Reversal of impurity pinch velocity in tokamak plasma with transport barriers

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1 Introduction

Impurity transport is an important issue for the success of the International Thermonuclear Experimental Reactor (ITER) as it can strongly influence the plasma performance. It is important to prevent impurity accumulation in order to maintain stationary plasma conditions \cite{1}. Impurity accumulation is predicted by the theory of collisional transport when the main ion density profile is peaked and thermal screening is negligible \cite{2}. However the predictions of neoclassical theory are rarely matched exactly by the observations. Turbulent transport is considered as a plausible candidate for explaining this discrepancy.

A standard phenomenology describes the steady state particle flux $\Gamma_s$ as a sum of a diffusive term and a convective term: $\Gamma_s = -D_s \nabla n_s + n_s V_s$, where $D_s$ is the diffusivity, $n_s$ is the density, and $V_s$ is the radial pinch velocity of species “s”. Several mechanisms have been identified in the framework of the quasilinear theory to explain the pinch velocity. First, perpendicular compressibility induces a curvature pinch velocity. Second, parallel compressibility is responsible for a second contribution that depends on the phase velocity of the fluctuations. And finally, the temperature gradient is responsible for a thermodiffusion term which also depends on the phase velocity.

In this work, the influence of transport barriers on the particle pinch is investigated. Transport barriers are observed in plasmas i) with reversed magnetic shear profile and zero or negative value of magnetic shear in the plasma core, and ii) with monotonic safety factor profile where the stabilization of the turbulence is provided by large $E \times B$ rotation shear. It is shown that transport barriers are a favorable configuration for getting a reversal of the impurity pinch velocity. This is an important issue for a fusion reactor as it allows the decontamination of the core plasma and prevents the degradation of confinement.

2 Model Equations

In collisionless plasmas, in the range of scales larger than an ion gyroradius ($k_i \rho_i < 1$), the main instabilities are the ion temperature gradient (ITG) and the collisionless trapped electron modes (TEM). In the following, we investigate the impurity turbulent transport using a three-dimensional nonlinear global fluid code TRB \cite{3, 4} which includes ITG modes and TEM. The study includes investigations of both monotonic and reversed $q$-profile configurations. The code solves the evolution equation of density and pressure for three species: deuterium, trapped electrons, and one impurity species. The geometry used in this simulation is a set of circular concentric magnetic surfaces.
A set of fluid equations is used here to describe a collisionless ITG/TEM turbulence:

\begin{align}
\frac{d_{1}n_s}{dt} &= -\mathbf{k}_s \cdot (n_s \nabla \phi + \nabla p_s/e_s) - \nabla \parallel (n_s v_{||s}) , \quad (1) \\
\frac{d_{1}p_s}{dt} &= -\mathbf{k}_s \cdot (p_s \nabla \phi + \nabla (p_s^2/n_s)/e_s) - \gamma \nabla \parallel (p_s v_{||s}) , \quad (2) \\
n_{3}s d_{3}v_{||s} &= -n_{3}s e_s \nabla \parallel \phi - \nabla \parallel p_s . \quad (3)
\end{align}

