$

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.

Henceforth we neglect recombination processes, leading to the overlap of regions occupied with different charge states. This is justified for the impurity species of interest, i.e. of low enough charge $Z$ and being localized in the source vicinity small compared with the whole magnetic surface. Indeed, for electron temperature typically above several electron-volts the recombination frequencies of carbon ions with $Z \leq 3$ and argon ions with $Z \leq 4$ is much smaller than the ionization ones. In such a case the three-dimensional profile of the density $n_Z$ of
impurity ions with the charge $Z$ and mass $m_Z$ is governed by the following continuity equation [4]:

$$\partial_t n_Z - \partial_r (r D_r \partial_r n_Z) / r - \partial_y (D_y \partial_y n_Z) + \partial_l \Gamma_Z = S_Z - \nu_Z n_Z$$

where the impurity ion transport in the radial direction $r$ and in the direction $y$ on the magnetic surface perpendicular to field lines is assumed as diffusion with some prescribed diffusivity components $D_r$ and $D_y$, respectively; $S_Z = \nu_{Z-1} n_{Z-1}$ is the source density.

The density $\Gamma_Z$ of the flux component parallel to the magnetic field is determined by the momentum balance equation:

$$\partial_t \Gamma_Z - \partial_r (r D_r \partial_r \Gamma_Z) / r - \partial_y (D_y \partial_y \Gamma_Z) + \partial_l (\Gamma_Z^2 / n_Z + n_Z T_Z / m_Z)$$

where $\nu_{Z_i} \sim Z^2$ is the friction coefficient due to coulomb collisions with the background ions [5].

The impurity ion temperature $T_Z$ is governed by the heat balance equation:

$$\partial_t E_Z - \partial_r (r D_r \partial_r E_Z) / r - \partial_y (D_y \partial_y E_Z) + \partial_l (2.5 T_Z \Gamma_Z)$$

where $E_Z = 1.5 T_Z n_Z$ is the thermal energy density of the $Z$-ions, $T_i$ is the temperature of the main ions; in equations (3) and (4) the impurity ion viscosity and heat conduction components perpendicular to the magnetic field are assumed related to the corresponding diffusivities. The last term in the r.h.s. of equation (3) is due to electric field; its component parallel to the magnetic field, $E_l$, arises in the presence of a parallel gradient in the electron pressure and is governed by the force balance for electrons:

$$e n_e E_l = -\partial_t (n_e T_e)$$

where $e$ is the elementary charge, $T_e$ the electron temperature and the electron inertia is neglected.

Figure 1. Regions and shells occupied by impurity ions of different charges $Z$. 

Shells of impurity ions of different charges

Plasma core

Regions occupied by different charge states

LCFS

Impurity neutrals
According to the plasma quasi-neutrality condition a localized impurity injection produces an inhomogeneity of the electron density, generating a parallel electric field. This and dependence of the ionization frequency on \( n \) makes the impurity spreading process non-linear already at low enough injection rates [1, 2].

### 3. Shell approximation

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, see figure 1. The \((Z-1)\)-shell with the dimensions \( l_{Z-1} \) along the magnetic field and \( \delta_{Z-1} \) 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 \( L_d \) and \( \delta_{Zd} \), respectively, due to ionization into the \( Z+1 \) state. Since the \( Z \)-shell is the source region for the \( Z+1 \)-ions, the following recurrent relationships can be applied:

\[
l_Z \approx l_{Z-1} + L_d, \quad \delta_Z \approx \delta_{Z-1} + \delta_{Zd},
\]

by starting with prescribed \( l_0 = \delta_0 = b \) in the case of neutrals, \( Z = 0 \).

The "shell"-structure can be roughly reproduced by using approximate solutions of transport equations (2) and (3) in a form with separated variables:

\[
n_Z (t, r, y, l) \approx \varphi_n (t, y) \psi_n (t, l) n_{Z0} (t, r) \quad (6)
\]

\[
\Gamma_Z (t, r, y, l) \approx \varphi_\Gamma (t, y) \psi_\Gamma (t, l) \Gamma_{Z0} (t, r) \quad (7)
\]

