A COMPUTATIONAL MODEL FOR TRANSPORT IN PARTIALLY ERGODIZED MAGNETIC FIELDS

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ABSTRACT

A 3-dimensional plasma fluid transport problem for fusion edge plasmas is considered. Conventional numerical methods from fluid dynamics or gas dynamics are not applicable, if the coordinate line along one of the main transport directions exhibits ergodic behaviour at least in some regions of the computational domain. In stellarator plasma edges, or in tokamaks with field line perturbations as foreseen for TEX-TOR under dynamic ergodic divertor (DED) operation, such complications can arise. We propose and discuss a novel "Multi-Coordinate System Approach" within the framework of a Monte Carlo procedure. A 3-dimensional plasma fluid code is developed, benchmarked and applied to a model with geometrical and magnetic field parameters chosen to fall in the range of parameters expected for TEXTOR with DED [1]. The resulting patterns in the computed plasma temperature field near the perturbation coils are in accordance with experimental observations of the radial modulation of the temperature field in TORE SUPRA, though under slightly different experimental conditions there.

I. INTRODUCTION

3 dimensional fluid simulations have become a more or less standard tool in computational fluid mechanics. In magnetised plasmas, however, even 2dimensional approximations still appear to be at the borderline of what is possible numerically. This due to several plasma physical peculiarities, such as the strong nonlinear character of transport coefficients themself, the high an-isotropicity, and the large differences of relevant timescales involved in one problem (electron energy transport along B, compared to particle transport across B, for example), leading to very stiff equations. Finally the sources and sinks (due to atomic ("chemical") processes) are, typically, both nonlocal (kinetic) and nonlinear. Still, extracting physical information from current magnetic fusion experiments requires computational assistence, due to the large number of individual processes competing with each other (detailed bookkeeping). See [2] for a recent review.

The situation is even more complicated in experiments, in which, for physical reasons, the 2 dimensional structure of the magnetic field is destroyed.

Intrinsic or even externally produced magnetic perturbations can provide a stochastic field topology in parts of fusion edge plasmas, both in tokamaks and in stellarators. In these edge plasma regions, ergodic zones, islands, and laminar zones can coexist and, certainly, mutually influence each other. Transport is inherently 3 dimensional here.

A further complication arises, since the so called "laminar zones" are not necessarily those found from field line tracing. Here we use the term "laminar zone" for that part of the flow field, in which the connection length from the source to the sink of any extensive quantity (say, for the plasma energy) along the magnetic field is short (only a few turns around the torus or less). This generalised terminology accounts for the **physical** properties and the influence of laminar zones upon the flow dynamics, distinct from the just **geometrical** characterisation in the more commonly used definition based upon field line length only.

In TEXTOR such stochastic regions will be produced deliberatly, by the the "Dynamic Ergodic Divertor" (DED), in the near future. In stellarators they will arise naturally, at increasing plasma- β .

We expect that TEXTOR-DED and stellarators will be "similar" in this sense and different from the intrinsically 2 dimensional (at least in an idealisation) axisymmetric divertor or limiter concepts.

Due to a 3D distribution of recycling sources and sinks there may be a complicated pattern of regions with short connection length to either a material boundary (sink), or to a sink region caused by neutral plasma interaction. In other words a dual character of the scrape off layer may be manifested, in which a pattern of regions of long and short connection length along the B-field to whatever sink (surface or volume distributed recycling sink) is produced.

The simplest possible model for the plasma flow under such conditions, therefore, must at least have the following ingredients:

- The complete field line pattern, including ergodic, island and "laminar" zones.
- A model for transport in these fields, with homogeneous boundary conditions only at the separa-

trix between perturbed (SOL) and unperturbed region, consistently linking the various regions inside the SOL.

• A model for the 3D recycling process. Distinct from regular (2D) boundary plasmas, as e.g., in ideal axisymmetric divertors or limiters, here we have to deal with a breaking of the symmetry between the magnetic topology (hence: the parallel plasma flow) on the one side and the vacuum chamber (hence: recycling) on the other side.

It is known since long, even from intrinsically 2D situations, that this "misalignment" between the plasma flow and the neutral particle recycling flow can, potentially, lead to complicated local flow patterns with flow reversal, perhaps even under globally low recycling conditions as expected for TEXTOR [3]. The terse physical cause here is an overloading of particular field lines (flux bundles) with recycling of plasma efflux from other, neighboring field lines.