Here, \(n_s, p_s, v_{||s}, \phi \) are the density, the pressure, the parallel velocity, and the electric potential, respectively. The labels “s” can be “e”, “i” and “z” which are for trapped electrons, ions, and impurities, respectively. We solve eight equations for \(n_e, n_z, p_e, p_i, p_s, \Omega, v_{||e} \) and \(v_{||z} \). Passing electrons are assumed to be adiabatic, while the dynamics of trapped electrons is described by Eqs. (1)-(3), with \(v_{||e} \) and \(v_{||z} \). The continuity equation for the main ion density \(n_i\) is taken into account in a different form: from the ambipolarity relation, one gets instead an equation for the the vorticity \(\Omega\), \(\Omega = f_\epsilon n_{e,eq} \frac{\delta \phi - \phi}{\nabla_{eq}} - (n_{i,eq} + \alpha n_{c,eq}) \nabla^2 \phi\). The curvature drift operator is \(\mathbf{k}_s = \frac{2}{n} B \times \nabla B \) for ion species. For trapped electrons, \(\mathbf{k}_s\) is replaced by the precession frequency in the toroidal direction, i.e., \(\mathbf{k}_s = \frac{1}{R} (1 + \frac{2}{3} \chi^2) \mathbf{e}_\phi\) here, \(\mathbf{e}_\phi\) is a unit vector of toroidal direction and \(R\) is the plasma major radius. Here, \(\dot{s} = (r/q)d\theta/dt\) is the magnetic shear. The Lagrangian time derivative is defined as \(\frac{d}{dt} = \frac{\partial}{\partial t} + v_{E} \cdot \nabla - D \nabla^2\), where \(D\) is a “collisional” diffusion operator and \(v_{E} = \frac{B_c}{B} V_{0}\) is the electric drift velocity. Note that the perturbed part of \(f_{i}n_{i}\) is the fluctuating density of trapped electrons, whereas \(n_{e,eq}\) is the total equilibrium electron density normalized to \(n_0\). The adiabatic compression index is \(\gamma = 5/3\). The normalization is of the gyroBohm type, as referenced in Ref.[4]. The fraction of trapped (respectively, passing) electrons is \(f_i = 2/\pi(2r/R)^{1/2}\) (respectively, \(f_e = 1 - f_i\)).

### 3 Theoretical description of anomalous particle transport

A common description for the impurity flux is a diffusion-convection equation [4, 5, 6, 7, 8, 9, 10],

\[ \Gamma_z = -D_z \nabla n_z + V_z n_z , \quad (4) \]

where \(n\) is the impurity density profile, \(D_z\) the diffusion coefficient and \(V_z\) the pinch velocity of the impurities. This formulation assumes that \(D_z\) and \(V_z\) are weak functions of \(n_z\) and \(\nabla n_z\), respectively. In steady state conditions and in plasma regions where the source can be neglected, the local logarithmic density gradient of an impurity \(1/L_{n_z} = -\nabla n_z/n_z\) is directly related to the ratio of the convection velocity to the diffusion coefficient, \(V_z/D_z\). Hence, the peaking of an impurity density is determined by the ratio \(-V_z/D_z\), or equivalently the normalized peaking factor \(-RV_z/D_z\). The peaking factor profile is an important parameter to characterize the impurity density pinch.

The diffusion-convection expression of the flux is consistent with the quasilinear theory. Indeed the radial turbulent flux of species \(s\) is \(\Gamma_s = (n_s v_{E}) = \sum_{k,\omega} n_{s,k,\omega} i k_{\theta} / \omega_{pe} \phi_{k,\omega}^e \). Replacing the density by its linear expression in this expression, one finds the quasilinear flux:

\[
\Gamma_s = \sum_{k,\omega} \frac{1}{N} \frac{e_s}{T_{s,eq}} \frac{i k_{\theta}}{\omega_{pe}} \left| \phi_{k,\omega}^e \right|^2 \left\{ -F \omega_{ps}^e - G \omega_{ps}^e + FG + \zeta G^2 \right\} n_{s,eq}, \quad (5)
\]
where \( F = \omega - 2\zeta \omega_{ds} - \zeta \frac{\omega^2}{\omega} \) \( G = \omega_{ds} + \frac{\omega^2}{\omega} \) and \( N = \omega F + \zeta \omega_{ds} G \). The curvature drift frequency is defined as \( \omega_{ds} = k_y \frac{T_E}{eB} \lambda_\delta \), where \( \lambda_\delta = (\cos \theta + \delta \sin \theta) \). The bracket is an average of the bounce motion for trapped particles, or the average of poloidal mode structure for passing particles. The vertical component of the wave number is \( k_y \) and the poloidal wave number is \( k_\theta \). The diamagnetic density and pressure frequencies are defined as \( \omega_n^* = \frac{\Gamma_{eB}}{T_e B} \frac{\partial n_{es}}{\partial t} \) and \( \omega_p^* = \frac{\Gamma_{eB}}{T_e B} \frac{\partial P_{es}}{\partial t} \), respectively, and the parallel transit frequency is \( \omega_\parallel = k_\parallel \sqrt{\frac{T_{es}}{m_e}} \).