For the factors \( \varphi_{n,\Gamma} (t, y) \) and \( \psi_{n,\Gamma} (t, l) \), describing the shape of solutions in the shells on magnetic surfaces, approximate analytical solutions of one-dimensional fluid equations have been utilized in Ref.[3]. Such solutions were obtained by applying a method from Ref. [6] to solve approximately parabolic partial differential equations, e.g., a diffusion one. This method 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 and 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. First consider the variation of \( n_Z \) along the coordinate \( y \). In the source region \( |y| \leq \delta_{Z-1} \), where the dominant process is the generation of the \( Z \)-ions, equation (2) is written in the form

\[
-D_y \partial_y^2 n_Z = S
\]

with the right hand side \( S \) assumed independent of the \( y \)-ordinates. In the region \( |y| > \delta_{Z-1} \) the decay of the \( Z \)-ions due to ionization is of the most importance and

\[
-D_g \partial_y^2 n_Z = -\nu n_Z
\]

with some still unknown but also assumed constant disintegration frequency \( \nu \). In this case the solution

\[
n_Z (y) = n_Z (y = 0) \varphi_n (y),
\]

vanishing far from the source, is given by:

\[
\varphi_n (|y| \leq \delta_{Z-1}) = 1 - \alpha (y/\delta_{Z-1})^2,
\]

\[
\varphi_n (|y| > \delta_{Z-1}) = \beta \exp \left[-(|y| - \delta_{Z-1})/\delta_{Zd}\right]
\]

where \( \delta_{Zd} = \sqrt{D_g/\nu} \). The factors \( \alpha \) and \( \beta \) can be determined from the continuity of the particle density \( n_Z \) and the flux density \(-D_g \partial_y n_Z\) at the source border \(|y| = \delta_{Z-1}\). This provides:

\[
\alpha = 1/ (1 + 2\delta_{Zd}/\delta_{Z-1}), \quad \beta = 1 - \alpha
\]

There is no reason for a variation of the parallel flux component \( \Gamma_Z \) in the perpendicular direction \( y \) different from that of \( n_Z \) and \( \varphi_\Gamma (y) = \varphi_n (y) \) is assumed henceforth. The situation is not, however, similarly straightforward in the case of the solution variation along the magnetic field. The continuity of \( n_Z \) presumes:
\[
\psi_n (|l| \leq l_{Z-1}) \approx 1 - \gamma \left( l/l_{Z-1} \right)^2, \\
\psi_n (|l| > l_{Z-1}) \approx (1 - \gamma) \exp \left[ - \left( |l| - l_{Z-1} \right) / l_{Zd} \right]
\]

which actually simply mimic the fact that the density profile is symmetric with respect to the source center and decays far from the source. However the continuity of the derivative \( \partial_\gamma n_Z \) cannot be exploited in this case. Indeed, by using motion equation (3) one the can express \( \partial_\gamma n_Z \) through such terms as \( n_Z, \Gamma_Z, \partial_\gamma \Gamma_Z \), etc, being continuous in space, and \( \partial_\gamma \Gamma_Z \). The latter is, however, discontinuous at the source boundary \( |l| = l_{Z-1} \), where the source density drops abruptly to zero, because \( S_Z \) and \( \partial_\gamma \Gamma_Z \) are directly related through the continuity equation (2) where other contributions are continuous. Even if one smooths the source profile in the vicinity of its border, the usage of the \( \partial_\gamma n_Z \) continuity would require the introduction of an intermediate region between the source and decay ones. Such a sophistication of the approach is out of a cope of the present consideration.

Thus, to quantify approximately the particle and parallel flux densities \( n_Z \) and \( \Gamma_Z \) in the shell approximation one has to know the variation with time \( t \) and minor radius \( r \) of the parameters \( n_{Z0}, \Gamma_{Z0} \), being the maximum values of \( n_Z \) and \( \Gamma_Z \) in the \( Z \)-shell, the characteristic dimensions of the decay region, \( l_{Zd} \) and \( \delta_{Zd} \), and the shape factor \( \gamma \). For this purpose we introduce new dependend "shell"-variables. These are the densities per unit length in the \( r \)-direction of the total number of \( Z \)-ions and their parallel momentum in:

the whole shell, \( 0 \leq |y|, |l| \):

\[
N_Z (t, r) = \int_{y \gg \delta_Z}^{y \gg \delta_Z} \int_{l \gg l_{Zd}}^{l \gg l_{Zd}} dy \int_0^{n_Z dl} = n_{Z0} \Delta_Z L_Z,
\]

its \( l \)-subregion, \( 0 \leq |y|, l_{Z-1} \leq |l| \):

