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Numerical solution of continuity equation with a flux non-linearly depending on the density gradient

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Abstract

An approach to integrate transport equations with fluxes being complex non-linear functions of physical parameters and their gradients, as it is predicted by theoretical models for micro-instabilities in plasma, is proposed. This approach operates without any splitting of the flux on diffusive and convective components often involved in transport calculations. As an example, computations of the density profile in a stationary state and during dynamic evolution are done with the Weiland's transport model. The results obtained by the proposed method and a conventional one with a flux splitting are compared.

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1. Introduction

By considering transport processes in fusion plasma it is conventional to speak about such characteristics as particle and heat diffusivities and advection velocity. This approach is originated in the traditional view on the mass and heat transfer as caused by collisions of individual particles. In hot magnetized plasma, such a situation is described by the classical theory in a straight magnetic field and by the neoclassical one in a toroidal geometry [1]. Under conditions, where these theories are relevant, they predict fluxes, e.g., of charged particles, as being uniquely represented by the sum of diffusive component proportional to the density gradient and convective one proportional to the density itself.

However, hot plasma prone to diverse micro-instabilities, which result in a complex turbulent motion of plasma particles and enhance mass and heat transfer tremendously [2]. The resulting anomalous transport

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exceeds the classical and neoclassical contributions by many orders of magnitude. There are several sophisticated transport models, in particular, multi mode model (MMM) [3], gyro Landau fluid model (GLF23) [4], which predict particle and heat fluxes by taking into account diverse instability mechanisms, e.g., due to radial gradients of ion and electron temperatures, the presence of trapped particles and so on. Since these instabilities are driven by the plasma inhomogeneities, the resulting fluxes are complex non-linear functions of the gradients.

By using these models in transport codes [5–7] for the computation of plasma parameter profiles, the fluxes are normally splitted on diffusive and convective contributions in order to apply well developed approaches for numerical integration of the second-order differential equations. Such a separation serves also as an approximate tool for interpretation of experimental data in customary concepts of diffusion and advection. However, a definitive answer to the question about the uniqueness of individual transport coefficients, both reconstructed from experimental measurements under usually ambiguous assumptions about the time and spatial behavior of these characteristics, and obtained by a splitting of theoretically predicted fluxes, is not provided yet.

Therefore, development of direct methods for integration of transport equations without flux splitting on diffusive and convective parts would be very helpful in order to clarify this situation and to offer a firm basis for the prediction of parameter profiles in future devices. In the present paper such an approach is elaborated and demonstrated on the example of the well known Weiland's transport model [2], being at the core of the MMM, for the charged particle flux. This model allows to calculate the contributions to the anomalous transport from ion temperature gradient (ITG) and collisionless trapped electron (TE) unstable modes. The predictions by the method outlined are compared with the results obtained by a standard approach involving the splitting of the flux into diffusive and convective parts.

In this paper, only the basic aspects of the method proposed will be presented. Therefore, no attempts are done here to compare the results of calculations with experimental measurements. Moreover, many details important for a sophisticated modeling of particular experimental conditions are omitted. For example, the magnetic surfaces are considered in a cylindrical approximation by ignoring such their features as elongation, triangularity or the presence of X-points. Nevertheless, the metric coefficients, in which these characteristics are involved by a one-dimensional consideration, can be straightforwardly taken into account. In addition, the particle source is assumed in a very primitive form, by describing the recycling neutrals at the plasma edge in a diffusion approximation. A more detailed source model can be, however, easily introduced.

2. Basic equations

Time evolution of the plasma density n is governed by the continuity equation. After averaging over cylindrical magnetic surfaces this looks like as follows:

$$\frac{\partial n}{\partial t} = S - \frac{1}{r} \frac{\partial (r\Gamma_r)}{\partial r} \tag{1}$$

where Γ_r is density of plasma flux along the radial co-ordinate r and S is the density of the charged particle source due to ionization of neutral particles. By discretization in time, i.e., with the replacement $\partial n/\partial t$ by $(n - n_{-})/\tau$, where n = n(t,r), $n_{-} = n(t - \tau, r)$ and the time step τ is small enough, one gets

$$n = n_{-} + \tau \left[S - \frac{1}{r} \frac{\partial(r\Gamma_r)}{\partial r} \right]$$
(2)

with S and Γ_r computed for n_- .