We wish to study the following simple model, carefully accounting for the above mentioned complications:

Field lines (flux bundles) are fed from the unperturbed core plasma and, mutually, from each other by anomalous cross-field diffusion normal to the field lines. With this competing is the fast plasma transport parallel to the magnetic field, which we assume to be as described by classical plasma transport theory (Braginskii).

Charged particles recombine upon impact on any material surface (limiter, vacuum vessel,...) and neutral atoms and molecules are released there, typically at an almost equal rate.

These neutrals are reionised, and, most importantly, not necessarily within the same fluxtube as the former ion.

Monte Carlo procedures are available (e.g. the EIRENE code, [4]), which can describe this neutral gas transport with sufficient accuracity, once the plasma profiles are given. Here we describe the conceptually new second module of such a code-package, which computes the plasma flow fields (e.g., temperature fields), for given recycling sources (e.g., ionisation profiles).

The computational task is to solve diffusion-advection equations for plasma transport in complex 3 dimensional magnetic field configurations including ergodic layers, i.e., with potentially chaotic (non-integrable) flow fields.

Existing 3D fluid codes for the stellarator periphery (EMC3, [5], BoRiS, [6]) are based upon one "global" magnetic coordinate system. Magnetic surfaces must exist everywhere, and the coordinate system must be perfectly aligned to them, also everywhere. Hence these procedures restricted to integrable flow fields, and are not suitable in the presence of ergodic layers.

Instead, our Multi-Coordinate System approach (see below) allows modelling of plasma transport in general magnetic field structures and still accounts for the detailed material boundary geometry of a device.

The main concepts followed here are:

- 1. A Monte-Carlo approach for diffusion-advection equations (Lagrangian discretization) is employed. Every "test particle" (fluid parcel) performs jumps (random steps) along and across the magnetic field in it's own moving coordinate system. Such sets of locally adequate coordinate systems (each one restricted to a sub-domain small compared to the Kolmogorov-length, and separated by cut-surfaces from the neighboring sub-domains) can readily be established, in the same way as Clebsch coordinates are constructed for open magnetic confinement configurations [7].
- 2. The link between two neighboring local coordinate systems (handing fluid parcels over from one to the next coordinate system) is done by a special "interpolated cell mapping", a well established procedure from nonlinear dynamics.
- 3. A second (global and more simple) Eulerian coordinate system is used to evaluate plasma parameters from the trajectories of the fluid parcels. This second mesh is chosen in order to represent the grid boundaries: e.g., vacuum vessel, limiters, divertor targets, etc., and, hence, the recycling process in a convenient way.

The rough scheme of the method is as follows. We start with an initial guess for the 3D profile of some hydrodynamical quantity A, preferably a specific extensive quantity (energy density, momentum density, mass density, etc..).

We then wish to find the result of the evolution of A after a time interval Δt . According to the Monte-Carlo technique, we scatter a number of "fluid parcels" ("test particles", by abuse of language) each of which represents some amount of A. The spatial distribution of the parcels must reproduce the initial profile $A(\vec{r}, t_0)$. Then each parcel performs a jump (in it's own, or local coordinate system) according to a law of motion derived from the balance equation for A and to the value of Δt chosen for the discretisation in time.

Hence, we solve a deterministic problem numerically by a Monte Carlo simulation of a concomitant probabilistic problem.

The new spatial distribution of the particles represents the new profile $A(\vec{r}, t_0 + \Delta t)$. This procedure (excluding the initial discretization) can be repeated either until a steady state is found, or the dynamical behaviour of the system itself is studied.

The mathematical task here is to derive the expressions for the components of a suitable random walk process, especially accounting for the particular combination of mapping and field line tracing, which we shall discuss below in more detail (see the next section)

According to the point 2, we need a preparation step to obtain all geometric (i.e., magnetic) information (interpolation coefficients for the mapping procedure, the components of the metric tensor etc.).

TEXTOR-DED, poloidal section methods to find approximations to solutions of sets of such conservation equations.

We do this by specifying a Markovian random walk process X_{rw} , which approximates (in the limit of small steps) a diffusion process X_d . We can then utilise relations between this diffusion process X_d and a Fokker-Planck equation and see, that our Monte Carlo procedure solves, indeed, our set of conservation equations.