In the case of the existence of external imposed \( \mathbf{E} \times \mathbf{B} \) velocity shear, the calculation of the quasilinear flux has to be modified. In the presence of an \( \mathbf{E} \times \mathbf{B} \) shear flow \( \mathbf{V}(r) \), the Lagrangian time derivative \( \frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v}_E \cdot \nabla \) should be modified as \( \frac{d}{dt} = \frac{\partial}{\partial t} + (\mathbf{v}_E + \mathbf{V}(r)) \cdot \nabla \). Here, \( \mathbf{V}(r) = V_0(r)e_\theta \), and \( V_0 = -\frac{E_x(r)}{B} \). Therefore, in the process of the linearization, the Fourier expression of the Lagrangian time derivative is given by \( -i\omega - i\omega + \frac{ik_y E(r)}{B} = -i(\omega - \omega_E) \). Here, the frequency of the \( \mathbf{E} \times \mathbf{B} \) shear velocity \( \omega_E \) is defined as \( \omega_E = -\frac{\Gamma_{eB}}{T_e B} \).

The Doppler shift due to this uniform flow component is adsorbed in to the frequency \( \omega \), i.e., \( \omega - \omega_E \rightarrow \omega \). A careful calculation accounting for the modification of the radial shape of the modes indicates that no change is expected due to Doppler shift.

The first term in Eq. (5), proportional to \( \nabla_r n_{eq} \), corresponds to the diffusive part of the flux. The other terms are referred to as pinch velocities. To identify the mechanisms underlying the pinch velocity, we assume now that one mode is dominant, and that the following ordering \( \omega_p^* \gg \omega \gg \omega_{ds} \gg \omega_\parallel \) holds. This ordering is consistent with the interchange character of ITG/TEM turbulence and the fluid approximation. Then it appears that the pinch velocity is the sum of three components. The first one, called curvature pinch, gives a peaking factor that mainly depends on the geometry \( \frac{V_{\perp eq}}{D} \sim -\left\{ \omega_{ds} + \frac{\zeta \omega_{ds}^2}{\omega - 2\zeta \omega_{ds}} \right\} \) [6, 7, 8]. It is caused by the compressibility of the \( \mathbf{E} \times \mathbf{B} \) drift velocity in an inhomogeneous magnetic field. This effect is related to turbulent equipartition (TEP) effect [6]. In the case where \( \omega \gg \omega_{ds} \), one has \( \frac{V_{\perp eq}}{D} \sim -2\lambda_\delta \). However, for lower frequencies, the pinch velocity can change sign. This change of sign occurs when \( \zeta \omega_{ds} < \omega < 2\zeta \omega_{ds} \). In particular the ratio \( VR/D \) is proportional to the parameter \( \lambda_\delta \), which also characterizes the canonical profile \( \exp\left\{ -\frac{2}{R} \int \lambda_\delta(r') dr' \right\} \). For trapped electrons, \( \lambda_\delta \) is related to the precessional frequency, thus depends on magnetic shear. For impurities, \( \lambda_\delta \) depends on \( \delta \) when modes are strongly ballooned. We note that TEP effects also exist for momentum pinch [11]. When the curvature pinch velocity is proportional to the magnetic shear, it is inward for a monotonic increasing \( q \)-profile and outward for reversed \( q \)-profile. It is independent of charge and mass. The second pinch velocity, called thermodiffusion is such \( \frac{V_{\perp eq}}{D} \sim \frac{2\lambda_\delta \omega_{ds}^2}{\omega - 2\zeta \omega_{ds}} \) [9, 7]. It originates from the compression of the diamagnetic drift velocity and is proportional to the impurity pressure gradient. Its magnitude is inversely proportional to the charge number. As a result the thermodiffusion pinch becomes negligible for high \( Z \) impurity [4]. The \( \mathbf{E} \times \mathbf{B} \) velocity shearing can break the balance of the intensity of the terms of the pinch velocities. The third contribution to the pinch velocity is connected with the parallel dynamics of the impurities \( \frac{V_{||}}{D} \sim -2\lambda_\delta \omega_{ds}^2 \) [10]. The magnitude of this pinch depends on the ratio \( Z/A \) and thus depends weakly on the impurity characteristics in realistic cases. The thermodiffusion pinch and the pinch linked to the parallel compressibility
can change sign depending on the direction of propagation of the fluctuations. The thermodiffusion pinch is inward for transport driven by instabilities rotating in the electron diamagnetic direction, such as TEM, and outward for transport driven by instabilities rotating in the ion diamagnetic direction such as ITG. In contrast, the pinch originating from the compression of parallel velocity has the opposite variation. Therefore, the total pinch, which is the sum of at least these three mechanisms, has a dependence on \( Z \) that is different depending whether instabilities rotate in the ion or the electron diamagnetic direction. The relative magnitude of these mechanisms can change depending on plasma conditions, such as \( q \)-profile, or impurity temperature gradient. Nevertheless the dependence on \( Z \) is usually weak since the curvature pinch velocity is the dominant contribution.