The explicit approach above requires normally very small time steps and becomes usually unstable if the particle source and flux are non-linear functions of n and $\partial_r n$. In order to cope with this situation, Eq. (2) is often reduced to a second-order equation with respect to the spatial co-ordinate r, for which reliable methods of numerical integration are elaborated, see, e.g., Ref. [8]. For this purpose, the flux density Γ_r is splitted on diffusive and convective parts, being proportional to $\partial_r n$ and n, respectively:

$$\Gamma_r = -D\partial_r n + V n \tag{3}$$

Such a splitting is unique only for a linear transport model when one can find D and V independent of $\partial_r n$ and n. For a non-linear flux one cannot justify that a certain splitting is the most preferable one. Moreover, the time evolution of the density profile is determined, according to Eqs. (1) and (2), by the total flux Γ_r and any splitting procedure should provide the same result. This is, however, not guaranteed *a priori* due to non-linearities involved in the problem and if different n(t,r) arise by using different splitting schemes, doubts about this approach are legitimate.

Here, we propose an implicit method to integrate Eq. (1) numerically without any artificial splitting of the flux into parts, which works reliably for strongly non-linear transport models. By taking into account that Γ_r reduces to zero at the plasma axis, r = 0, Eq. (2) is multiplied by r and integrated from r = 0 to the radial position in question. As a result one gets the flux continuity relation:

$$\Gamma_r = \Phi(r) \tag{4}$$

with

$$\Phi(r) \equiv \frac{1}{r} \int_0^r \left(S - \frac{n - n_-}{\tau} \right) r \,\mathrm{d}r \tag{5}$$

With the known density profile at the previous time moment, $n_{-}(r)$, and some approximation for n(r), one can computes $\Phi(r)$. The procedure for computing of the next approximation to n(r) is started from the last closed magnetic surface r = a. Here, a boundary condition, relating the local values of n and $\partial_r n$, is normally imposed:

$$\alpha n(a) + \beta \partial_r n(a) = \delta \tag{6}$$

The transport model prescribes Γ_r as a non-linear function of n, $\partial_r n$ and other parameters p_j : $\Gamma_r = \Gamma_r(n, \partial_r n, p_j)$. In this study, which includes only particle transport, p_j are known functions of r. Eqs. (4) and (6) combined provide a non-linear algebraic equation for n(a):

$$\Gamma_r\left[n(a), \frac{\delta - \alpha n(a)}{\beta}, p_j(a)\right] = \Phi(a) \tag{7}$$

which can be solved by some numerical approach. In order to find n(a - h), where h is the spatial grid increment, the gradient at r = a - h is determined by interpolating linearly the behavior of n(r) on the interval $a - h \le r \le a$: $\partial_r n(a - h) \approx [n(a) - n(a - h)]/h$. This results in the following equation for n(a - h):

$$\Gamma_r\left[n(a-h), \frac{n(a)-n(a-h)}{h}, p_j(a-h)\right] = \Phi(a-h)$$
(8)

Note that through the function $\Phi(r)$ Eqs. (7) and (8) contain the information about the particle source S, which is especially important at the plasma edge. In a steady state the source term provides the only contribution to Φ . In the following section, by considering a particular example, we discuss how to proceed in the case when Eq. (8) has more than one solution.

The procedure above is continued to the plasma axis, providing a new approximation for the density profile, $n_{\text{new}}(r)$. The new approximation to Φ is calculated according to the relation:

$$\Phi_{\text{new}} = (1 - A_{\text{mix}})\Phi + A_{\text{mix}}\Phi(n_{\text{new}})$$

where $\Phi(n_{\text{new}})$ is determined from Eq. (5) with $n(r) \equiv n_{\text{new}}(r)$. Iterations are repeated till the deviations between two consequent approximations of some control parameters, n(r = 0), n(r = a), and $\Gamma_r(r = a)$, become smaller than $10^{-4}A_{\text{mix}}$. The maximum level of the mixture factor A_{mix} is restricted by the condition of the iteration convergence, as discussed in the following section.

