THE HENRYK NIEWODNICZAŃSKI
INSTITUTE OF NUCLEAR PHYSICS
POLISH ACADEMY OF SCIENCES
UL. RADZIKOWSKIEGO 152, 31-342 KRAKÓW, POLAND

**WWW.IFJ.EDU.PL /BADANIA/PUBLIKACJE/RAPORTY/**

KRAKÓW, JANUARY 2020

---

REPORT NO. 2103/AP

# Screening effect of partially ionized high-Z impurities in relativistic electron Fokker-Planck calculations and runaway electron dynamics

## Part 1 – Preliminary work towards statistical study of partial screening effect in WEST tokamak discharges

***KRZYSZTOF KRÓL***

**Abstract**

In this report, the problem of tungsten impurities in tokamak plasmas is introduced and the related phenomenon of partial screening occurring during Coulomb collisions between suprathermal electrons and tungsten impurity ions is discussed. The report also introduces the first code among a chain of numerical tools: ALOHA, C3PO, LUKE and R5X2, available for collaborators in CEA Cadarache, where the WEST tokamak is located. This chain of codes has recently been upgraded to take into account the partial screening effect. This set of tools will allow to carry out statistical investigations on the impact of partial screening on the fast electron dynamics in tokamak plasmas.

WYDANO NAKŁADEM INSTYTUTU FIZYKI JĄDROWEJ IM. HENRYKA NIEWODNICZAŃSKIEGO
POLSKIEJ AKADEMII NAUK
KRAKÓW 2020

## The problem of impurities in tokamak plasmas

Nowadays, tokamaks represent the most promising device to achieve a thermonuclear power plant in the future. In the south of France in Cadarache, countries from the whole world build together ITER - International Thermonuclear Experimental Reactor, which will be the biggest tokamak in history. The main goal of this reactor is to prove, by achieving a net energy gain $Q = P_{fusion} / P_{heating} > 1$, that the construction of a thermonuclear power plant based on magnetic confinement is possible.

Among many components, the divertor is a part of tokamak structure that must sustain intense heat and particle fluxes from the plasma edge. This means that the materials used for the divertor design must have a high melting point. Historically, the main plasma-facing components in previous tokamaks, operating with hydrogen or deuterium were made of carbon composites, which exhibit satisfying properties for this purpose. However, deuterium-tritium fusion reactions will occur in the future thermonuclear power plants. Tritium is a radioactive isotope with half-time of decay roughly equal to 12.5 years. Operation of a tokamak with tritium is much more complicated due to radioprotection and safety regulation issues. It means that the material used for the divertor cannot allow for high tritium retention. For this reason, carbon was rejected as a material for the divertor. After many considerations, fusion research community opted for tungsten, the metallic element with the highest melting point and with much lower tritium retention than carbon, as the main element for the ITER divertor. But a new problem arises because of the high temperature of the plasma. Indeed, the divertor surface will be continuously eroded and will sputter tungsten impurities into the plasma. Such tungsten impurities, despite of their small amount, cause a major issue. Tungsten ions tend to accumulate in the plasma core and to cool down the plasma by electromagnetic radiation. This can even trigger the end of the plasma discharge through plasma disruption, which consists in a sudden collapse of the plasma confinement. Nowadays, most of tokamaks work in a pulsed way - single discharges with a time duration from hundreds of milliseconds to a few seconds - while future thermonuclear power plants are foreseen to operate in a continuous way and without any disruptions. Another issue of tungsten is the increase of the bremsstrahlung losses, that decrease significantly the fusion performances of the plasma. The conclusion is that among several problems that must be solved on the road to thermonuclear power plants, the issue of tungsten impurities is a critical one to be solved.

Up to now, some researches have been performed on the melting behavior of tungsten and tungsten impurity transport on the JET tokamak. From now, one of the main key tokamaks devoted to these investigations will be the French device WEST – standing for W (tungsten) Environment in Steady State Tokamak, located in Cadarache. In WEST, not only the divertor is covered of tungsten, but also the other plasma-facing components of the vacuum chamber. WEST is thus an ideal device to investigate the behavior of tungsten impurities in tokamak plasmas.