4 Characterization of the impurity transport

Various simulations have been performed to investigate the basic properties of impurity transport in core plasma ITG/TEM turbulence with and without internal transport barriers (ITBs). The simulated impurities are Helium (He, \( Z = 2, A = 4 \)). Note that the Helium ash will be a primary impurity in the core of burning plasmas. The choice of Helium as impurity is a natural choice, since even if other impurities are not present, there will be Helium in a burning plasma.

In L-mode plasmas, a monotonic \( q \)-profile is chosen as shown in Fig. 1. The radial profiles of the electron temperature, the ion temperature, and the ion density are plotted. The ion density shows a peaked profile which indicates the existence of an inward pinch velocity. The turbulence has been reached to steady state.

Knowing the values of the diffusion coefficient and pinch velocity, one can test the prediction of the quasilinear theory for various \( q \)-profiles. Let us note that three terms contribute to the r.h.s. of Eq. (1): \(-\kappa_t \cdot (n_s \nabla \phi)\) which is related to curvature pinch, \(-\kappa_t \cdot (\nabla p_s / e_s)\), which is the thermodiffusion contribution, and the parallel compressibility term \(-\nabla_\parallel (n_s v_\parallel)\). Each of these three terms can be switched on or off in the numerical simulations for the impurity species (\( s = \z \)). It can be shown from quasilinear theory that switching on one of these terms, and the others off, provide the corresponding contribution to the pinch velocity. This gives a
way to compute numerically each contribution to the pinch velocity. Figure 2 shows the pinch velocity $V_z$ for each case. The total pinch velocity is labeled $V_z$, $V_{\perp cz}$ stands for the curvature pinch, the thermodiffusion pinch is $V_{\nabla T z}$, and the parallel compressibility pinch is noted $V_{\parallel cz}$. The pinch velocity $V_z$ is different for each pinch contribution. The curvature pinch velocity $V_{\perp cz}$ is the dominant contribution of the total pinch velocity $V_z$ as shown in Fig. 2, and is directed inward. The thermodiffusion pinch is $V_{\nabla T}$ is also directed inward and its intensity is small compared to $V_z$ and $V_{\perp cz}$. The parallel pinch velocity $V_{\parallel cz}$ is the smallest, and is directed outward. The total pinch velocity $V_z$ is directed inward, which leads to peaked impurity profile in the core. Let us note that other impurities behave basically the same.

