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Fundamentals of and Recent Advances in the Theory and Simulation of the Magnetised Plasma-Wall transition (MPWT)*

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1. INTRODUCTION
What is the Magnetised Plasma-Wall Transition (MPWT)?

- If a plasma is bounded by some material wall, a complexly structured region termed "plasma-wall transition (PWT)" forms between the unperturbed (bulk) plasma and the wall.
- If, as in the case of a tokamak, a magnetic field oblique or parallel to the wall is present, we speak of a “magnetised plasma-wall transition (MPWT)”
The mandatory next step: ITER

- The name ITER stands for “International Thermonuclear Experimental Reactor” or (Latin) “The way (to fusion)”
- ITER is a reactor-scale tokamak test facility which will eventually produce > 500 MW of fusion power.
- ITER is being built at Cadarache, France, and scheduled to start operation in about 10 years from now.
- The ITER project is supported by a consortium of countries representing more than half of the world's population (EU, Japan, USA, Russia, China, South Korea, and India, with more countries likely to join along the way).
Recent ITER Design
(From ITER homepage)

ITER Tokamak Cutaway
(Dec. 2006)
S. Kuhn et al., Trieste, 23 July 2008

Nested Poloidal Flux Surfaces
in ITER Nominal Configuration
(2001)
Structure of the tokamak discharge in terms of regions/subsystems:

- Core
- Core to SOL transition (pedestal), including Last closed magnetic surface (LCMS, separatrix)
- Bulk SOL
- SOL - divertor PWT
- Divertors
- SOL - first wall transition (outer or far SOL)
- First wall
- Private region
- External circuits and systems!
The need for *predictive* tokamak modelling

- Challenges and costs of fusion research are enormous: 50 years of fusion research already, ITER project costs € 10 billion.
- Hence, understanding and optimising the ITER discharge to the maximum extent possible is mandatory even before ITER will start operating.
- This requires, on the one hand, careful exploitation and evaluation of present-day tokamak experiments (JET in Culham, UK, and ASDEX Upgrade in Garching, Germany, and many others).
- On the other hand, the inherent nonlinearity of plasma behaviour rules out simple extrapolation of these experimental results to a significantly larger device like ITER, so that a massive *theoretical and numerical* ("modelling") effort aimed at *predicting* the behaviour of ITER is indispensable as well.
Predictive tokamak modelling must be integrated!!

- Like any other plasma device, the tokamak is a "globally self-consistent" dynamical system, i.e., all of its subregions interact simultaneously with, rather than evolving independently of, each other.

- **Basic postulate:** any modelling effort aiming at realistically and reliably predicting the overall performance of a tokamak discharge must be integrated in the sense that it correctly and simultaneously describes not only the subregions themselves but their mutual interactions as well.

- **In contrast,** the conventional “regional” approach to tokamak modelling has widely been to treat relevant subregions (such as the core) or groups of subregions (such as the SOL), as separate entities, leading to uncertainties primarily with respect to their coupling.
Some implications of Integrated Tokamak Modelling (ITM)

• The integrated-modelling “philosophy” was officially adopted by the EU’s Fusion Programme by the setting up of the EU's Integrated Modelling Task Force (ITM TF) in 2003.

• Goal of the ITM TF: create a complete “numerical tokamak” within the next 10 years or so.

• To summarise: With respect to the physics and numerics involved, ITM requires both correct/improved descriptions of the various subregions themselves plus, as the essential new ingredient, correct treatment of the coupling between them.

• Beyond this technical aspect, ITM in addition offers an encouraging perspective for all fusion groups and scientists to collaborate in and contribute to fusion research in a more coordinated and concrete manner than may have been possible hitherto:

• Development of “modules” for the numerical tokamak!
What does the our present subject (MPWT) have to do with this?