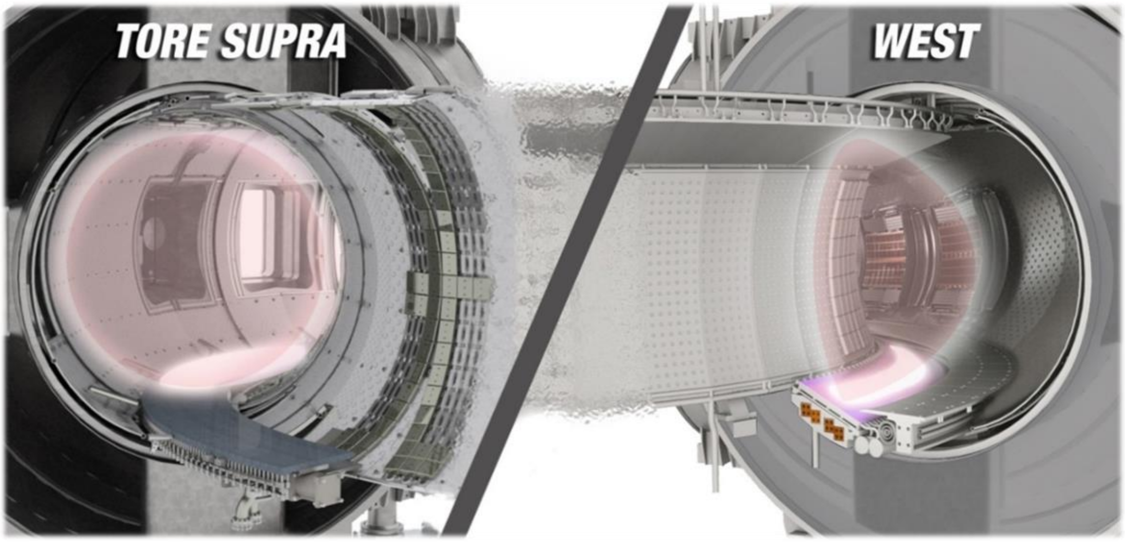


Fig. 1. French thermonuclear device upgraded from Tore Supra to WEST configuration [1].

Besides the tungsten impurities issue, a suprathermal electron population of kinetic energies of the order of 100 keV can arise in tokamak plasmas due to electron heating – e.g. by Lower Hybrid Current Drive (LHCD) method, or at much higher energies of the order of 1 MeV during a tokamak disruption (so-called runaway electrons). While the first ones can allow to control the electric current flowing into the plasma, essential for the generation of the poloidal component of the magnetic field, the latter ones (runaways) can damage the in-vessel components when the plasma confinement is lost, especially after a plasma disruption. There are therefore two different situations when considering the interaction between fast electrons and tungsten ions in a tokamak plasma. In the case of LHCD, collisions of fast electrons with tungsten ions could decrease the efficiency of the current drive. In the case of plasma disruptions, the fast electron beam (runaway electrons) can be mitigated by a massive gas injection that can slow down the fast electron beam by collisions with the injected impurities.

Both above situations need a proper description of Coulomb collisions between fast electrons and tungsten ions. Up to know, investigations have shown that the main reason for the mismatch between experimental data and theory is the so-called partial screening effect [2, 3].

**Coulomb collision operator**

One can describe fast electron dynamics in tokamak plasmas by the Fokker-Planck equation. For solving this equation, the LUKE code was developed by Y. Peysson and J. Decker [4]. This code, together with ALOHA [5], C3PO [6] and R5X2 [7], gives a chain of simulation tools for modelling fast electron dynamics in the case of LHCD heating.

Let us consider two species of particles in plasma – species *a* and *b*. Considering the special case when species *b* has a Maxwellian distribution, the Coulomb collision operator takes the form:

$$C^{ab} = \nu_D^{ab}\mathcal{L}(f_a) + \frac{1}{p^2}\frac{\partial}{\partial p}[p^3\left(\nu_S^{ab} f_a + \frac{1}{2}\nu_\parallel^{ab}\frac{\partial f_a}{\partial p}\right)] \tag{1}$$