\[
N_{Zl} (t, r) = \int_{y \gg \delta_Z}^{y \gg \delta_Z} \int_{l \gg l_{Zd}}^{l \gg l_{Zd}} dy \int_{l_{Z-1}}^{n_Z dl} = n_{Z0} \Delta_Z L_{Zd},
\]

and \( y \)-subregion, \( \delta_{Z-1} \leq |y|, 0 \leq |l| \):

\[
N_{Zy} (t, r) = \int_{y \gg \delta_Z}^{y \gg \delta_Z} \int_{l \gg l_{Zd}}^{l \gg l_{Zd}} dy \int_0^{n_Z dl} = n_{Z0} \Delta_{Zd} L_Z,
\]

where \( \Delta_Z = \Delta_{Zs} + \Delta_{Zd}, \quad \Delta_{Zs} = \delta_{Z-1} (\delta_{Z-1}/3 + \delta_{Zd}) / (\delta_{Zd} + \delta_{Z-1}/2), \quad \Delta_{Zd} = \delta_{Zd}^2 / (\delta_{Zd} + \delta_{Z-1}/2), \quad L_Z = l_{Z-1} (1 - \gamma/3) + L_{Zd}, \) and \( L_{Zd} = l_{Zd} (1 - \gamma). \)
Equations for shell variables follow directly from the integrals of equations (2) and (3) over the corresponding regions:

\[ \partial_t N_Z - \partial_r \left( r D_r \partial_r \frac{N_Z}{r} \right) = \nu_{Z-1} N_{Z-1} - \nu_Z N_Z \]  \hspace{1cm} (10)

\[ \partial_t N_{Zy} - \partial_r \left( r D_r \partial_r \frac{N_{Zy}}{r} \right) = G_{Zy} - \nu_Z N_{Zy} \]  \hspace{1cm} (11)

\[ \partial_t N_{Zl} - \partial_r \left( r D_r \partial_r \frac{N_{Zl}}{r} \right) = G_{Zl} - \nu_Z N_{Zl} \]  \hspace{1cm} (12)

\[ \partial_t \Lambda_Z - \partial_r \left( r D_r \partial_r \frac{\Lambda_Z}{r} \right) = \nu_{Z-1} \Lambda_{Z-1} - (\nu_Z + \nu_i Z) \Lambda_Z + \frac{T_Z + Z T_e / \alpha Z}{m_Z} \frac{N_Z}{L_Z} \]  \hspace{1cm} (13)

\[ \partial_t \Lambda_{Zl} - \partial_r \left( r D_r \partial_r \frac{\Lambda_{Zl}}{r} \right) = - (\nu_Z + \nu_i Z) \Lambda_{Zl} + \frac{4}{1 - \gamma} \left( \frac{\Lambda_Z - \Lambda_{Zl}}{l_{Z-1}} \right)^2 \frac{L_Z}{N_Z} + \frac{T_Z + Z T_e / \alpha Z}{m_Z} 0 (1 - \gamma) \frac{N_Z}{L_Z} \]  \hspace{1cm} (14)

where

\[ G_{Zy} = - \int_0^{l \gg l_{Z-1}} D_y \partial_y n_Z (t, r, \delta_{Z-1}, l) \, dl = n_{Z0} \frac{D_y L_Z}{\delta_{Zd} + \delta_{Z-1}/2} \]

and

\[ G_{Zl} = \int_0^{y \gg \delta_{Z}} \Gamma_Z (t, r, y, l_{Z-1}) \, dy = \Gamma_{Z0} \Delta_{Z} \]

The last terms on the right hand side in equations (13) and (14) are due to the impurity pressure gradient, the \( T_Z \) contribution, and electric field, the \( T_e \) one. The latter, can be estimated with an accuracy of 20% by adopting \( \alpha Z = 1 + \frac{n_i Z}{n_{Z0}} \frac{\Delta_{V}}{m_{\mu Z} \delta_{Zd}/4} \). The temperature \( T_Z \) of \( Z \)-ions is assumed the same in the whole \( Z \)-shell and its variation in time and along the minor radius \( r \) is governed by the following equation resulting from the integration of a combination of equations (2) and (4) over the shell:

\[ \partial_t T_Z - \partial_r (D_r \partial_r T_Z) - D_r (2 \partial_r \ln N_Z - 1/r) \partial_r T_Z \]

\[ = (T_{Z-1} - T_Z) S_Z / N_Z + 2 \nu_{Z} (T_i - T_Z) \]  \hspace{1cm} (15)