It should be noticed that the approach outlined above requires iterations even in the case of a linear transport model when the splitting of the flux on convective and diffusive parts is unique. Therefore, in such a situation it seems to be more time consuming than standard approaches like finite volume method [8]. However, it does not happen automatically because the source of charged particles depends non-linearly on their density and thus iterations are necessary by any approach. For a flux varying non-linearly with the density gradient the number of iterations needed for convergence is consequently increased. Many technical aspects, e.g., approximations for time and spatial derivatives are considered above on a very simple level. More sophisticated approaches can improve the convergence and reduce time consumption significantly. One important issue is, e.g., the use of more accurate methods for the time integration. A simple one-sided finite difference approximation applied above implies a linear time variation of the solution. In situations, where this exceptional behavior is by far not realized, the centered time derivative is more preferable. In this case $(n - n_{-})/\tau$ provides the derivative at $t - \tau/2$. The most straightforward way to estimate the right-hand side of Eq. (1) at this time is to use the arithmetically averaged of its values at times t and $t - \tau$, although, more sophisticated methods may be also applied.

For very small τ an explicit representation of the time derivative, through the values of the variable at previous time steps only, is more advantageous than the implicit one chosen above. This is due to the large error arising if the current approximation to n(t,r) is even slightly different from the "correct" one. As it is shown in the following section the latter results in the increasing number of iterations with decreasing τ when this is below a certain level. An appropriate combination of both explicit and implicit representations of the time derivative has to be used by a further development of the method proposed.

3. Example of application

3.1. Transport model

In order to demonstrate the approach proposed, this is applied to the continuity equation (1) with the particle flux given by the Weiland's transport model [2]. It takes into account drift instabilities due to the ion temperature gradient and collisionless trapped electrons. Small perturbations of the plasma density, electric potential, ion and electron temperatures, \tilde{n} , $\tilde{\phi}$ and $\tilde{T}_{i,e}$, respectively, induced by instabilities are assumed in the form of Fourier harmonics proportional to $\exp(ik_x x + ik_y y - i\omega t)$. The components of the wave vector in the radial direction x and in the direction y perpendicular to x and the magnetic field, k_x and k_y , respectively, define the complex eigen frequency ω through the dispersion relation obtained from linearized fluid equations and quasi-neutrality condition [2]:

$$\frac{\widehat{\omega}(1-\epsilon) + \epsilon\left(\frac{7}{3} - \eta - \frac{5}{3}\epsilon\right) - k_y^2 \rho_s^2(\widehat{\omega} + 1 + \eta)\left(\widehat{\omega} + \frac{5}{3}\epsilon\right)}{\widehat{\omega}^2 + \frac{10}{3}\epsilon\widehat{\omega} + \frac{5}{3}\epsilon^2} = 1 - f_t + f_t \frac{\widehat{\omega}(1-\epsilon) - \epsilon\left(\frac{7}{3} - \eta - \frac{5}{3}\epsilon\right)}{\widehat{\omega}^2 - \frac{10}{3}\epsilon\widehat{\omega} + \frac{5}{3}\epsilon^2}$$
(9)

where $\hat{\omega} = \omega/\omega_*$, $\omega_* = c_s \rho_s k_y/L_n$ is the electron drift frequency; $c_s = \sqrt{T/m_i}$, m_i , $\rho_s = c_s/\Omega_{ci}$ and Ω_{ci} are the ion sound speed, mass, Larmor radius and frequency, respectively; $L_n = -n/\partial_r n$, $L_T = -T/\partial_r T$ the radial *e*-folding lengths for the density *n* and temperature *T*, whose unperturbed values are assumed the same for electrons and ions; $\epsilon = 2L_n/R$, $\eta = L_n/L_T$ and $f_t = \sqrt{2r/(R+r)}$ the fraction of trapped particles with *R* being the major torus radius.