**Elastic collisions** part

**Inelastic collisions** part

**Parallel diffusion** part

$$\mathcal{L}(f_a) = \frac{1}{2}[\frac{1}{sin\delta}\frac{\partial}{\partial\delta}\left(sin\delta\frac{\partial f_a}{\partial\delta}\right) + \frac{1}{sin^2\delta}\frac{\partial^2 f_a}{\partial\varphi^2}]$$ - definition of so-called Lorentz scattering operator

$\nu_D^{ab}$ - deflection frequency

$\nu_S^{ab}$ - slowing-down frequency

$\nu_\parallel^{ab}$ - parallel-diffusion frequeny

$C^{ab}$ - collision operator for collision between particles a and b

$p$ - normalized momentum

$f_a$ - the distribution function of species a particles

The operator consists of three parts. The most important to consider for the partial screening effect are the first two terms. The deflection and slowing down frequencies are parameters responsible for elastic and inelastic collisions.

**Partial screening effect**

Investigations on screening effect of partially ionized high-Z impurities (like tungsten) are necessary to properly describe the fast electron dynamics in tokamaks. When considering heavy impurities, for example tungsten of atomic number $Z$ = 74 in a typical tokamak temperature range $T$ = 1 – 10 keV, different ionization states of tungsten impurities coexist. The effective electric charge of the impurity ions results from the screening of the ion nucleus by the remaining electron cloud. In this case, free incident electrons from the plasma with a sufficiently high kinetic energy can probe this electron cloud, resulting in the partial screening of the ion nucleus as depicted in Fig. 2. The effective charge of the impurity ion is then higher than from a full-screening assumption.

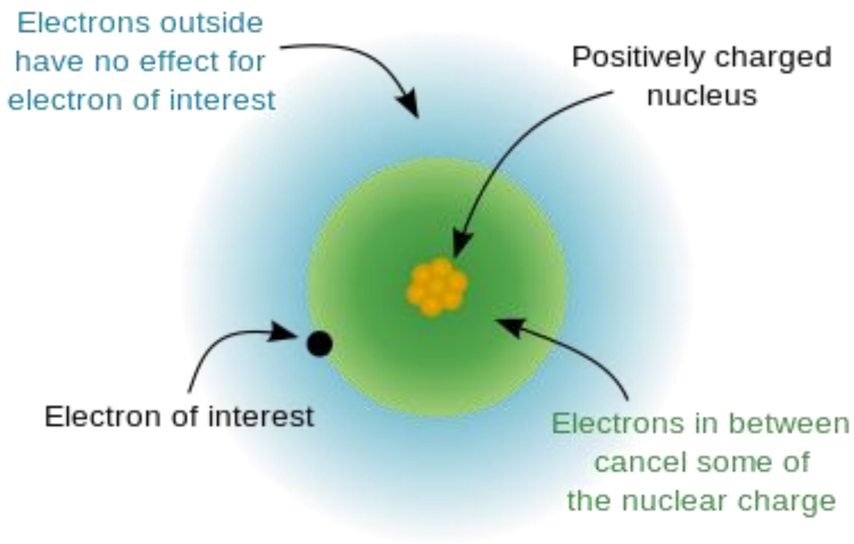


Fig. 2. Symbolic picture of partial screening effect.

The effective charge $Z$ of the ion can be obtained by subtracting the so-called atomic form factor $F_j(q)$ from number of protons $Z_j$ in the nucleus:

$$Z = Z_j - F_j(q) \tag{2}$$

where $q$ denotes the modified momentum [2] of the incident electron. The form factor is a measure of the scattering amplitude in the plane wave approximation and can be associated to an equivalent or effective number of screening electrons, therefore $0 \leq F_j(q) \leq Z_j$. For light impurities - fully ionized in the plasma core, like carbon or nitrogen – considered up to now, $F_j(q) = 0$ such that the partial screening effect can be neglected. However, for heavy impurities like tungsten, $F_j(q) > 0$ and an estimation of the form factor becomes necessary. The form factor can be expressed as the Fourier transform of the radial density of the electron cloud in the momentum space:

$$F_j(q) = \int \rho_{e,j}(r) e^{-iqr/a_0}\, dr \tag{3}$$

This means that the form factor of a particular ion can be estimated by calculating the radial density of its electron cloud. To do so, one can consider a few models like the Thomas-Fermi model, the Tseng-Pratt model or the Density Functional Theory [8, 9].

