Effect of sonic poloidal flows in determining flow and density asymmetries for trace impurities in the tokamak edge pedestal

E. Fable, T. Pütterich, E. Viezzer, and the ASDEX Upgrade team
Max-Planck-Institut für Plasmaphysik, EURATOM Association, 85748 Garching, Germany
E-mail: emiliano.fable@ipp.mpg.de

Abstract. The structure of poloidal and toroidal flows of trace impurities in the edge pedestal of tokamak plasmas is studied analytically and numerically. Parallel momentum balance is analysed upon retaining the following terms: poloidal and toroidal centrifugal forces (inertia), pressure force, electric force, and the friction force. It is shown that, when the poloidal flow is such to produce a properly defined Mach number of order unity somewhere on the flux surface, shock fronts can form. The shock fronts can modify the predicted asymmetry structures in both the flow and the density profile along the poloidal arc. Predictions of the theory are shown against experimental observations in the ASDEX Upgrade tokamak, showing good qualitative and quantitative agreement if the inertia term associated with the poloidal flow is retained.
1. Introduction

Understanding the behaviour of impurities in the edge pedestal of tokamak H–modes is a fundamental requirement to be able to predict impurity penetration in the plasma core. The available theory, and it is referred here in particular to neoclassical theory, can very well predict flux–surface averaged transport fluxes and species poloidal flows and their relationship with the toroidal flow and the particle density, see for example [1] for a thorough review, and [2, 3] for more detailed calculations.

It is well known that flows and density equilibration on a flux surface are regulated by collisional processes (mainly friction for trace impurities) and strong damping of acoustic modes perturbations. However, the exact shape of the density and flow profile on the flux surface is not provided by standard neoclassical theory. Previous works in this direction have been produced, assuming dominant impurity–on–bulk ions friction [4], or rigid toroidal rotation of the whole plasma [5, 6]. In Ref. [4] in particular the outcome of the predicted flow and density poloidal profiles on the radial transport is discussed. However, previous works have not considered the inertial term in the parallel momentum balance. As it turns out and will be shown later on, that term is necessary when dealing with flows that can become super–sonic along the poloidal arc. In fact, standard neoclassical ordering breaks down for sonic flows, as in that case the perturbation to a ’global’ Maxwellian is of the same order of the equilibrium function.

Previous works on the impact of sonic poloidal flows on the bulk species behavior and on the magnetic equilibrium have been published [7, 8], however here the focus is on the impurities, while bulk species are assumed sub–sonic in flow speed. In this work it is shown, through both analytical and numerical calculations, how the poloidal structure of the flow and density of a trace impurity emerges by the interplay of inertia, friction, and the pressure and electric drive. Since the magnetic field acts effectively as a nozzle, it can be easily seen that static shock fronts can form as the poloidal Mach number, properly defined, goes through one. Peculiar of the toroidal plasma is that the nozzle is periodic and radially coupled, meaning that shock fronts at different poloidal positions appear at the different radial locations, implying that radial coupling and a three–dimensional flow structure can form around the shock fronts [9].

The present work has been inspired following charge exchange measurements [10, 11] and observations of poloidal asymmetries of impurity flows in the edge pedestal [12, 13, 14] in the ASDEX Upgrade (AUG) tokamak. Observations on other machines have been reported as well, see e.g. [15].

The manuscript is organized as follows: in section 2 the main assumptions and equations are introduced. In section 3 the main results are derived analytically. In section 4 numerical examples are computed and qualitatively compared to experimental observations. Section 5 draws the conclusions.
2. Main assumptions and equations

2.1. Some definitions and assumptions

The background magnetic field is defined by its toroidal component $B_\phi = FR$ (F being the diamagnetic flux function and $R$ the local major radius) and its poloidal component $B_\theta = |\nabla \psi|/R$, where $\psi$ is the poloidal magnetic flux and $R$ is the local major radius. An appropriate coordinate system is defined as the triplet $(\psi, \theta, \phi)$, with $\theta, \phi$ respectively the poloidal and toroidal angle (with $\theta$ increasing upwards from the outboard side and $\phi$ increasing clockwise when the torus is viewed from above). The actual signs of the fields are also introduced: $\sigma_\phi, \sigma_\theta$ respectively for the toroidal and the poloidal field. As such in the following it assumed strictly that $B_\phi, B_\theta > 0$, while the signs are explicited in the equations through $\sigma_s$. A reference location on the poloidal angle is chosen as $\theta = 0$, the outboard mid–plane position, and will be identified in the following with the pedix $'L'$, while the inboard mid–plane position on the high field side will be identified with the pedix $'H'$. The usual flux–surface–average (FSA) is defined as $\langle f \rangle = \partial/\partial V \int f dV$, where $V$ is the plasma volume enclosed by the local flux surface. It is reminded a basic property of the FSA: $\langle B \cdot \nabla f \rangle = 0$.