For this purpose, we first have to rewrite the prototypical equations in Fokker-Planck form.

The fluid equations, in this form and in some general curvilinear coordinates x^i read:

oloidal cross section of TEXTOR model, showing:
ALT-II toroidal limiter, DED target and Poincare $\frac{\partial \Phi}{\partial t}$ $\frac{\partial \Phi}{\partial t}$ $\frac{\partial \Phi}{\partial x^i} \sqrt{g} \left(\chi^{ij} \frac{\partial \Phi}{\partial x^j} - V^i_{Drift} \Phi \right) + Q_{\Phi}$, Fig.1: P

We will c hoose, below, cuts θ =whomsty in the unsitric determinant toroidal coordinate system as the balleron thehedliffusivity related to the conductivity mapping procedure. This choice is somewhat (a/bi) may $n\chi$. n denotes the number density and it is made here because of the particular situm northy onents arising in the drift term are of the TEXTOR limiters and perturbation coils. On each such (Poincarè-) section a regular 2D (r, ϕ) $P_{rijt}^{\text{nesh}} = \frac{5}{3}V_{\rho}^{i} + \chi^{ij}\frac{\partial}{\partial x^{j}}\log n$, is defined. We solve (numerically) the equations of the magnetic field line through the knots of such a mesh where V are fluid velocity components. The source from a given section to the next and to the previous one, and interpolate the resulting transformation functions (i.e., the coordinates of final points as functions in the particular case of the energy balance equation of the coordinates of the starting points by means and ions in a single ion species of bicubic splines (hence the name: "interpolated cell; 1, 1, 1; c. of bicubic splines (hence the name: "interpolated cell plasma we readily identify

mapping") It is useful to define a "limiter shadow" of dead and dead density. dead and dead are dead and dead are dead density. dead d

Moving from these "shadowed zones, along the fields results in the termination of the trajectory on a material surface, before the next section is reached." From now on is taken to be of the material surface, before the next section is reached.

$$\chi^{ij} = \chi_{\perp} g^{ij} + (\chi_{||} - \chi_{\perp}) h^i h^j, \tag{5}$$

II. BASIC EQUATIONS

where $g^{ij} = (\nabla x^i)(\nabla x^j)$ and $h^i = \mathbf{h} \nabla x^i$ are contravariant components of the metric tensor and of The main goal of the present wherking two developing the magnetic field ${f h}={f B}/B$.

a computational tool, which permits to solve $\|a_{\perp} + c(n)\|$ and κ_{\perp} are classical parallel prototypical balance equations of thadypromalous perpendicular heat conductivity coefficients, respectively

$$\frac{1}{\partial t} = \nabla \vec{\Gamma}_{\Phi} + Q_{\Phi} \qquad (1)$$

Here Φ is a specific quantity (per unit mass), ρ is the mass density, and $\vec{\Gamma}_{\Phi}$ is the flux of Φ .

ALT

DED

 Q_{Φ} comprises all terms (sources, sinks) that do not fit into the divergence of the flux Γ_{Φ}

We specialise the flux $\vec{\Gamma}_{\Phi}$ to diffusive-advective

$$\vec{\Gamma}_{\Phi} = \kappa \vec{\nabla} (\rho \Phi) + \vec{V} \rho \Phi. \tag{2}$$

 κ is the diffusivity (or: conductivity) coefficient, and $\nabla(\rho\Phi)$ is the thermodynamic force driving the dissipative part of the flux

Again, all remaining terms can be put into Q_{Φ} .

This is the general differential equation governing the evolution of the extensive quantity (per unit volume) $\rho\Phi$

Because of the geometrical and physical complications mentioned above, we will employ Monte Carlo III. MULTI COORDINATE SYSTEM APPROACH (MCSA)

For the numerical solution of eqs. (3) a set of many (typically $M \sim 20$) local magnetic coordinate systems S_m , m = 1..M is used in combination with a mapping procedure derived from field line tracing [8]. This permits to avoid artificial cross-field transport otherwise caused by a numerical mixing of parallel and perpendicular fluxes. Every local coordinate system is chosen such that for two coordinates (e.g., labelled 1 and 2) the condition

$$\mathbf{h} \cdot \nabla x_m^i = 0, \qquad i = 1, 2. \tag{6}$$

holds. I.e. two coordinates are chosen normal to B for each coordinate system.