- The SOL-divertor MPWT couples the bulk SOL with the divertor plates.
- The entire SOL couples the core-SOL transition (pedestal) region to the divertor plates.
- Hence, our results are modules which should eventually be implemented in the numerical tokamak.
- Note however: Implementation of modules in the numerical tokamak require personal involvement and initiative of the authors!
2. GENERAL STRUCTURE OF THE MPWT
GENERAL STRUCTURE OF THE MAGNETIZED PLASMA-WALL TRANSITION (PWT)

Magnetic field oblique to the wall

- The magnetized plasma-wall transition is a crucial element in overall tokamak behavior.
- Understanding it is of utmost importance to tokamak modeling and operation.
- The vast majority of existing plasma-wall transition models is of an approximate character.
- Better understanding contributes to more accurate simulations, especially via improved fluid boundary conditions.

```
<table>
<thead>
<tr>
<th>Unperturbed plasma</th>
<th>Collisional presheath</th>
<th>Magnetic presheath</th>
<th>Debye sheath</th>
</tr>
</thead>
<tbody>
<tr>
<td>BCs</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>
```

Scale lengths:

\[ l_c \leq l_i \sim \rho_i \sim \lambda_D \]
The magnetized PWT, more physical view
(from Stangeby, 2000)
3. CLASSICAL STUDIES OF THE MAGNETIZED PWT

3.1 Riemann’s fluid model of the entire magnetized presheath
(not splitting up a priori!)


Considering a time-independent plasma consisting of electrons and one species of singly charged ions
Basic equations

ion continuity equation
\[ \nabla \cdot (n_i u) = 0 \]
ion momentum equation
\[ m_i (u \cdot \nabla) u = e \{ E + u \times B \} - \frac{1}{n_i} \nabla p_i - \nu_c m_i u \]
ion polytropic law
\[ \nabla p_i = \gamma k T \nabla n_i \]
with polytropic coefficients
\[ \gamma = 1, \quad \gamma = 5/3, \quad \gamma = 3 \]
Boltzmann-distributed electrons
\[ n_e = n_s \exp \left( \frac{e \varphi}{k T_e} \right). \]
electric field definition
\[ E = -\nabla \varphi \]
quasineutrality
\[ n_i = n_e \]

Scaling assumptions

Asymptotic 3-scale approximation
\[ \lambda_D \ll \rho_i \ll l_c \]
\[ \Rightarrow \] Debye sheath \[ \Rightarrow \] non-neutral, \( \sim \) collisionless
\[ \Rightarrow \] Magnetic presheath \[ \Rightarrow \] \( \sim \) quasineutral, \( \sim \) collisionless
\[ \Rightarrow \] Collisional presheath \[ \Rightarrow \] \( \sim \) quasineutral, collisional
Magnetic field lies in x-z plane

ion gyrofrequency vector:

\[ \omega = \frac{e}{m_i} B \]
Component equations

The problem basically reduces to solving the 3 equations for $v_x$, $v_y$ and $v_z$.

The ion continuity equation

$$n_i u_z = n_s u_s$$

with $s$ referring to the “sheath edge,” to be defined below.

$x$ component of ion mom. eq.

$$v_z \frac{du_x}{dz} = \omega_z u_y - v_c u_x$$

$y$ component of ion mom. eq.

$$v_z \frac{du_y}{dz} = \omega_x u_z - \omega_z u_x - v_c u_y$$

$z$ component of ion mom. eq.

$$\frac{du_z}{dz} = (-\omega_x u_y - v_c u_z) \frac{u_z}{u_z^2 - c^2}$$

with $c$ the ion sound velocity

$$c = \left[ k(T_e + \gamma T_i)/m_i \right]^{1/2}$$

and the gyrofrequency comp's

$$\omega_x = \frac{e}{m_i} B \cos \alpha, \quad \omega_y = 0$$

$$\omega_z = \frac{e}{m_i} B \sin \alpha$$

Quasineutrality + Boltzmann electrons + ion continuity

$$\Rightarrow \quad \varphi = \frac{k T_e}{e} \ln \frac{u_z}{u_s}.$$
Sheath edge singularity and Bohm criterion

Clearly, a singularity \( \frac{du_z}{dz} \to \infty \) ("sheath edge singularity") occurs for \( u_z = c \) ("marginal Bohm criterion")

This position marks the breakdown of the quasineutral approximation and may be interpreted as the sheath (entrance) as seen on the presheath scale, so we may set \( u_s = c \).
Normalized parameters and variables