The dispersion relation is solved as an algebraic equation for ω and the mode with the maximum growth rate $\gamma = Im\omega$ is selected. This and the requirement that the perturbations are not suppressed by Landau damping result in $k_y \simeq 0.3/\rho_s$ and $k_x \simeq 2\sqrt{2}\pi/\rho_s \times L_n \hat{s}/(qR)$ [2], with q being the safety factor and $\hat{s} = d \ln q/d \ln r$ the magnetic shear.

The density of the particle flux is determined as $\Gamma_r \equiv \tilde{n} \tilde{V}_E^* + c.c.$, where $\tilde{V}_E = -ik_y c \tilde{\phi}/B$ is the radial drift velocity due to perturbed electric field, which is estimated in a quasi-linear approximation providing for the perturbation of electrostatic potential $\tilde{\phi} \simeq \gamma B/(ck_x k_y)$ [2]; B is the magnetic field. This results in

$$\Gamma_r = f_t n V_* \frac{g_1}{g_2} \frac{\gamma^3}{\epsilon^4} \tag{10}$$

with $V_* \simeq 0.6 \left(\frac{q\rho_s}{\pi sR}\right)^2 c_s$, $g_1 = |\widehat{\omega}|^2 (1-\epsilon) - \widehat{\omega}_r \left(\frac{14}{3} - 2\eta - \frac{10}{3}\epsilon\right) \epsilon - \frac{5}{3} \left(-\frac{11}{3} + 2\eta + \frac{7}{3}\epsilon\right) \epsilon^2$ and $g_2 = [\widehat{\omega}_r^2 - \gamma^2 - \frac{10}{3}\widehat{\omega}_r \epsilon + \frac{5}{3}\epsilon^2]^2 + 4\gamma^2 \left(\widehat{\omega}_r - \frac{5}{3}\epsilon\right)^2$.

Fig. 1 displays the ϵ -dependence of Γ_r computed for the parameters in the interior of tokamak TEXTOR [9]: R = 1.75 m, r = 0.3 m, $B_T = 2.25$ T, q = 2, s = 1, $n = 4 \times 10^{19}$ m⁻³, T = 500 eV, $L_T = 0.3$ m. One can see that the flux is a complex non-linear function of the density *e*-folding length, which even changes its sign for



Fig. 1. Particle flux density versus the parameter $1/\epsilon = R/2L_n$ computed according to the Weiland's transport model [2].

small density gradient $\partial_r n = -2n/(\epsilon R)$. Normally, this is interpreted as the presence of an inward convective flux component, the so-called pinch-effect.

With a linear approximation applied in the previous section in order to estimate $\partial_r n(r)$, one gets the relation $\epsilon(r) = \frac{2}{1-n(r+h)/n(r)} \frac{h}{R}$. Thus, Eq. (4) is a non-linear algebraic equation for n(r) with a unique solution for $\Phi(r) > 0$, see Fig. 2, that can be found easily numerically. In the case $\Phi(r) \leq 0$, which can happen on the density ramp up stage with $n > n_-$, the solution is not unique if $\Phi(r) > \Gamma_r^{\min}$. In order to cope with this, we have to extend the transport model also for negative ϵ corresponding to a positive density gradient. The assumptions in the transport model used are not satisfied in this case and for $\epsilon < 0$ we assume $\Gamma_r = -D_0\partial n/\partial r \equiv 2D_0n/(R\epsilon)$ with some prescribed D_0 . Fig. 2 shows the resulting N-like ϵ -dependence of Γ_r for $D_0 = 0.1 \text{ m}^2/\text{s}$. Thus, there are three solution exists again. Since at the last closed magnetic surface (LCMS), r = a, Γ_r is always positive, $\epsilon(a)$ and n(a) are defined uniquely and the total n(r) profile is also unique. At the positions, where $\Phi(r) = 0$ and $\Phi(r) = \Gamma_r^{\min}$ the density gradient undergoes a sharp change between I and III branches of the $\Gamma_r(\epsilon)$ curve. The gradient values corresponding to the unstable branch II cannot be realized in the framework of the present transport model with quasi-stationary determined amplitudes of perturbations.