The third coordinates x_m^3 are chosen such that their coordinate surfaces $x_m^3 = constant$ are nowhere tangent to \mathbf{B} , e.g.: $\mathbf{h} \cdot \nabla x_m^3 > 0$. As a result, the parallel flux has only one nonzero component. This can be seen, e.g., from the form of the general diffusion tensor,

$$D^{ij} = D_{\perp} g^{ij} + (D_{||} - D_{\perp}) (\mathbf{h} \nabla x^3)^2 \delta_3^i \delta_3^j$$
 (7)

where δ_3^i is the Kronecker symbol.

Particular sets of local coordinate systems used below are constructed in quasitoroidal coordinates r, θ, φ . Here r is the small radius, θ the poloidal and φ the toroidal angle, respectively. The third variable x_m^3 is chosen to coincide with the poloidal angle, $x_m^3 = x^3 = \theta$. The cuts ("Poincaré sections") are introduced at the surfaces

$$\theta = const. = \theta_m \equiv (m-1)\Delta\theta, \qquad m = 1, \dots, M$$
 (8)

where $\Delta \theta = 2\pi/M$ (see fig.1).

Consider an arbitrary point $P = (r, \theta, \varphi)$. The coordinates $x_m^1(P), x_m^2(P)$ in the system S_m are defined as the small radius and the toroidal angle of the projection along the magnetic field line to the Poincaré section m. Hence x_m^1, x_m^2 are linked with the quasitoroidal coordinates by the characteristics of eq. (6),

$$x_m^1 = \rho(r, \theta, \varphi; \theta_m), \qquad x_m^2 = \chi(r, \theta, \varphi; \theta_m), \qquad (9)$$

which satisfy the magnetic field line equations,

$$\frac{\partial \rho}{\partial \theta'} = \frac{h^r(\rho, \theta', \chi)}{h^\theta(\rho, \theta', \chi)},$$

$$\frac{\partial \chi}{\partial \theta'} = \frac{h^\varphi(\rho, \theta', \chi)}{h^\theta(\rho, \theta', \chi)},$$
(10)

and initial conditions

$$\rho(r, \theta, \varphi; \theta) = r, \qquad \chi(r, \theta, \varphi; \theta) = \varphi.$$
(11)

Here $h^r(r,\theta,\varphi)$, $h^{\theta}(r,\theta,\varphi)$, $h^{\varphi}(r,\theta,\varphi)$ are contravariant components of the vector **h** in quasitoroidal coordinates.

IV. MONTE-CARLO PROCEDURE

The mathematical justification for the Monte Carlo procedure used here is well known from standard textbooks. Essentially, we simulate random walks from a discontinuous Markov-process, which approximates a (continuous) diffusion process. Averaging over the trajectories we obtain an approximate solution to this Fokker-Planck equation, hence also to the heat balance equation. The internal energy contained in the system is distributed between an ensemble of N_p "test particles". Thus, the internal energy density averaged over a given cell is estimated as the sum of the weights of particles in this cell devided by the cell volume.

In order to derive the elementary time step we rewrite (3) in conservative Fokker-Planck form for the pseudoscalar density N of test particles $N = u\sqrt{g}\Omega/w$.

w is the weight of test particles and Ω is the plasma volume,

$$\frac{\partial N}{\partial t} = \frac{\partial}{\partial x^i} \left[\frac{\partial}{\partial x^j} D^{ij} N - V_c^i N \right] + Q_N, \tag{12}$$

where

$$V_c^i = V^i + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^j} \sqrt{g} D^{ij}. \tag{13}$$

The source terms $Q_N = Q_u \sqrt{g}\Omega/w$ are accounted for by weight adjustment, and here we describe the dynamics of test particles only. The random process governing the test particle motion is

$$x^{i}(t + \Delta t) = x^{i}(t) + \Delta x^{i}, \tag{14}$$

where Δx^i are small random steps and $\Delta t \ll \tau_{min}$. Here τ_{min} is the shortest relaxation time corresponding to parallel relaxation: $\tau_{min}^{-1} = D_{\parallel}/L_{\parallel}^2$, L_{\parallel} is the parallel spatial scale of plasma and magnetic field parameters. The Fokker-Planck equation for the density of test particles N subjected to random process (14) coincides with (12) if

$$\langle \Delta x^i \Delta x^j \rangle = 2D^{i,j}(\mathbf{x}(t))\Delta t, \quad \langle \Delta x^i \rangle = V_c^i(\mathbf{x}(t))\Delta t,$$
(15)