- Magnetic field inclination: \( \delta = \tan \alpha = \frac{\omega_z}{\omega_x} \)
- Collision frequency: \( \nu = \frac{v_c}{\omega_x} \)
- Position variable: \( \zeta = \frac{z}{\rho_i} = \frac{\omega_x}{c} z \)
- Potential: \( \chi = -\frac{e\phi}{kT_e} \)
- Ion velocity components: \( u = \frac{u_z}{c}, \quad v = \frac{u_y}{c}, \quad w = \frac{u_x}{c} \)

Geometry & collisionality assumptions:
- Small inclination angle: \( \omega_x \gg \omega_z \iff \delta \ll 1 \)
- Strongly magnetized: \( \omega_x \gg v_c \iff v \ll 1 \)
Normalized component equations

\[ u_x \text{ equation} \quad u \frac{dw}{d\zeta} = \delta v - \nu w, \]
\[ u_y \text{ equation} \quad u \frac{dv}{d\zeta} = u - \delta w - \nu v, \]
\[ u_z \text{ equation} \quad \frac{du}{d\zeta} = (-\nu - \nu u_z) \frac{u}{u^2 - 1} \]

quasineutrality \( \chi = \ln u \).

Only two dimensionless parameters: \( \delta, \nu \)
Solve \( u_x, u_y \) and \( u_z \) equations first, then find potential \( \chi \)
Bohm criterion now reads \( u = 1 \)
Numerical solutions of normalized component equations: Potential profiles*

FIG. 2. Potential profiles $\ln(v_x/c_s) = -eU/kT_e$ for $\delta = \tan \alpha = 0.01$ and various values of $v = v_x/\omega_x$; $p_i = c_s/\omega_x$. Broken lines: B, Behnel's approach ($\alpha = 0$, $v = v_x/\omega_x = 0.03$); C, Chodura's approach ($v = 0$, $c = v_{\parallel}/c_s = 1$, see Sec. III).

*From Riemann, 1994
Numerical solutions of normalized component equations: $v_x$ profiles*

*From Riemann, 1994

FIG. 3. Velocity component $v_x$ (approximately the B direction) for $\delta=\tan \alpha=0.01$ and various values of $v=v_c/\omega_x$; $\rho_i=c_s/\omega_x$.
Numerical solutions of normalized component equations: $v_y$ profiles*

*From Riemann, 1994

FIG. 4. Velocity component $v_y$ (the $E \times B$ direction) for $\delta = \tan \alpha = 0.01$ and various values of $\nu = v_c/\omega_x$; $\rho_i = c_i/\omega_x$. 

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2. CLASSICAL STUDIES OF THE MAGNETIZED PWT

3.2 Chodura’s fluid model of the collisionless magnetic presheath


Special case of Riemann’s model of Sec. 2.1:

\[ \nu \equiv \frac{\nu_c}{\omega_x} \rightarrow 0 \]

Simplest possible model: quasineutral and collisionless.
Hence most basic reference case!
Normalized component equations

Noncollisionality \( v = 0 \)

\[ u \frac{d\nu}{d\zeta} = \delta v \]

\( u_\xi \) equation \[ u \frac{dv}{d\zeta} = u - \delta w \]

\( u_\zeta \) equation \[ \frac{du}{d\zeta} = \frac{-u \, v}{u^2 - 1} \]

Quasineutrality \( \chi = \ln u \)

From the \( u_\xi, u_\eta, u_\zeta \) equations we find

Energy conservation \( u^2 + v^2 + w^2 = 2 \ln \frac{u}{u_0} + C^2. \)

Where for \( \zeta \to -\infty \)

\[ u \to u_0 = C \sin \alpha \]

\[ w \to w_0 = C \cos \alpha, \quad v \to 0 \]
Eliminating $v$ and $w$ we find the following differential equation for $u$ only:

$$\left(\frac{1-u^2}{u}\right)^2 u'^2 = f(u)$$

where $f(u) = C^2 + 2\ln\frac{u}{u_0} - u^2 - \left[\frac{C + 1/C}{\cos\alpha} - \delta(u + \frac{1}{u})\right]^2$

This equation is found to have physical solutions only for

$$C \geq 1 \iff u^B \geq c \iff u_z \geq c \sin \alpha$$

This condition is called the **Bohm-Chodura condition**. It represents an important boundary condition at the magnetic presheath entrance and is usually applied in its marginal form:

$$u^B_i = C$$
Summary: In the simplest magnetic presheath model (Chodura's fluid model: quasineutral and collisionless), the magnetic presheath is usually defined by the clear-cut boundary conditions

\[ \mathbf{u}_i \parallel B = C \]  
(Bohm-Chodura condition)

at the magnetic presheath entrance, and

\[ \mathbf{u}_i \perp w = C \]  
(Bohm condition)

At the Debye sheath entrance.