Equations (10)-(15) for shell variables can be straightforwardly integrated numerically, however by iterating them, since their right hand sides are interrelated non-linearly. Moreover, the inversion relations between the shell and original variables \( n_{Z0}, \Gamma_{Z0}, l_{Zd}, \delta_{Zd} \) and \( \beta \) have explicit analytical form:

\[ n_{Z0} = \frac{N_Z}{L_Z \Delta_{Z}}, \Gamma_{Z0} = 2 \frac{\Lambda_Z - \Lambda_{Zl}}{l_{Z-1} \Delta_{Z}} \]
\[
\delta_{Zd} = \delta_{Z-1} \frac{1 + \sqrt{(4N_Z/N_{Zy} - 1)/3}}{2(N_Z/N_{Zy} - 1)} \]

\[
l_{Zd} = \frac{l_{Z-1}}{2\Lambda_Z/\Lambda_{Zl} - 2}
\]

and

\[
\gamma = \frac{N_Z/N_{Zl} - 1 - l_{Z-1}/l_{Zd}}{N_Z/N_{Zl} - 1 - l_{Z-1}/(3l_{Zd})}
\]

Thus the time evolution of three-dimensional profiles of the impurity ion densities \( n_Z(t, r, y, l) \) can be approximately modeled by solving one-dimensional equations (1) and (10-15). The boundary condition to equation (1) is a prescribed density of neutrals at the injection outlet, \( n_0(t,a) \); boundary conditions to \( N_Z, N_{Zy}, N_{Zl}, \Lambda_Z, \Lambda_{Zl} \) and \( T_Z \) follow from those for \( n_Z, \Gamma_Z \) and \( T_Z \), corresponding to zero derivatives on the plasma axis \( r = 0 \), \( \partial_r N_Z = \partial_r N_{Zy} = \partial_r N_{Zl} = \partial_r \Lambda_Z = \partial_r \Lambda_{Zl} = \partial_r T_Z = 0 \), and prescribed decay lengths \( \delta_n, \delta_\Gamma \) and \( \delta_T \) at the LCFS \( r = a \), \( \partial_r N_Z/N_Z = \partial_r N_{Zy}/N_{Zy} = \partial_r N_{Zl}/N_{Zl} = -1/\delta_n, \partial_r \Lambda_Z = \partial_r \Lambda_{Zl} = -1/\delta_\Gamma \) and \( \partial_r T_Z = -1/\delta_T \).

4. Verification of "shell" approach

In this section we verify the relationships for the functions \( \varphi_{n,\Gamma} \) and \( \psi_{n,\Gamma} \) deduced in the previous section on the basis of approximate solutions of transport equations (2) and (3). It is done by comparing the results of calculations performed in "shell" approximation and obtained by direct numerical solution of one-dimensional transport equations. Consider the diffusion transport in the perpendicular direction \( y \) described by the following generic equation in dimensionless variables:

\[
\partial_t n_Z - \partial^2_y n_Z = \Theta (\delta_0 - |y|) - \nu n_Z
\]

where \( \Theta (y < 0) = 0, \Theta (y \geq 0) = 1 \) is the Heaviside function. The time evolution of the "shell" variables \( N_Z \) and \( N_{Zy} \) is governed by ordinary differential equations:

\[
\frac{dN_Z}{dt} = \delta_0 - \nu N_Z
\]

\[
\frac{dN_{Zy}}{dt} = \frac{4N_Z/N_{Zy} - 4}{[1 + \sqrt{(4N_Z/N_{Zy} - 1)/3}]^2} \left( N_Z - N_{Zy} \right) - \nu N_y
\]

Figure 2a shows \( n(t, y) \) computed by solving numerically equation (16) and figure 2b - equations (17) for \( \delta_0 = 0.03, \nu = 10 \), initial condition \( n_Z(0, y) = 0 \) and boundary conditions \( \partial n_Z/\partial y (t,0) = \partial n_Z/\partial y (t,1) = 0 \). The difference in the central values \( n_Z(t,0) \) does not exceed 20%; the maximum deviation is approached at \( t \approx 0.1 \).