5 Effect of a transport barrier on impurity transport

The impurity transport in two cases of the transport barriers have been performed, a reversed magnetic shear configuration and an external $E \times B$ shear flow.

5.1 Magnetic shear reversal

Simulations have been performed with reversed $q$-profiles as shown in Fig. 3. A strong barrier is created in the reversed magnetic shear case. The position of zero magnetic shear is $r/a = 0.55$. Steepening is found in the profiles of the ion temperature, the electron temperature, and the ion density. The main focus of this work is the dynamics in the “core” region. Figure 4 shows the radial profiles of various components of the pinch velocities in the core tokamak plasma. The barrier regions are defined as $0.45 < r/a < 0.62$ where the diffusion coefficient drops by approximately 50 percents from its peak value.

When the magnetic shear is negative, the direction of the curvature pinch velocity $V_{\perp cz}$ in the core region ($r/a < 0.45$) is opposite to the one obtained for monotonic $q$-profile, i.e., is in the outward direction as shown in Fig. 4. This is consistent with the quasilinear theory which predicts a curvature pinch proportional to $\nabla q/q$. The curvature pinch provides the main contribution to the total velocity so that the latter is mainly directed outward. In the barrier region ($0.45 < r/a < 0.62$), the turbulence intensity is small. Therefore, it is not expected
that quasilinear theory applies. It appears that the pinch velocity changes sign and is directed outward (inward) when magnetic shear is positive (negative).

The thermodiffusion pinch $V_{\nabla T_z}$ is negative for monotonic $q$-profile and reverses its sign when the magnetic shear is reversed as shown in Fig. 2 and 4. The parallel compressibility pinch $V_{\| c_z}$ behaves in the opposite way, i.e., is positive for monotonic $q$-profile and negative for reversed $q$-profile.

### 5.2 Externally imposed $E \times B$ velocity shear

Another way to produce a transport barrier is to impose an $E \times B$ velocity shear, which acts on the growth and radial extent of turbulent eddies in the plasma.

The radial profile of the safety factor $q$, the ion temperature, the electron temperature, and the ion density are plotted in Fig. 5. The safety factor is monotonic profile. The transport barrier is produced by externally imposed $E \times B$ shear flow at $r/a = 0.5$.

Figure 6 shows the radial profiles of (a) diffusion coefficients $D_z$ and (b) pinch velocities $V_z$ of the total pinch, the curvature pinch $V_{\perp c_z}$, the thermodiffusion pinch $V_{\nabla T_z}$, and the parallel compressibility pinch $V_{\parallel c_z}$ contributions. The barrier region is defined as $0.44 < r/a < 0.55$ as shown in Fig. 6(a). Figure 6 indicates that the total pinch velocity $V_z$ is shifted to be positive than the case of L-mode plasma which is shown in Fig. 2(b). The characteristics of the pinch velocities that contributes to the total pinch velocity are changed from the case of the L-mode plasma. When the external $E \times B$ velocity shear is induced, the direction of the curvature pinch velocity $V_{\perp c_z}$ in the core region ($r/a < 0.44$) is opposite to the one obtained for L-mode plasma (Fig. 2), i.e., is in the outward direction. The thermodiffusion pinch $V_{\nabla T_z}$ and the parallel compressibility pinch $V_{\parallel c_z}$ are negative (inward direction) in the core plasma. However, the total pinch velocity is shifted in the outward direction since the contribution of the curvature pinch has a positive sign. Therefore, the steady state radial profile of impurity density is hollow, as shown in Fig. 6(b). The interpretation of the mechanisms is explained in next section.
6 Interpretation of the simulation results