The partial screening effect impacts the fast electrons dynamics through both the Born-Rutherford cross-section (Coulomb collisions) and the bremsstrahlung differential cross-section.

**Input, output and general description of ALOHA code**

To perform the whole simulation chain ALOHA-C3PO-LUKE-R5X2, firstly one must have access to experimental tokamak data as inputs for the chain of codes. The WEST tokamak is considered here. For ALOHA – Advanced Lower Hybrid Antenna code, the experimental inputs from the WEST database are the incident powers, phases and reflection coefficients of each module of the LHCD antenna. ALOHA can calculate derivative of power over the parallel component of the refractive index – power spectrum at the output of the antenna, which is then an input for C3PO. C3PO is a ray-tracing code which can model the propagation of the LH wave in the plasma from edge to the core of the plasma. Based on this, the LUKE code can calculate the electron velocity distribution function. This electron distribution function can be further used in the last code – R5X2 to calculate the hard X-ray radiation. The electron distribution function allows also calculating the current density in the plasma. The workflow of these simulation tools can be drawn in the following way:

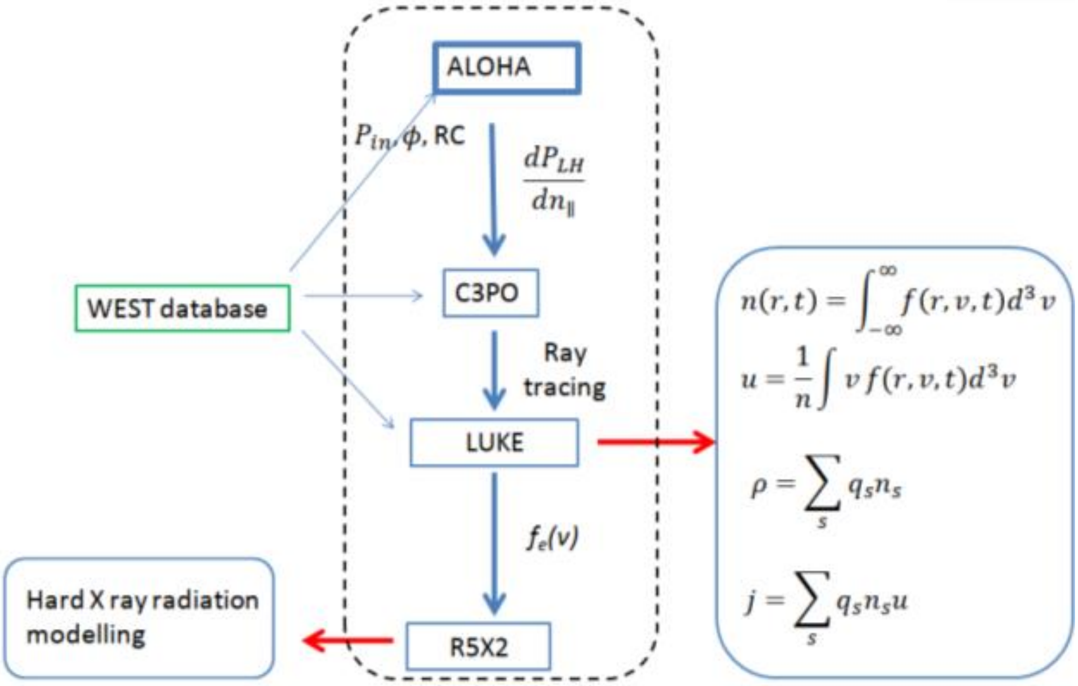


Fig. 3. Schematic picture of the ALOHA-C3PO-LUKE-R5X2 simulation workflow.