Motion along the magnetic field is modeled by the following system of continuity and momentum equations:

\[
\partial_t n_Z + \partial_l \Gamma_Z = \Theta (l_0 - |l|) - \nu n_Z
\]

\[
\partial_t \Gamma_Z + \partial_l (n_Z + \Gamma_Z^2/n_Z) = -\mu \Gamma_Z
\]

In this case the "shell" model equations look as follows:

\[
\frac{dN_Z}{dt} = \delta_0 - \nu_N Z
\]
Figure 2. Solution of the diffusion equation (16) found by solving it numerically (a) and by integrating ordinary differential equations (17) deduced in the “shell” approximation (b).

Figure 3. Solution of the continuity equation (18) and equation of motion along the magnetic field (19) found by solving them numerically (a) and by integrating ordinary differential equations (20-23) deduced in the “shell” approximation (b).

\[
\frac{dN_{Zl}}{dt} = 2\frac{\Lambda_Z - \Lambda_{Zl}}{l_Z} - \nu N_{Zl} \tag{21}
\]

\[
\frac{d\Lambda_Z}{dt} = -\mu \Lambda_Z + \frac{N_Z}{L_Z} \tag{22}
\]

\[
\frac{d\Lambda_{Zl}}{dt} = -\mu \Lambda_{Zl} + (1 - \gamma) \frac{N_Z}{L_Z} + \frac{4}{1 - \gamma} \left(\frac{\Lambda_Z - \Lambda_{Zl}}{l_{Z-1}}\right)^2 \frac{L_Z}{N_Z} \tag{23}
\]

Figure 3 shows \( n(t, y) \) computed for \( \delta_0 = 0.03, \nu = 10, \mu = 20, \) with initial \( n_Z(0, y) = 0 \) and boundary conditions \( \partial n_Z/\partial y(t, 0) = \partial n_Z/\partial y(t, 1) = 0. \) Also in this case the difference between the results obtained by solving original transport equations (18), (19), see Fig. 3a, and those found from the integration of the "shell" approximation equations (20-23), see Fig. 3b, does not exceed 20% for the central values \( n(t, 0). \)

5. Example of applications
In several tokamaks, such as JT-60 [7], DIII-D [8], JET [9, 10], argon impurity has been puffed into H-mode plasmas with the edge transport barrier (ETB) in a narrow region \( a - \Delta \leq r \leq a, \Delta \ll a, \) where the parameter gradients are very sharp. This presumes a sudden alteration in the transport coefficients at the border between the plasma core and ETB. Here we describe the whole radial profile of \( D_{r,y} \) as follows:

\[
D_{r,y} = \frac{D_{core} + D_{ETB}}{2} + \frac{D_{core} - D_{ETB}}{2} \tanh\left(\frac{a - \Delta - r}{\delta}\right) \tag{24}
\]
Figure 4. Time evolution of the radial profiles of the surface averaged (a) and maximum (b) densities of singly charged argon ions $Ar^{1+}$.

Figure 5. Time evolution of the radial profiles of the surface averaged (a) and maximum (b) densities of $Ar^{4+}$ ions.

with $D_{\text{core}} \ll D_{ETB}$ and $\delta \ll \Delta$. One can see that deeply enough in the ETB, $r \gtrsim a - \Delta + 2\delta$, the relation above reproduces the diffusivity in the barrier, $D_r \approx D_{ETB}$, and in the core, $r \lesssim a - \Delta - 2\delta$, $D_r \approx D_{\text{core}} \gg D_{ETB}$. Figures 4 and 5 show the time evolution of the radial profiles for the surface averaged impurity ion densities $\langle n_Z \rangle$ and the maximum densities $n_{Z0}$ in shells of the ions $Ar^{1+}$ and $Ar^{4+}$ calculated for argon puffing experiments on JET with $R = 3m$, $a = 1m$ and $\Delta = 0.05m$ [9, 10]. It was assumed that neutral argon atoms enter the plasma with a thermal velocity at the room temperature, $V_0 = 250 \text{ ms}^{-1}$; their density at the inlet of the jet with the side length $b \approx 0.03m$ is constant in time and $n_0(t, a) = 10^{20} \text{ m}^{-3}$. The diffusivity of impurity ions is characterized by $D_{\text{core}} = 0.1 + 0.9 (r/a)^2$, $D_{ETB} = 0.1$ measured in $\text{m}^2 \text{s}^{-1}$ and $\delta = 0.001m$. One can see that at last closed flux surface at $r = a$ the maximum density of singly charged ions $Ar^{1+}$ exceeds the local plasma density before injection of $5 \times 10^{18} \text{ m}^{-3}$. Thus the electron density is significantly perturbed by the injection. This effect can not be taken into account by calculating with standard one-dimensional codes for impurity transport. Even for significantly strongly charged ions $Ar^{4+}$ there is a noticeable localization near the injection position and their maximum density on the magnetic surfaces exceeds by order of magnitude the surface averaged one. This is of importance by estimating the radiation heat loads on the wall elements. More results of calculations with the “shell” model can be found in Ref.[3].
6. Conclusion