The main ion species Mach number is defined as $M_{a,i} = |U_i|/v_{th}^i$, with $U_i$ the species flow and $v_{th}^i = \sqrt{T_i/M_i}$ the species thermal speed. The impurity Mach number is defined as $M_{a,Z} = |U_Z|/v_{th}^Z$, with $U_Z$ the impurity velocity and $v_{th}^Z = \sqrt{T_i/M_Z}$ the impurity thermal speed. In the following it is assumed that bulk ions are strongly subsonic, $M_{a,i} \ll 1$, while there is no limit to the speed at which the trace impurities can rotate.

It is now clarified what is the definition of ‘trace’ as used in the following for the impurities: it is assumed that $Zn_Z \ll n_i$, where $n_Z$ is the impurity density and $n_i$ the main ions density. This means that the background geometry and electrostatic potential are determined by the bulk species only. On the other hand, to be able to treat the impurities in a fluid context, it is assumed that the parallel Knudsen number, defined as $K_{n,||} = v_{th}^Z/(Rq\nu_{ZZ}) < 1$, with $\nu_{ZZ}$ the impurity self–collisional frequency and $Rq$ the parallel connection length. Also, the Knudsen number associated to the impurity–ion collisions is given by $K_{n,||,Z} = v_{th}^i/(Rq\nu_{Zi}) < 1$. Both Knudsen numbers being below unity, means that the impurity distribution function can be represented as a local Maxwellian, which describes an isotropic pressure tensor, and for which the parallel fluid flow will be influenced mostly by friction with the bulk ions.

Finally, it is assumed that the ions species temperature is a flux function, $T_i = T_i(\psi)$, while the impurity density can acquire poloidal dependence. The main ion density is assumed to be a flux function as well, since it is considered here a situation in which $M_{a,i} \ll 1$.

In the remainder, the pedix $Z$ characterizing the impurity species is implicitly assumed for density, temperature, and velocities. It will be explicited when needed (e.g. for main ions or electrons).
2.2. Particle continuity equation for the impurity

The particle continuity equation is written (for impurity species) as:

$$ \nabla \cdot (nU) = 0 \quad (1) $$

where the $\partial/\partial t$ term is neglected (it is of the order of the cross-field flow). The flow is predominantly on a flux surface, i.e. $|U \cdot e_\psi| \ll |U|$. In this case equation (1) reduces to the well known poloidal dependence of the poloidal flow component $U_\theta$:

$$ U_\theta(\psi, \theta) = K(\psi) \frac{B_\phi(\psi, \theta)}{n(\psi, \theta)} \quad (2) $$

where $K$ is a yet to be determined flux function. Working on the general velocity expression $U = U_\parallel b + U_\perp = U_\phi e_\phi + U_\theta e_p$, one finds the toroidal and parallel velocity components expressed as:

$$ U_\phi = \sigma_\phi \sigma_\theta K \frac{B_\phi}{n} + \sigma_\theta R \Omega $$

$$ U_\parallel = \sigma_\theta K \frac{B}{n} + \sigma_\theta \sigma_\phi F \Omega $$ \quad (3)

with $\Omega = -\partial \Phi_0 / \partial \psi$ the rigid rotator speed. Note that it is assumed here an 'ideal-like' Ohm’s law $E + U \times B = 0$, with $E = -\nabla \Phi_0$. The diamagnetic term $\propto \nabla P/(Zn)$ is neglected at this stage. As such the electric field is computed from the known flow velocities at one specific poloidal position. The role of the diamagnetic flow will not be investigated further and is left for future work. The zero–order electrostatic potential $\Phi_0(\psi)$ is a flux function. As such also $\Omega$ is a flux function. A relation between $K$ and the FSA parallel velocity can also be found:

$$ K = \sigma_\theta \frac{\langle BU_\parallel \rangle}{\langle B^2/n \rangle} - \sigma_\phi \frac{F \Omega}{\langle B^2/n \rangle} \quad (4) $$

Note that a pure toroidal flow can be sustained by choosing $\langle BU_\parallel \rangle = \sigma_\theta \sigma_\phi F \Omega$, however a poloidal flow is always accompanied by a toroidal flow with in–out asymmetries (Pfirsch–Schlütter flow).