The results of computations done by the method proposed have been compared with those obtained by a flux splitting on diffusive and convective parts. The splitting is done according to the recipe:

$$D = \sigma \frac{\partial \Gamma_r}{\partial (-\partial_r n)}, \quad V = \frac{\Gamma_r + D\partial_r n}{n}$$
(11)



Fig. 2. Particle flux density versus the parameter $1/\epsilon$ continued into the range of positive density gradient. The value ϵ at the radial position r is determined by the equality $\Gamma_r = \Phi(r)$.

Here, σ is a free parameter assumed constant over the plasma radius. It is introduced in order to examine the influence of a deviation in the flux splitting from the prescription with $\sigma \equiv 1$ adopted in the MMM [3]. The latter would provide the correct unique diffusivity in the case of a linear transport model. In addition, the diffusivity *D* is restricted by the minimum value 0.1 m²/s to avoid unphysical non-positive values. Fig. 3 shows the ϵ -dependence of the transport coefficients obtained according to Eq. (11) with $\sigma = 1$ for the flux displayed in Fig. 1.

3.2. Results of calculations

For particular calculations it was assumed that the particle source is due to neutral beam injection and ionization of neutrals recycling through the LCMS. The beam source density, S_b , is determined by the beam power P_b , the energy of injected particles E_b , and the shape of the power absorption, which is assumed as a Gaussian one with the characteristic width r_b :

$$S_{\rm b} = \frac{P_{\rm b}}{2\pi^2 R r_{\rm b}^2 E_{\rm b}} \times \frac{\exp\left(-\frac{r^2}{r_{\rm b}^2}\right)}{1 - \exp\left(-\frac{a^2}{r_{\rm b}^2}\right)} \tag{12}$$

The recycling source density, $S_r = n_a k_i n$, is determined with the neutral density n_a computed in a diffusive approximation [10]. This implies that the rate coefficient of charge-exchange with ions, k_{cx} , is much larger than that of ionization by electrons, k_i . Therefore, cold primary neutrals, which enter the plasma volume, undergo charge-exchange and acquire the ion energy much earlier than they could be ionized. In this case, n_a is mainly given by the hot neutral density, which is governed by the continuity equation:

$$\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(-rD_{\mathrm{a}}\frac{\mathrm{d}n_{\mathrm{a}}}{\mathrm{d}r}\right) = -k_{\mathrm{i}}nn_{\mathrm{a}} \tag{13}$$

where $D_{a} = \frac{T}{m_{a}(k_{i}+k_{ex})n}$ and m_{a} are the diffusivity and mass of atoms, respectively. It is assumed here that the temperature of hot neutrals is the same as that of the plasma. The diffusion approximation allows, nevertheless, to take into account a difference between these characteristics and, therefore, the heat transfer between neutrals and ions by charge-exchange processes [11]. Moreover, the neutral model assumed can be easily extended by including cold neutrals explicitly [11].



Fig. 3. The diffusivity and pinch-velocity found from the particle flux density displayed in Fig. 1 according to Eq. (11) with $\sigma = 1$ and D restricted by the minimum value 0.1 m²/s.

The boundary condition at the LCMS implies a given probability R_{rec} for neutrals to recycle back into the plasma after recombination of ions and electrons on the wall:

$$D_{\rm a}\frac{{\rm d}n_{\rm a}}{{\rm d}r}(a) = \Gamma_r(a)R_{\rm rec} \tag{14}$$

At the LCMS the *e*-folding length δ_n for the plasma density is fixed, i.e., $\alpha = 1$, $\beta = \delta_n$ and $\delta = 0$ are assumed in Eq. (6). Computation have been done for the TEXTOR parameters cited above and $P_b = 1.5$ MW, $E_b = 50$ keV, $r_b = 0.3$ m, a = 0.46 m, $R_{rec} = 0.98$, $\delta_n = 0.1$ m. This study deals with the particle transport only and does not include any consideration of the heat transfer or redistribution of the electric current. Therefore, prescribed radial profiles of the plasma temperature *T*, assumed the same for electrons and ions, and of the safety factor *q* have been used, see Fig. 4. The initial profile of the plasma density, n(0,r), is also shown there.