The shell model for impurity spreading from a localized source in plasmas of fusion devices is elaborated further and verified by comparing with numerical solutions in the cases of one-dimensional diffusion across the magnetic field and flow along field lines. Additionally to impurity densities averaged over magnetic surfaces, being usually calculated in standard impurity transport codes, it allows to determine the dimensions of shells occupied by low charged ions, produced and vanishing at distances from the source much smaller than the magnetic surface dimensions. The penetration depth of such ions along the magnetic field is determined from their parallel momentum balance equation and is controlled by the competition of forces due to the electric field, own pressure gradient and friction due to collisions with the main plasma ions, and by the life time till ionization into the higher charge state. Both the ionization rate and the electric field are governed by the electron density which changes in the presence of impurity ions in order to maintain the plasma quasi-neutrality. The difference between the results from the shell approach and numerical solution of transport equations does not exceed 20%. With such a really tolerable error the shell model allow to calculate the maximum density of low charged impurity ions, which cab be by orders of magnitude larger than the surface average values provided by standard impurity transport codes.

To our knowledge, presently there are no three-dimensional non-stationary calculations of impurity transport over the whole plasma volume, from the separatrix to the axis. Therefore, it is difficult to assess firmly how significantly the computational time can be reduced by proceeding from three-dimensional calculations to a one-dimensional modeling on the basis of the "shell" approach outlined in the present paper. A rough estimate can be done by analogy with calculations for the global heat transport induced by the formation of a cold plasma cloud near the impurity injection position. This is also a three-dimensional problem, requiring calculations with very tiny steps in time and space. In Ref.[12] the study was limited to a non-stationary two-dimensional heat transport modeling on a single magnetic surface. Calculations were performed for MGI experiments on JET, by using a non-equidistant mesh with $100 \times 100$ grid points in the toroidal and poloidal directions on a magnetic surface close to the separatrix, during a total time of $10^{-3}s$ covered in 100 time steps increased from $10^{-6}s$ in a geometrical progression. These calculations required roughly 100 hours of CPU time on an Intel core with a speed of 1.2 GHz. If we assume that at least 100 magnetic surfaces have to be taken into account by calculating the total radial structure, a CPU time exceeding 1 year is required. For modeling of impurity transport $3Z_{\text{max}}$ three-dimensional equations have to be solved for each element, with $Z_{\text{max}}$ being the maximum number of charged states in question. This results in an astonishing estimate of several decades of CPU time needed only for a single argon study . In spite of the crudeness of this estimate, the necessity to reduce the calculation time drastically, by orders of magnitude, is obvious. In the case of heat transport we recently elaborated an analytical model to assess the heat losses along the magnetic surface to the cold area [11]. By using this, the time evolution of the average value of the electron temperature on the magnetic surface, $\langle T_e \rangle$, can be computed by solving a zero-dimensional equation. This requires a CPU time by a factor of $3 \times 10^4$ smaller than that needed for two-dimensional calculations. Remarkably, the results obtained by both approaches differ less than by 6%! Roughly the same reduction factor is expected if instead of three-dimensional profiles of the temperature the time evolution of the $\langle T_e \rangle$ radial profile will be calculated from a one-dimensional heat balance equation. By returning to the impurity transport, we get, with the same reduction factor, a CPU time of several hours needed for calculations of argon transport by using one-dimensional equations, in a rough agreement with the CPU time actually spent on the computations of radial impurity ion density profiles.

Thus the “shell” model proposed allow to model the impurity penetration process with a good accuracy during a reasonable calculation time. Moreover, the plasma reaction on the impurity
spreading can be described in the framework of this approach. This provides good chances for a self-consistent coherent description of the impurity transfer and its impacts on the background plasma in a near future.

References