For more realistic situations, the usefulness and validity of these boundary conditions must be critically questioned and discussed!
4. COMPREHENSIVE ANALYTIC STUDY OF THE MPWT


GENERAL STRUCTURE OF THE MAGNETIZED PLASMA-WALL TRANSITION (PWT)

Magnetic field oblique to the wall

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- Understanding it is of utmost importance to tokamak modeling and operation.
- The vast majority of existing plasma-wall transition models is of an approximate character.
- Better understanding contributes to more accurate simulations, especially via improved fluid boundary conditions.

**Scale lengths:**

\[ \leq l_c \sim \rho_i \sim \lambda_D \]
4.1. The asymptotic three-scale limit

The “asymptotic three-scale limit” is defined by the extreme ordering

$$\lambda_D \ll \rho_i \ll \lambda_c$$

i.e.

$$\varepsilon_{Dm} = \frac{\lambda_D}{\rho_i} \to 0 \quad \text{and} \quad \varepsilon_{mc} = \frac{\rho_i}{\lambda_c} \to 0$$

In this limit, the three subregions of the MPWT can be characterized as follows:

Debye sheath (DS): non-neutral, unmagnetised, collisionless
Magnetic presheath (MPS): quasi-neutral, magnetised, collisionless
Collisional presheath (CPS): quasi-neutral, strongly magnetised, collisional

These characterisations break down at

- the DS-MPS transition (DS entrance)
- the MPS-CPS transition (MPS entrance)

These transition regions have for the first time been investigated in detail.
4.2. Model and basic equations

The uniform magnetic field is assumed to lie in the $xz$-plane, making a small angle $\alpha$ with the wall.

$$T_i \to 0, \quad n_e = n_0 \exp(e\Phi / kT_e).$$

In the dimensionless variables

$$\left( \frac{v_z}{c_s} \right) \Rightarrow u, \quad \left( -e\Phi / kT_e \right) \Rightarrow \varphi,$$

$$\left( \frac{n_i}{n_0} \right) \Rightarrow n, \quad \left( \frac{c_s}{\omega_c} \right) \Rightarrow \rho,$$

the basic equations become

$$\left( \frac{\partial n u}{\partial z} \right) = \lambda_i^{-1} \exp(-\varphi)$$

$$\left\{ D^2 + \rho^{-2} \right\} Du = \left\{ D^2 + \sin^2 \alpha \cdot \rho^{-2} \right\} (\partial \varphi / \partial z)$$

$$\lambda_B^2 (\partial^2 \varphi / \partial z^2) = n - \exp(-\varphi)$$

where

$$\lambda_i = c_s / \nu_i, \quad D = u (\partial / \partial z) + \lambda_i^{-1}, \quad \lambda_i^{-1} = \lambda_{cx}^{-1} + \lambda_i^{-1} e^{-\varphi} / n, \quad \lambda_{cx} = c_s / \nu_{cx},$$

Note that by introducing the operator $D$ we have recuced the system of the 3 component equations of motion to a single equation for $u$. 
4.3. DS-MPS transition

\[ \varepsilon_{Dm}, \varepsilon_{mc} \ll 1 \]

\[ \left( \frac{1-u^2}{u} \right) \left( \frac{du}{dz} \right)^2 = \frac{1}{\rho^2} f(u) + \lambda_D^2 \left( u^2 \left( \frac{d\phi}{dz} \right)^2 + \frac{1}{\rho^2} \sin^2 \alpha \cdot \Phi \right), \]

\[ \Phi = \frac{1}{2} \left( \frac{d\phi}{dz} \right)^2 + \frac{\varepsilon^2}{\rho^2}, \quad \text{and} \]

\[ f(u) = \cos^2 \alpha \left[ u_1^2 \ln \left( \frac{u}{u_1} \right) - u_1^2 \right] - \left( u_{11} + u^{-1} - \sin \alpha \left( u + u^{-1} \right) \right)^2, \]

\[ u = 1 + \delta u \quad \text{and} \quad \varphi = \varphi_* \approx \delta u \ll 1 \quad (\varphi_* \text{ is the potential at the DS entrance}). \]

**Intermediate scale \( \zeta = z/l \)**

The characteristic intermediate scale \( l \) is chosen as the position where the contribution of the magnetic field has the same order as that of the charge separation.