The error in the representation of the distribution function of test particles subjected to the above random process is quadratic in Δt after one time step. Within this precision during one time step one can model separately different types of transport processes using the independent sets of random numbers for each process. The diffusion and convection can be modelled separately as well,

$$\Delta x^i = \Delta x_D^i + \Delta x_C^i. \tag{16}$$

The convection step is carried out as in any conventional deterministic Lagrangian discretisation scheme. The non-trivial part is the term with the second derivative. This diffusion step, in our local coordinates $x^{1,2}$, is carried out by a stochastic perturbation of Lagrangian trajectories. It is given by

$$\Delta x_D^i = \sqrt{2\Delta t} \alpha^{ik} \xi_k + \frac{D^{i3}}{D^{33}} \Delta x_D^3, \qquad i, k = 1, 2.$$
 (17)

Here α^{ik} is the square root matrix,

$$\alpha^{ik}\alpha^{jl}\delta_{kl} = D^{ij} - \frac{D^{i3}D^{j3}}{D^{33}}, \qquad i, j, k, l = 1, 2 \quad (18)$$

and ξ_i is a set of random numbers, satisfying the conditions $\langle \xi_i \rangle = 0$ and $\langle \xi_k \xi_l \rangle = \delta_{kl}$, δ_{kl} is Kronecker symbol. The matrix on the right hand side of (18) is non-negatively definite since the diffusion tensor is non-negatively definite. Therefore the square root matrix α^{ik} is real.

Up to the precision of the map $\{\rho, \chi\}$ the random process introduced above induces no artificial cross field transport, i.e., our procedure is perfectly aligned despite of the possibly ergodic character of the magnetic field. The maps $\{\rho(r, \theta_m, \varphi, \theta_{m+1}), \chi(r, \theta_m, \varphi, \theta_{m+1})\}$,

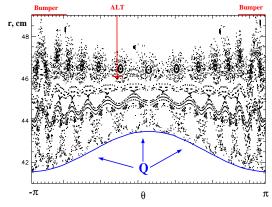


Fig.2: Typical Poincarè plot for a TEXTOR-DED model magnetic field at $\varphi = const$

 $\{\rho(r,\theta_m,\varphi,\theta_{m-1}),\chi(r,\theta_m,\varphi,\theta_{m-1})\},\ m=1,\ldots,M,$ are precomputed by numerical integration of eqs. (10) for the mesh of r,φ values. They are then reconstructed during the Monte Carlo computation by means of bicubic splines which provide sufficient mapping accuracy.

We introduce time intervals Δt small compared with characteristic relaxation time of the relevant plasma parameters. The transport coefficients required are computed from the estimates of plasma parameters from the previous time step and are kept constant during Δt . This "explicit" procedure is repeated until a stationary solution is reached.

V. SAMPLE APPLICATIONS

The new code E3D is employed here to study the heat transfer in the edge plasma, expected during the DED operation in TEXTOR.

We have to assume, so far, that the dominant heat transport mechanism along the B-field is conduction, i.e., that a certain temperature gradient parallel B is maintained. Under typical (low recycling) limiter conditions, parallel ion heat transport is convection limited by the electrostatic sheath in front of the limiter. In the applications described below, addressing electron heat transfer, the convective component along B is omitted.

The magnetic field enters into our procedure via the field line equations, i.e., numerically, via field line tracing. All formulae above are written for the most general case, i.e., for the completely numerical treatment of the equations of the field lines (10) (as, e.g., described in [1] using the DIVA- GOURDON code combination there). However, for special purposes (as, e.g., fast parameter studies, program debugging, code validation and comparison to theoretical results etc.) we have implemented a simple analytical model for the magnetic field as well, which preserves all main features of the real configuration, ranging from almost unperturbed magnetic surfaces through chains of islands to the complete ergodicity, depending upon the parameters of that model-field.

Results presented here have been obtained with such a "model magnetic field", see figure 2.