2.3. Parallel force balance for impurities

The parallel force balance equation is simply:

$$ MnB \cdot [(U \cdot \nabla) U] = -TB \nabla \parallel n - Zn B \nabla \parallel \Phi + B \mathcal{F}_\parallel \quad (5) $$

where the self–viscous term and the inductive electric force are neglected, the first for the trace assumption, the second since most H–modes work at low edge loop voltage. $\mathcal{F}_\parallel$ is the parallel component of the friction force, which is considered between the impurity and the main ions only:

$$ \mathcal{F}_\parallel = -Mn\nu_{Zi}(U_\parallel - U_{i,\parallel}) \quad (6) $$

where $\nu_{Zi}$ is the impurity–to–main ions collisional frequency. The poloidally varying potential $\Phi$ is assumed as a small perturbation with respect to the dominant one $\Phi_0$. 

The inertial term, i.e. the first term on the left–hand–side of equation (5), can be manipulated as 
\((\mathbf{U} \cdot \nabla) \mathbf{U} = \nabla \left( \frac{U^2}{2} \right) - \mathbf{U} \times (\nabla \times \mathbf{U})\). Upon substituting formulas (3), after some algebra, the following equation is obtained:

\[
\mathbf{M} \mathbf{B} \cdot \nabla \left( \frac{K^2 B^2}{n^2} - R^2 \Omega^2 - \mathbf{M} \nu_{Zi} B(U - U_i) \right) = -TB\nabla|\log n - ZB\nabla|\tilde{\Phi} - \mathbf{M} \nu_{Zi} Z_i B(U - U_i) \quad (7)
\]

As a remark, notice that the collisional frequency, being \(\nu_{Zi} \propto n_i/T^{3/2}\), is a flux function. This fact allows to compute the averaged parallel velocity from the FSA of equation (7) simply as: \(\langle BU \rangle = a_U = \langle BU_i \rangle\), leading to \(K = \frac{\sigma_\phi a_U - \sigma_\phi F\Omega}{\langle B^2/n \rangle}\). The main ions averaged parallel flow term \(a_U\) is computed using information from the flow profiles obtained at one specific poloidal location of reference.

Equation (7) is finally recast in Bernoulli–like form \(v_{th} = \sqrt{T/M}\):

\[
\mathbf{B} \cdot \nabla \left[ \frac{K^2 B^2}{n^2} - R^2 \Omega^2 + 2v_{th}^2 \left( \log n + \frac{Z\tilde{\Phi}}{T} \right) \right] = -2\nu_{Zi} B(U - U_i) \quad (8)
\]

2.4. Pfirsch–Schlueter \(\tilde{\Phi}_{PS}\) and centrifugal potential \(\tilde{\Phi}_\omega\)

To evaluate the source \(\tilde{\Phi}\), to enter in equation (8), it is first followed Ref. [16], which deals with the Pfirsch–Schlüter potential, leading to:

\[
\tilde{\Phi}_{PS} = \sigma_\phi \eta F P' \int_L^l \frac{dl}{B_\theta} \left( 1 - \frac{1}{g_3 R^2} \right) \quad (9)
\]

Since \(P'\) is negative, and at the LFS both \(B_\theta\) is smaller and \((g_3 - 1/R^2)\) is positive, it turns out that \(\tilde{\Phi}\) is negative at the HFS equatorial mid–plane.

In addition, one can also include the centrifugal potential [6], which is given by

\[
\tilde{\Phi}_\omega = \frac{1}{4} \frac{\omega^2 R_L^2}{v_{th}^2} \left( \frac{R^2}{R_L^2} - 1 \right) \quad (10)
\]

where \(\omega\) is the toroidal angular rotation frequency of the main ions. The resulting potential perturbation is thus \(\tilde{\Phi} = \tilde{\Phi}_{PS} + \tilde{\Phi}_\omega\).