For the renormalized potential \( w = s \cdot (\varphi - \varphi_*) \) we obtain

\[ \left( \frac{d^2 w}{d\zeta^2} \right)^2 = f(1) + \left( \frac{d^2 w}{d\zeta^2} \right)^2, \quad \text{(a)} \]

The intermediate scale is found as

\[ l = (\rho \cdot \lambda_D^2)^{1/3} \quad \text{and} \quad s = (\rho / \lambda_D)^{2/3}. \]

For the potential in the intermediate region we ultimately obtain in leading order

\[ \frac{d^2 w}{dz^2} = w^2 + \sqrt{f(1)} (\zeta = \zeta_*), \quad \text{--- the Painlevé equation.} \]
5. PIC SIMULATION OF A COLLISIONAL MAGNETIZED PWT

5.1 Fundamentals of PIC simulation
Developments of the electrostatic PIC (particle-in cell) code BIT1

Particle mover
\[
\frac{d}{dt} \vec{V}_i = \frac{q_i}{m_i} (\vec{E} + \vec{V}_i \times \vec{B}),
\]
\[
\frac{d}{dt} \vec{X}_i = \vec{V}_i, \quad i = 1, 2, \ldots, N,
\]

Poisson solver
\[
\nabla \vec{E} = \frac{\rho}{\varepsilon_0},
\]
\[
\vec{X}_i, \vec{V}_i, \rho
\]

Charged-neutral particle and Coulomb collisions

Neutral-neutral particle collisions

Plasma-surface interactions

New:
(i) Multi-neutral model;
(ii) elastic, excitation, charge-exchange and ionization collisions for all atomic hydrogen isotopes
(iii) A simplified model of plasma-surface interactions

Future plans:
(i) Collision-optimized approach;
(ii) Self-consistent neutral model;
(iii) More reliable model for plasma-surface interactions

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(i) Multi-neutral model;
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Future plans:
(i) Collision-optimized approach;
(ii) Self-consistent neutral model;
(iii) More reliable model for plasma-surface interactions
3.2 PIC simulation of a collisional magnetized PWT

Pioneer in PIC simulations of the (collisionless) magnetized PWT:

Here: D. Tskhakaya and S. Kuhn, EPS 2001, Funchal

Magnetized PWT structure

PIC simulation geometry
PIC code used: **BIT1** ("Berkeley-Innsbruck-Tbilisi")
developed by **D. Tskhakaya (jr)**
on the basis of **XPDP1** from U.C. Berkeley:

**J.P. Verboncoeur** et al., JPC (1993)

- **Input parameters** are chosen so as to be relevant to fusion divertor plasmas
- **Fixed background** of atomic hydrogen
- **Ions undergo elastic collisions** with background neutrals
- **Electrons are collisionless**
- **Ions and electrons are injected with half Maxwellian distribution functions**
- **A careful injection scheme** is required to maintain quasineutrality and avoid an artificial source sheath
Steady state after a few ion transit times
\[ L/\left(\sin \alpha \sqrt{kT_i/m_i}\right) \]

Profiles of different plasma parameters in the PWT region:
- (a) potential \( \Phi \);
- (b) electric field \( E \);
- (c), (d) particle densities \( n_e, n_i \);
- (e), (f) fluid velocity components \( V_{ex}, V_{ix} \);
- (g) Temperatures \( T_e, T_i \).

Remarkable result from (e), (f): Quasineutrality already breaks down for \( |V_{ix}| < c \), so the Bohm criterion is not satisfied. This is not surprising because the conditions for the latter are not fulfilled here.

Averaging over a few plasma oscillations leads to fluctuation levels < 5 \%.
Velocity and energy distributions

Electron and ion velocity distributions
- at the MPE (a), (d) and
- at the DSE (b), (e).
- Energy distributions of electrons and ions absorbed at the wall (c), (f).