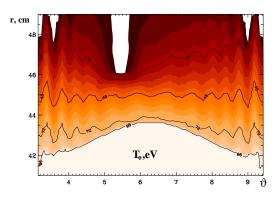
In addition to the typical TEXTOR data [1], we have chosen the following input parameters (boundary conditions) for the simulations shown here:

- radius of the perturbation coils $r_c = 53cm$;
- number of Poincaré sections M=19;
- heat flux from core into SOL $(r = 42cm) Q_{e,i} = 0.45MW$ in electrons and ions each;
- cross field heat conduction coefficient $\chi_{\perp} = n\kappa_{\perp}$ with $\kappa_{\perp} = 5m^2/s$;
- plasma density $n = 7 \times 10^{12} cm^{-3}$;
- perturbation field \tilde{B} varied from 0 to 0.1 T.

The numerical results illustrate the influence of the perturbation field on the temperature profile and the power load distribution on the TEXTOR limiters, see figure 3a and 3b for typical 3D temperature fields. plotted in one selected poloidal cross section. The parallel heat transport is fast enough for electrons and ions to result in regular radial and poloidal patterns, following the field structure. Related findings have already been reported from the ergodic divertor experiments at TORE SUPRA [10]. The heat load pattern on the TEXTOR limiters (figure 4) is also found to be strongly influenced by the effect of the perturbation field. Even with maximal foreseen currents in the perturbation coils with stationary (i.e. not yet dynamical) fields, clear heat load patterns on the first wall components prevail, however with some redistribution between the toroidal ALT pump-limiter, the inner bumper (i.e., "divertor target") and the vessel. This is an indication of near field effects, i.e., the existance of so called "laminar zones"

The results seem to confirm the qualitative picture of the heat flux patterns on the bumper limiter ("divertor target"), [11], essentially as a consequence of the field structure in the "laminar region" alone. Quantitatively, however, we find that the geometric origin field lines carrying the main heat, which is deposited on the "divertor target" is located in the ergodic parts of the SOL, i.e., on fieldlines with a rather deep radial penetration, distinct from the ad hoc pre-selection of field lines of short geometrical length. Furthermore, and as expected, we find a redistribution of global heat load from the ALT limiter to the wall and bumper. However, due to the localization of the heat flux into narrow stripes, the peak power load on the bumper is increasing about 2 times faster with increasing perturbation field. The proper balance between requirements for pumping (strong localisation of plasma fluxes) and heat removel (spreading of plasma efflux over a large area) seems to remain a critical issue even for fusion reactor design, also with ergodic divertors.

We conclude from this first applications to a strongly simplified (and hence: still physically obvious) case that the procedure seems to work both correctly and economically (turn around time: 2 hours on CRAY-T3E with the fully parallelized version).



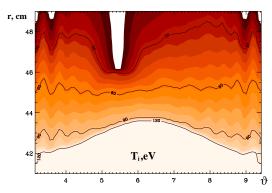
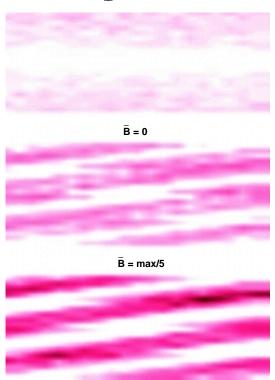


Fig.3a,b: top: electron temperature field bottom: ion temperature field

$\chi_{\perp} = 5 \text{ m}^2/\text{s}$



 $\tilde{B} = max$

Fig.4: heat load pattern on inner divertor targets top: no perturbation field middel: 20 % perturbation field bottom: maximum perturbation field

VI. CONCLUSIONS

A fully parallelized 3D MC fluid code has been developed for the solving transport equations in tokamak edge plasmas with arbitrary magnetic field topology (including ergodic zones, islands and laminar zones).

The efficiency of the code is sufficient for modelling the DED operation in TEXTOR on CRAY T3E (turn around time about 2 hours).

The computational model should prove general enough to allow also the simulation of partially ergodic stellarator edge plasma conditions without a principal modification of the existing code.

It has been shown that the power flux to the bumper limiter in TEXTOR is significantly increasing with the increase of the amplitude of the perturbation magnetic field. Further studies with varied radial position of the main (ALT-) limiter still need ot be carried out to identify optimal operation windows.

At the same time, the power flux to bumper limiter becomes localized within a few helical stripes. This produces an increase in peak power flux value, approximately two times faster than the total flux to bumper limiter. Dynamic divertor operation, however, even at low frequencies (below 100 Hz) stongly reduces this peak power loading again.

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