The chain of codes starts from ALOHA written in MATLAB. The code allows calculating the coupling between the LH wave in the antenna and the plasma edge. One of the main features of this code is the ability to obtain the power density spectrum at the output of the antenna. The power spectrum for the WEST shot #55539 is shown below as an example:

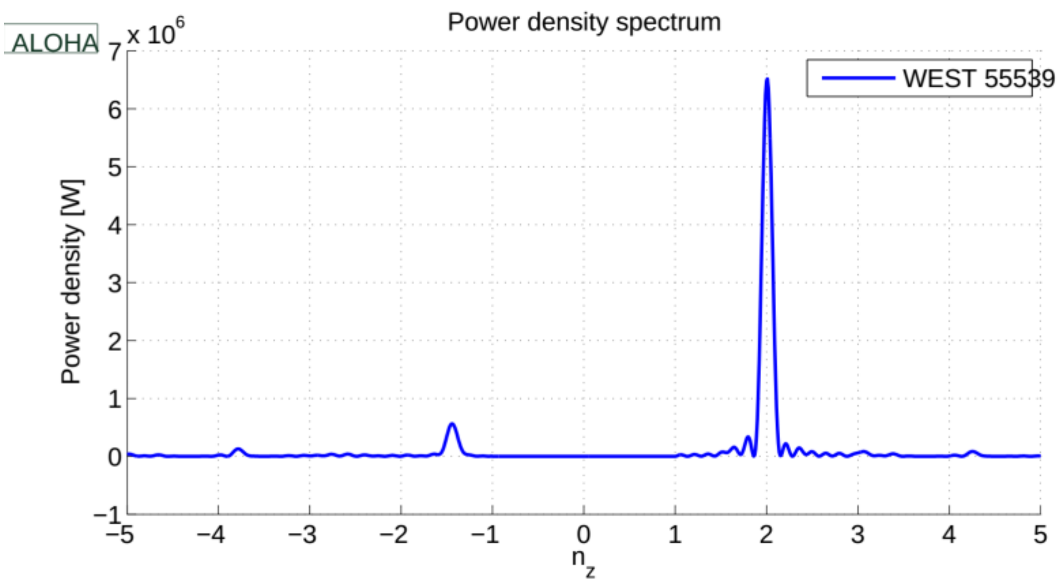


Fig. 4. Power density spectrum for WEST LH antenna, shot number 55539.

One of the most important inputs in ALOHA is the electron density in the private plasma region, see Fig. 5, at the mouth of the antenna. In the WEST tokamak, there are two Lower Hybrid

Antennas: FAM (Full Active Multijunction) and PAM (Passive Active Multijunction) antennas. The interface between the antenna and the plasma edge is depicted on Fig 5.

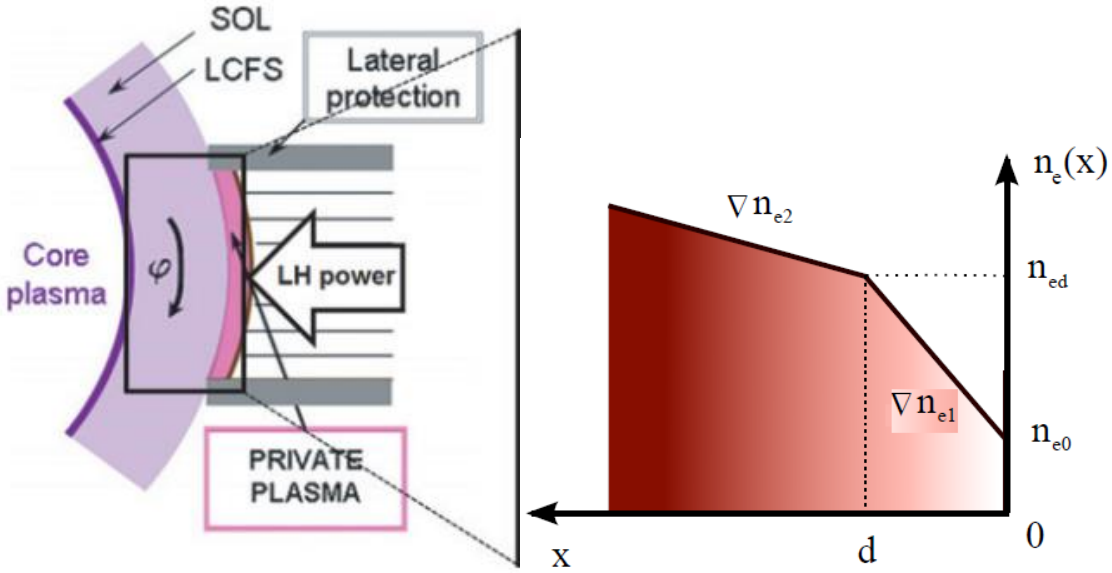


Fig. 5. Left: Interface between the LHCD antenna and the tokamak plasma. Right: plasma density as a function of the distance from the mouth of LH antenna [10].