2.5. Phenomenological diffusion

It is shown in the next section that equation (8) can develop shock fronts [8]. Since along the radial direction, these shocks appear at different poloidal locations (basically the shock front poloidal location is determined by the density and the collisionality), it is expected that a smooth structure finally is sustained [9]. Note that gyrokinetic turbulence is not a candidate here since turbulence structures are of the order of the Larmor radius. On the other hand, parallel transport due to free streaming can also smooth the shock front.
2.6. Consistency with the gyrokinetic equilibrium

It is now shown that equation (5) can be derived from the equilibrium gyrokinetic equation, demonstrating its consistency. The gyrokinetic equation for the impurity equilibrium distribution function $F$ is:

$$\nabla \cdot \left[ (v_{\parallel} b + v_E) BF \right] + \frac{\partial}{\partial v_{\parallel}} \left( \dot{v}_{\parallel} BF \right) = C$$

(11)

where $v_E = E \times B / B^2$, $E = -\nabla \Phi_0$, and $C$ is the collision operator. All terms inversely proportional to the charge $Z$ have been neglected (i.e. the curvature and centrifugal drifts). The parallel acceleration is given by: $\dot{v}_{\parallel} = -\mu b \cdot \nabla B - Z e / M b \cdot \nabla \Phi + v_{\parallel} \frac{v_E \cdot \nabla B}{B} + v_E \cdot (v_E \cdot \nabla) b$, where it is important to retain both terms involving $v_E$. The distribution function $F$ is assumed as an isotropic local Maxwellian $F \propto n e^{-0.5(\nu_1 - U_{\parallel})^2 - \mu B}$ and for reference it is set (mass, temperature) $M = T = 1$.

First integration of the equation in velocity space $\int d\mu d\nu_{\parallel}$ leads to the continuity equation $\nabla \cdot (n U_{\parallel} b + n v_E) = 0$. Then, integrating with $\int v_{\parallel} d\mu d\nu_{\parallel}$ leads to the parallel force balance equation:

$$\nabla \cdot \left( n U_{\parallel} ^2 b + nb + n U_{\parallel} v_E \right) +$$

$$\frac{n}{B} b \cdot \nabla B + Z nb \cdot \nabla \Phi - n U_{\parallel} \frac{v_E \cdot \nabla B}{B} - n v_E \cdot (v_E \cdot \nabla) b = R_{\parallel}$$

(12)

where $R_{\parallel}$ is the parallel friction term. After some algebra it is finally found that equation (12) coincides with equation (5), where the relevant identity $v_E \cdot (v_E \cdot \nabla) b = b \cdot \nabla \left( \frac{R^2 \Omega^2 B_{\theta}^2}{2 B^2} \right)$ has been derived.

3. Poloidal flow structure and density distribution of the trace impurity

Equation (5) is now studied in detail by first putting it into dimensionless form as:

$$\frac{\partial}{\partial x} \left[ \alpha f^2 - r^2 + \beta (\gamma - \log f) \right] = v_1 + v_2 f + \mu \frac{\partial^2 f}{\partial x^2}$$

(13)

where the unknown $f = \langle B^2 / n \rangle^{-1} B^2 / n$, and the other parameters are defined as: $\alpha = K \langle B^2 / n \rangle / (2 B^2 v_{th})$, $r = R^2 \Omega^2 \langle 2 K \langle B^2 / n \rangle \rangle$, $\beta = v_{th} / (K \langle B^2 / n \rangle)$, $\gamma = \log B^2 + Z \Phi / T$, $v_1 = \delta (\sigma_{\theta U} B^2 - \sigma_{\theta} F \Omega B_{\theta}^2) / \langle B^2 \rangle$, $v_2 = -\delta (\sigma_{\theta U} - \sigma_{\theta} F \Omega) / (K \langle B^2 / n \rangle)$, $\delta = R_{\perp} \nu_{\theta} / (B_{\theta} v_{th})$. The choice of the independent variable $f$ is such that $\langle f \rangle = 1$ is an automatic constraint of the problem, additionally to $f$ being periodic in $x$ after one poloidal turn. The coordinate $x$ is defined such that $dx = d\theta / (R_L |\nabla \theta|)$. The physical meaning of the different terms is respectively: (left–hand–side) poloidal centrifugal energy, toroidal centrifugal energy, nozzle striction effect from magnetic field and electric potential energy, pressure drive, (right–hand–side) friction breaking from toroidal and poloidal rotation of the main ions, and finally the phenomenological diffusion term.