Electrons $\sim$ maxwellian
Ions $\sim$ cut-off shifted maxwellian

Main observation:
Bohm criterion not well satisfied here, due to non-negligible
- ratio $\lambda_D/l_c$
- collisionality

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6. EFFECT OF NONUNIFORM CROSS ELECTRIC FIELD

The assumption of uniform $E_c$ used so far is somewhat incorrect:

The $E$ component parallel to the (conducting) wall vanishes at the wall, hence has a strong gradient normal to the wall.

Neglecting ion collisions with neutrals and the diamagnetic drift we find that the ion velocity at the MPE equals

$$v_{\parallel 0} = c_s \left( \sqrt{1 + \eta^2} - \eta \right) + \frac{E_y}{B} \cot \theta,$$

with

$$\eta = \pm \frac{1}{2} \frac{\cot \theta}{1 + \frac{T_i}{T_e}} \rho_i \left( \frac{1 + T_e}{T_i} \right)^{1/2} \frac{L_y}{L_x}, \quad L_y^{-1} \left| \frac{\partial_z E_y}{E_z} \right|_{z \to -\infty}$$

The last two terms on the rhs can be shown to be of the same order, hence must be considered together.

For $\eta \to 0$ we also have $E_y/B \to 0$ and thus retrieve the classical Bohm-Chodura condition

$$v_{\parallel 0} = c_s$$

PIC simulations of nonuniform cross electric field effects

To demonstrate the importance of the drift gradient, we have run two PIC simulations with imposed $E_y (∥ \text{wall})$:

(a) $E_y$ constant, with $E_y \approx c_s B \sin \theta$ (Fig 1, solid line)

(b) $E_y$ constant inside most of the CP, but decreasing linearly in and beyond the MP (Fig. 1, dashed line).

Fig. 1

\[ |E_y| \text{ [kV/m]} \]

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Fig. 2. Profiles of the parallel component of the ion velocity \((v_n = 0)\) near the MPE. The MPE is located at 2 mm. Solid, dashed, and dotted lines correspond to nonuniform \(E_y\) (the gradient of \(E_y\) starts at 2.4 mm), to constant \(E_y \neq 0\), and to \(E_y = 0\), respectively.
6. Fluid model of the magnetic presheath in turbulent plasmas (1)

The ion flux density at the MPSE accounting for turbulence

\[ \Gamma_{i,z} = n_{MPSE}^r c_s \sin \alpha + \Gamma_{i,z,MPSE}^{turb}, \]

where there is a magnetic field oblique to the surface, can be applied to the boundary conditions of the fluid transport codes used for modelling tokamak SOL plasmas

Fluid model of the magnetic presheath in turbulent plasmas (2)

New expressions for the fluid Bohm criterion at the SE, and for the ion flux (z-perpendicular to the wall)

\[ n_{SE}^r v_{z,SE}^r + \Gamma_{i,z,SE}^{turb} - \frac{n_{SE}^r c_s^2}{v_{z,SE}^r} = 0 \]

\[ \Gamma_{i,z,SE} = n_{SE}^r c_s \sqrt{1 + \left( \frac{\Gamma_{i,z,SE}^{turb}}{2 n_{SE}^r c_s} \right)^2} + \frac{\Gamma_{i,z,SE}^{turb}}{2} \]

where the turbulent flux (in RED) is a new term representing the chosen turbulence model
7. CONCLUSIONS

1. Magnetized-PWT studies are important for, e.g.,
   (a) Fluid boundary conditions for SOL codes, and
   (b) Conditioning of particle and heat loads to divertor plates,
   which is especially important for a costly project like ITER

2. “Simple” magnetized-PWT models are indispensable for
   basic and reference information, but for practical applications
   more realistic investigations are needed in addition.

3. In this talk we have illustrated some steps towards more
   realistic magnetized PWT studies, namely
   (a) more refined analytic studies, (b) use of PIC simulations,
   (c) non-uniform cross electric field, (d) turbulent magnetic
   presheath

4. Ultimately, all of these more or less small-scale results should
   be brought together judiciously in the framework of
   INTEGRATED TOKAMAK MODELLING, which is required
   for reliably interpreting and predicting the behavior of
   tokamaks, and ITER in particular.
THANK YOU!