The antenna has two lateral protections (bumpers). The plasma between the mouth of the antenna and the surface determined by the end of the bumpers is called private plasma. The plasma density at the mouth of the antenna – on the scheme marked by $n_{e0}$ is a critical input for ALOHA. In ALOHA, it is assumed that the plasma density profile is linear, see the Fig. 5.

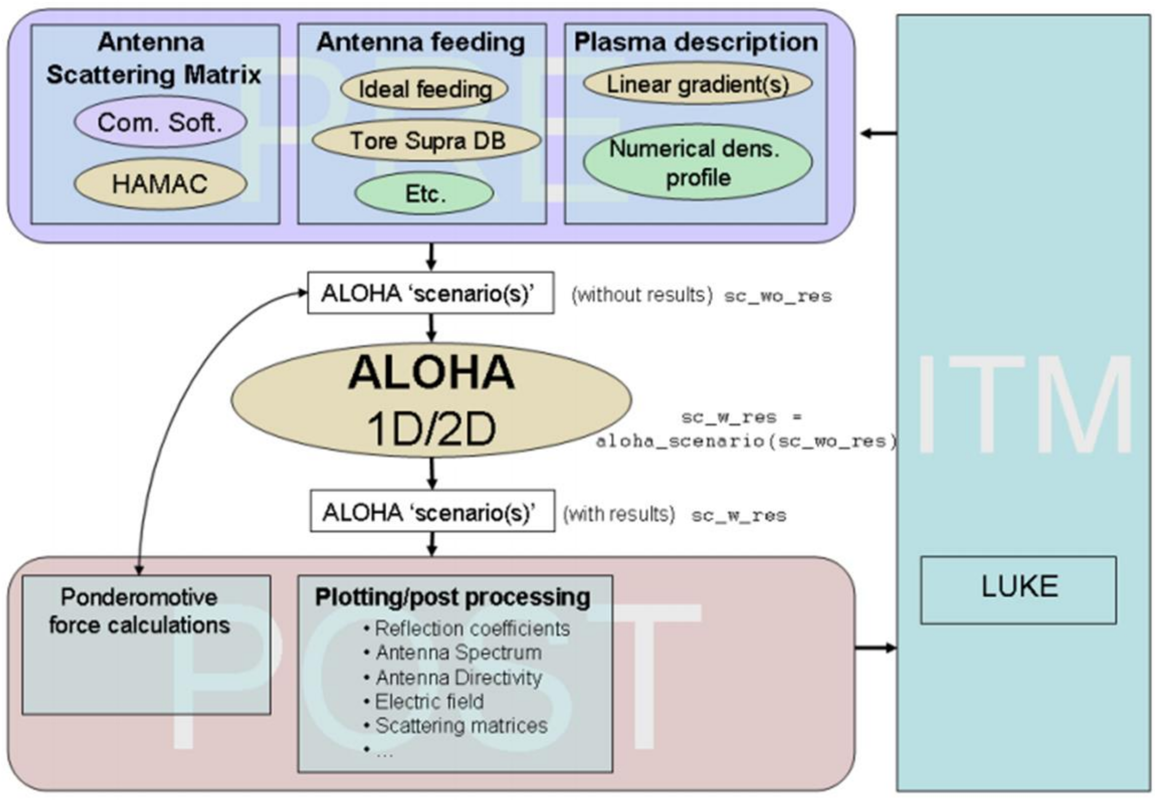


Fig. 6. Simulation workflow of ALOHA [11].