The mathematical structure of equation (13) is that of a viscous Burger equation with external forcing, while the case $\mu = 0$ is equivalent to the inviscid Burger equation with additional linear contributions. The latter, inviscid limit, can be rewritten very
Impurity flow structure in the tokamak edge pedestal

compactly as \((2\alpha f^2 - \beta) \frac{\partial f}{\partial x} + af^3 + bf^2 + cf = d\). The latter form shows clearly that a singularity in the equation appears when \(f = \sqrt{\beta/(2\alpha)}\), except if, at the same time, for said value of \(f\), \(af^3 + bf^2 + cf - d = 0\). In principle such a location, where \(\frac{\partial f}{\partial x}\) is finite despite its coefficient vanishing, exists along the poloidal arc. On the other hand, because the system is periodic, there has to be another location at which both conditions will not be satisfied. This results in a shock front appearing, producing a finite jump in \(f\), i.e. in density, poloidal and toroidal flow. This phenomenon will always appear as soon as a location where \(f = \sqrt{\beta/(2\alpha)}\) is present. Note that said condition is physically the fact that the Mach number associated with the quantity \(U_\theta B/B_\theta\) is unity. In usual H–mode edge plasmas such Mach numbers can be easily reached for the impurities, which are not subject to poloidal flow damping when being in trace concentration.

As example of analytical limits of equation (13), consider the cases \(\beta \gg \alpha\) and low collisionality, then one obtains \(f \sim B^2\), which results in the density \(n\) being a flux function. Another case is when the toroidal centrifugal term \(r\) is dominant, leading to the well known outboard impurity accumulation [6]. The limit of infinite collisionality as studied in [4], leads to \(f = 1\), i.e. \(n \sim B^2\), which provides inboard impurity accumulation. The limit found when, neglecting collisions, \(\alpha \gg \beta\), leads again to \(f \approx 1\), i.e. \(n \approx B^2\). In this respect a super–sonic collisionless flow and a strongly collisional flow are indistinguishable from the point of view of the density poloidal distribution. On the other hand, when \(\alpha \sim \beta\), with or without collisions, a peculiar structure appears, i.e. the shock front, which has observable characteristics. Realistically most edge H–mode plasmas are in this regime of mixed transonic–collisional flow where all terms in equation (13) are important.

4. Numerical applications and comparison with experimental observations

Equation (13) is solved numerically by employing a numerical scheme based on 'convergent time evolution', i.e. adding a time derivative term on the left–hand–side and make it relax through numerical diffusion, and spatially by using upwind Euler scheme which is automatically stable for large flow velocities, however it has intrinsic numerical diffusion. The upwind Euler scheme nicely resolves the static shock front and automatically stabilizes the artificial 'sound' waves generated by the convective non–linearity. Iterations are also employed to solve for the unknown term \(\langle B^2/n \rangle\). The time step is chosen to reach steady–state and the spatial grid is sufficiently large to resolve the poloidal structures and the diffusion layer (of the order of \(\sqrt{\mu}\)). The numerical scheme has been validated by benchmarking against analytical expressions of the equation in different limits and by checking conservation of \(\langle f \rangle = 1\).

The input profiles are taken from charge exchange measurements of both LFS and HFS poloidal and toroidal rotation in ASDEX Upgrade [11], for boron B\(^{5+}\). Also the LFS impurity density and temperature are measured and used as input. The values of \(a_U\) and \(\Omega\) are computed from the measured flow velocities, while the deuterium
density, relevant for the impurity–ion collisionality, is taken as having the same impurity density profile, but rescaled such that the pedestal top value matches the one from the experimentally measured electron density. The magnetic fields are taken from the equilibrium reconstruction code CLISTE [17]. Note that in the standard magnetic configuration of AUG $\sigma_\phi = +1, \sigma_\theta = -1$. Profiles of the input quantities can be found in figure 1(a,b,c). In figure 1(a), a modified poloidal velocity is also used (dot–dashed line), which has constant velocity from the position of the maximum ($\rho_\phi \approx 0.99$) up to the separatrix. The reason for using this modified velocity profile is to somewhat consider eventual uncertainties in separatrix position with respect to the rotation measurements and in experimental uncertainties.