Fig. 5 shows comparison of the plasma density profiles found in the steady state with $\tau = \infty$ by the present and standard methods. All solutions are converged with an accuracy of 10^{-5} . Although the agreement between different approaches is good enough, the difference between the profiles exceeds significantly the error of computations. The difference is much more pronounced in the case of computations with a small τ . Fig. 6 displays the change in the density profile, Δn , with respect to the initial one after one time step $\tau = 3$ ms. One can see that the results obtained by the standard method and represented by dashed curves, differ significantly for σ varying in a relatively narrow range. The drop in the density at $r \leq 0.25$ m for the flux splitting case is due to the fact that in this plasma region, more exactly from the position, where the density profile makes the break, the particle diffusivity is equal to its minimum value $0.1 \text{ m}^2/\text{s}$ and the pinch-velocity is very close to zero. Therefore, the initially peaked profile is flattened by the diffusion and the central density decreases. Attempts to reduce the minimum level of diffusivity results in a very unstable operation of the solver for the continuity equation because the factor by the highest second-order derivative becomes too small. The dependence on the splitting scheme, being in contradiction to the fact that only the total flux defines the profile evolution, seems to be intrinsic for the splitting approach. It is rooted not in some drawbacks of the numerical scheme but in the non-linear dependence of the flux on the plasma density and its gradient, which requires many iterations to get a converged solution. In the case of a non-linear flux no one of splitting schemes can pretend to be the most truthful one. Therefore, this approach does not provide the unique profile evolution, which nevertheless exists and is determined by the total flux. Namely, this evolution is given by the approach proposed here and displayed by the solid curve in Fig. 6.

In order to reduce time consuming the possibly largest mixture factor A_{mix} has to be used. It turns out that the maximum level of A_{mix} , above which iterations do not converge, depends essentially on the time step. The



Fig. 4. Radial profiles of the plasma temperature T, safety factor q and initial density n(t = 0) used in computations.



Fig. 5. Density profiles in the stationary state computed by the approach with the flux splitting (dashed lines) and by the presently developed method (solid line).



Fig. 6. Density change with respect to the initial state after time $\tau = 3$ ms computed by the approach with the flux splitting (dashed lines) and by the proposed method (solid line).

restriction $A_{\text{mix}} < \min(1,10\tau)$, with τ measured in ms, has been envisaged for the conditions modelled above. Also the total number of iterations necessary for one time step depends on τ . Computations on a grid with 300 equidistant knots and with $\tau = \infty$ provide directly the stationary state after 367 iterations; one time step with $\tau = 1$ s, 0.1 s, 0.01 s and 1 ms requires, respectively, 242, 64, 163 and 737 iterations. The increase of the number of iterations with τ decreasing below a certain level demonstrates an advantage to use an explicit approach to evaluate the time derivative for small τ . In general, the method proposed has good convergence properties, i.e., the error always steadily reduces with consequent iterations. This is because integration is generally a more numerically stable procedure than differentiation.

4. Conclusion

Fluxes predicted by theoretical transport models are complex non-linear functions of parameter gradients. An approach to integrate continuity equation with such a flux, without a splitting on diffusive and convective parts, is proposed. Computations were performed with the Weiland's transport model taking into account drift instabilities due to the ion temperature gradient and collisionless trapped electrons. The profiles provided by this approach do not coincide with those obtained by making a flux splitting, which are different for different splitting procedures in contradiction to the fact that only the total flux is of importance.

There are no principal limitations to apply the approach proposed to model plasma conditions closer to those in ITER, i.e., with edge or/and internal transport barriers. Such a development will be done in near future.

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