The ALOHA inputs can be divided into 3 groups. Based on the parameters of a particular lower hybrid antenna, a special plug-in named HAMAC calculates the scattering matrix of the antenna. The second required input is the so-called antenna feeding - necessary experimental data for each module of antenna: incident powers, phases and reflection coefficients. The third input is related to the plasma itself. The most crucial parameter is the plasma density at the mouth of the antenna. This quantity can be either experimentally measured using Langmuir probes, or derived iteratively by matching the observed and predicted reflection coefficients. The power spectrum depends on the value of the edge density. So, after a first guess of this quantity, further optimization is needed. To perform a simulation with ALOHA, the first step is to create a so-called scenario data .mat structure. This can be done using a special ALOHA script. Then, it is possible to use the main MATLAB function of ALOHA aloha_scenario which takes as an input the scenario structure and performs all calculations. This optimization process starts with first aloha_scenario calculations and calculates predicted values of reflection coefficients for all modules of the antenna. Then, using the method of mean square error optimization, an optimization script is looking for the optimal value of the plasma density based on an iterative comparison between calculated reflection coefficients and experimental ones.

For the users who want to perform simulations in this framework, the following quantities must be set:

1. WEST antenna port variable – it is necessary to choose for which antenna calculations will be done. One ALOHA simulation can model the coupling of one LH antenna with the plasma.

2. WEST shot number – provide the reference number of the WEST tokamak discharge for a particular simulation.

3. Edge density – first initial guess of electron density at the mouth of the antenna.

4. Start and stop times for measurement averaging, that will be used for antenna feeding. User should check before the simulation if experimental data from this particular shot and period are correctly processed.

Optionally, it is possible to choose the length of the scrape-off layer and also to choose the method of calculation with two models of density gradients.

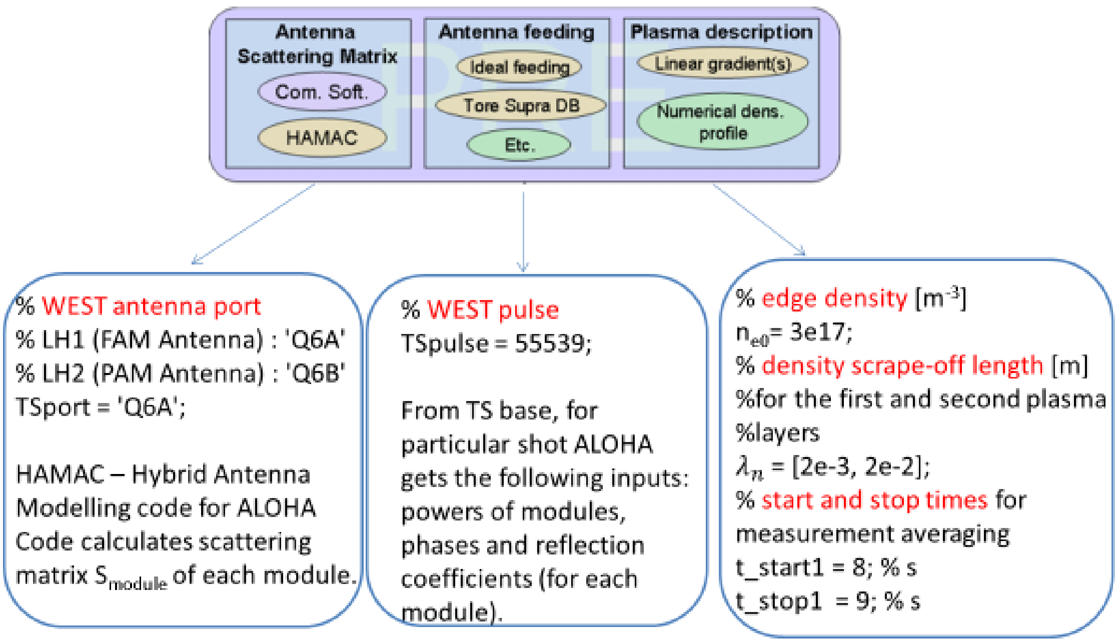


Fig. 7. Inputs of ALOHA separated in three groups.

Table 1 (see [12]) shows the importance of performing the optimization of the input plasma density. For the Tore Supra shot #31527 in Table 1(a), the results of the first row do not include any plasma density optimization, while the results of the second row include the plasma density optimization process. It is shown that the calculated current $I_{LH}$ driven by LH wave and based on Langmuir probes measurements is far away from the experimental current (value in brackets). But after application of the density optimization process, the new $I_{LH}$ value is much closer to the experimental one. This proves that the plasma density optimization based on the reflection coefficients is the most adapted to obtain robust results of current drive as calculated by the LUKE code.