In figures 2, 3, and 4 the results of the calculations are shown, where in subplots (a) the inertia term proportional to $\alpha$ and $r$, as well as diffusion, are set to zero, whereas in subplots (b) the equation is solved in its entirety. Here the viscosity parameter is chosen of the order of $\mu \approx 0.01$, which does not disturb the resulting profiles but helps in smoothing the shock front. At present the exact value of $\mu$ can not be determined from principles, thus requiring in future to perform global simulations as for example proposed in Ref. [20]. Notice that in figure 2(c), the modified poloidal velocity of figure 1(a) has been employed. In figure 3(c) the poloidal distribution of the resulting toroidal flow is also shown, for the case with all terms retained in the numerical calculation.

From the results displayed in the figures, several points can be clarified:

1. while the friction force alone can give a reasonable agreement in the poloidal flow asymmetry (not shown), it fails in reproducing the toroidal flow asymmetry, as can be seen in figure 2(a);
2. the ”poloidal” centrifugal force, at Mach of order unity, provides that additional poloidal structure that leads to matching both the poloidal and toroidal flow radial variations on LFS and HFS, as can be seen from figure 2(b,c). Notice also that the LFS value of the poloidal flow regulates the behavior of the toroidal flow asymmetry, as when the former quantity drops, also the latter behave differently, as comparing figure 2(b) and figure 2(c);
3. there is a strong indication that at the top of the plasma the toroidal flow has reversed direction with respect to both LFS and HFS, as can be seen in figure 3(c). This is a testable prediction of the calculations presented here;
4. smoothing of the shock structure is essential, as seen in comparing figure 4(a) and figure 4(b).

5. Conclusions

The poloidal structure of flows and density of trace impurities is studied by employing parallel momentum balance and retaining the non–linear convective (or inertial) terms that produce additional effects with respect to previous results [4, 6]. In particular the non–linear term arising from the poloidal flow is necessary to properly introduce shock fronts and poloidal shock structures that drastically change the resulting impurity
density profiles when the associated flow goes from sub to super-sonic along the poloidal arc.

The findings reported here show that it should be rather generic, in the H-mode edge, for these structures to exist since trace impurities can be strongly accelerated in the poloidal direction by the background electric field even in the absence of average parallel rotation of the main ions. A remark has to be made with respect to the type of impurity, since the effects presented here should be valid for low and moderate-Z impurities, while for high-Z impurities the role of the poloidally asymmetric potential and of the toroidal centrifugal force could become important and modify the outcome [18, 19].

Comparison of the discussed theory against experimental observations in ASDEX Upgrade is showing that all terms are important to reproduce the observed flow structures, at least on the LFS and HFS. Measurements on the top of the plasma should provide a key answer since the shock front will deeply influence the LFS-top-HFS profile.

Additional effects that can play a role in the pedestal and are not considered here are: diamagnetic flow, local sources, orbit loss, global effects, application of localized radio-frequency heating. It is expected that the orbit loss mechanism in particular would be important since the pedestal region has a width which is usually of the order of the impurity poloidal Larmor radius, as well as global effects [20].

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Impurity flow structure in the tokamak edge pedestal

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Figure 1. Radial profiles with error bars, on the \( \rho_\psi \) coordinate, of experimentally measured (a) LFS poloidal rotation \( U_\theta \) (solid), HFS poloidal rotation (dashed), and (b) LFS (dashed) and HFS (dashed) toroidal rotation \( U_\phi \); (c) LFS impurity density. In subplot (a), the dot–dashed line is the poloidal velocity, modified such that the value stays constant from the position of maximum value up to the separatrix. This example is taken from ELMy H–mode AUG discharge #28093.
Figure 2. (a) Comparison of radial profiles of LFS and HFS toroidal rotation for the case with $\alpha = \mu = 0$; (b) same comparison but including all terms; (c) same comparison but here the input poloidal rotation profile has a constant value from the position of the maximum velocity ($\rho_\psi \approx 0.99$) up to the separatrix.
Figure 3. (a) Poloidal variation of impurity density for different radial locations (in legend) for the case with $\alpha = \mu = 0$; (b) same plot but with all terms included; (c) Poloidal distribution of the toroidal rotation profile for different radial locations (in legend), case with all terms included.
Figure 4. (a) Poloidal variation of Mach number when both friction and viscosity are neglected for three radial locations (in legend); (b) same plot but with all terms included.