6.1 Reversed magnetic shear

When the magnetic shear is negative, the direction of the curvature pinch velocity $V_{\perp cz}$ is reversed and is directed outward. This is consistent with the quasilinear theory which predicts a curvature pinch proportional to $\nabla q/q$. The thermodiffusion pinch $V_{VTZ}$ is negative for monotonic $q$-profile and reverses its sign when the magnetic shear is reversed. The parallel compressibility pinch $V_{\parallel cz}$ behaves in the opposite way, i.e., is positive for monotonic $q$-profile and negative for reversed $q$-profile. This is consistent with the turbulence dominated by TEM for monotonic $q$-profile and by ITG modes for reversed $q$-profile. We observe that the results of Figs. 2 and 4 agree with the quasilinear prediction of Section 3. Hence the simulations agree with quasilinear theory predictions for all configurations. Moreover, it appears that the negative magnetic shear plays a favorable role in turbulent impurity transport as it leads to an impurity decontamination [12]. Note that this work does not include the neoclassical pinch which may be directed inward within the ITB.

6.2 Externally imposed $E \times B$ shear flow

The mechanism of the reversal of the curvature pinch is different from the reversal pinch velocity in the magnetic shear reversal. The pinch velocity is proportional to the magnetic shear, but it does not depend explicitly on the external imposed $E \times B$ shear velocity.

To identify the mechanisms underlying the pinch velocity, we have assumed that one mode is dominant, and that the following ordering holds $\omega_{ps}^* \gg \omega \gg \omega_{ds} \gg \omega_{||}$. For ITG/TEM modes, the growth rate scales as $\omega \sim \sqrt{\omega_{ps}^* \omega_{ds}}$. Furthermore, $\omega_{ps}^* > \omega_{ds}$ so that the inequality $\omega_{ps}^* \gg \omega \gg \omega_{ds}$ is satisfied. In the hydrodynamic regime, one has $\omega_{||}/\omega_{ds} \gg 1$. Hence this ordering is consistent with the interchange character of ITG/TEM turbulence and the fluid approximation.

In the presence of the external $E \times B$ shear velocity, the behavior of the pinch velocity changes dramatically. The nonlinear effects change the ordering in the frequencies in the process of the time integration. The simulations are performed to be self-consistent taking into account the changing of the ordering of the frequencies. The results of quasi-linear calculation indicate that the sign of pinch velocities agree with a new hierarchy $\zeta \omega_{dz} < \omega < 2\zeta \omega_{dz}$. Nevertheless, the reversal of the curvature pinch velocity remains less pronounced than for the negative magnetic shear case. This is consistent with the result shown in Fig. 6. The pinch velocities in the core plasma ($0.25 < r/a < 0.45$) follow the new ordering, i.e., the curvature pinch is directed outward while other pinch velocities are directed inward.

7 Conclusion

Impurity turbulent transport has been studied in configurations with positive and negative magnetic shear, in L-mode, reversed $q$-profile, and with external $E \times B$ shear flow. This has been done by developing a quasilinear theory that accounts for compressibility effects and thermodiffusion. In addition, 3D fluid simulations have been performed. This simulation
shows that the predictions of the quasilinear theory are robust. In particular it is found that the curvature pinch is the main component in monotonic $q$-profiles, hence leading to impurity peaking. However, transport barrier configuration leads to a reversal of the curvature pinch velocity which becomes outward. This is due to reversal of the curvature pinch velocity with the magnetic shear. Also, the sign of the thermodiffusion and parallel compressibility pinch velocities changes with the phase velocity of fluctuations i.e., depends on the underlying instability (ITG or TEM). These velocities are subdominant for monotonic $q$-profile, but play a significant role in the reversed $q$-profile. The reversal of pinch velocities is also found in monotonic $q$-profile plasma in presence of $\mathbf{E} \times \mathbf{B}$ shear flow. However, the mechanism is different from the one with reversed magnetic shear. The reversal of the curvature pinch is a consequence of the modification of the ordering of the frequencies. Consequently, the total pinch velocity is directed outward. This behavior is favorable for fusion plasmas since it expels the impurities from the core plasma. Hence, it appears that a transport barrier configuration is the main control parameter, which leads to a positive value of pinch velocities. This is favorable for the plasma decontamination in the core.

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