Table 1 - Comparison of ALOHA and LHCD simulations with and without plasma density optimization [12].

| (a) TS # 31527 (C3) | $n_{\mathrm{edge}}$ ($\times 10^{17}$ m$^{-3}$) | RC (%) | $D$ | $I_{\mathrm{LH}}$ (kA) |
|---|---|---|---|---|
| $n_{\mathrm{edge}} = n_{\mathrm{Langmuir}}$ | 4.0 | 2.1 (5.0) | 0.48 | 618 (425) |
| $RC_{\mathrm{ALOHA}} = RC_{\mathrm{Exp.}}$ | 1.3 | 5.0 (5.0) | 0.32 | 416 (425) |
| (b) TS # 45525 (C4) | $n_{\mathrm{edge}}$ ($\times 10^{17}$ m$^{-3}$) | RC (%) | $D$ | $I_{\mathrm{LH}}$ (kA) |
| $n_{\mathrm{edge}} = n_{\mathrm{Langmuir}}$ | 3.0 | 3.1 (1.4) | 0.38 | 420 (438) |
| $RC_{\mathrm{ALOHA}} = RC_{\mathrm{Exp.}}$ | 1.1 | 1.4 (1.4) | 0.55 | 599 (438) |

**Summary**

During the year 2019, the HARMONIA team started the preparation of a theoretical and numerical framework for the investigations on collisions between tungsten ions and fast electrons in tokamak plasmas. This report describes the preliminary study performed towards a MATLAB script for the statistical analysis of the impact of the partial screening effect on fast electron dynamics using a database of WEST tokamak discharges. This work will allow determining the importance of partial screening effect on Lower Hybrid current drive efficiency and bremsstrahlung losses.

**Acknowledgements**

This research was supported in part by the PL-Grid Infrastructure and by the HARMONIA Grant nr 2018/30/M/ST2/00799. I am grateful to the members of the HARMONIA team: Didier Mazon, Yves Peysson, Marek Scholz, Jakub Bielecki, Axel Jardin and Dominik Dworak for their collaboration with me and inspiring discussions.

**Bibliography**

[1] IRFM CEA, Cadarache, http://west.cea.fr/en/index.php.

[2] L. Hesslow et al., Effect of Partially Screened Nuclei on Fast-Electron Dynamics, Physical Review Letters, vol. 118, Iss. 25 – 23 June 2017.

[3] L. Hesslow et al., Generalized collision operator for fast electrons interacting with partially ionized impurities, J. Plasma Phys. (2018), vol. 84.

[4] J. Decker, Y. Peysson, DKE: a fast numerical solver for the 3-D relativistic bounce-averaged electron Drift Kinetic Equation, MIT Plasma Science and Fusion Center report.

[5] J. Hillairet et al., ALOHA: an Advanced LOwer Hybrid Antenna coupling code, (2010) Nucl. Fusion 50 125010

[6] Y. Peysson et al., A versatile ray-tracing code for studying rf wave propagation in toroidal magnetized plasmas, (2012) Plasma Phys. Control. Fusion 54 045003

[7] Y. Peysson and J. Decker, Fast electron bremsstrahlung in axisymmetric magnetic configuration, Physics of Plasmas 15, 092509 (2008)

[8] Berthold-Georg Englert. Semiclassical Theory of Atoms. Springer-Verlag, 1988.

[9] R. H. Pratt and H. K. Tseng. Behavior of electron wave functions near the atomic nucleus and normalization screening theory in the atomic photoeffect. Phys. rev. A, 5(3) :1063, 1972.

[10] M. Preynas, Phd thesis (English version), Etude du couplage linéaire et non-linéaire de l'onde hybride basse aux plasmas de tokamaks, (2012).
https://user.iter.org/filesharing/FileInfo.aspx?uid=86ffe55f-615c-4a8d-b75e-efe149db1732

[11] J. Hillairet, ALOHA Manual,
https://github.com/jhillairet/ALOHA/blob/master/doc/ALOHA_Manual.pdf

[12] E. Nilsson et al., Comparative modelling of lower hybrid current drive with two launcher designs in the Tore Supra tokamak, Nucl. Fusion 53, 083018, (2013).