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Applications of Bayesian Temperature Profile Reconstruction to Automated Comparison with Heat Transport Models and Uncertainty Quantification of Current Diffusion

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²*See the Appendix to G. Falchetto et al., Nucl. Fusion 54 (2014) 043018*

**See annex of F. Romanelli et al, "Overview of JET Results",
(25th IAEA Fusion Energy Conference, Saint Petersburg, Russia (2014)).*

ABSTRACT

In this work we are showing two more applications of the developed expert system described in [12]. The first application shown in the present paper is devoted to the development of an automated comparison method between the experimental plasma profiles reconstructed using Bayesian methods and time dependent solutions of the transport equations. The method was applied to model validation of a simple heat transport model with three radial shape options. It has been tested on a database of 21 Tore Supra and 14 JET shots. The second application aims at quantifying uncertainties due to the electron temperature profile in current diffusion simulations. A systematic reconstruction of the N_e , T_e , T_i profiles was first carried out for all time slices of the pulse. The Bayesian 95% highest probability intervals on the T_e profile reconstruction were then used for i) data consistency check of the flux consumption and ii) defining a confidence interval for the current profile simulation. The method has been applied to one Tore Supra pulse and one JET pulse.

1. INTRODUCTION

As tokamak experiments produce large quantities of data (50 Gbytes of data per second is expected for an ITER pulse), automated processing will be required to systematically analyze these data. Physicists are usually interested in computing a number of plasma physical quantities from the measured data and this is typically done by a chain of codes for “plasma reconstruction”. What is done quite rarely is a systematic comparison of the results obtained from experimental data to the ones produced by physics models verified for other shots (and possibly other tokamaks).

Such comparison, using application-specific criteria to judge the quality of the agreement, may be used to detect unexpected phenomena in an experiment (if validated models are available) or for systematic model validation against experiments. Automated data consistency checks can also be integrated to detect issues on measurements or on their processing by the plasma reconstruction chain.

To implement these functionalities, we developed an expert system carrying out in an integrated way:

1. The Plasma Reconstruction from the measurements, using Bayesian methods. This includes a first level of internal consistency checks of the experimental data and validity of the reconstruction
2. The prediction of the reconstructed quantities, according to the chosen integrated models (a concrete application will be shown in this paper for the density peaking models)
3. An intelligent comparison of the first two steps providing an automated analysis and reporting on the quality of the comparison according to a set of well-defined criteria

The first application of this expert system was shown in our previous article [12] for the comparison of experimental density profile reconstruction with models. The analysis performed in the paper was done for a number of Tore Supra and JET shots, showing a comparison with simple 0D models

of density profile peaking based on independent time slices. The statistics obtained from Bayesian reconstruction were used in the definition of criteria qualifying the quality of the agreement, thus allowing an automation of the comparison. Nevertheless, in this first proof-of-principle of our automated analysis concept, no attempt was made to take into account the dynamics of the plasma discharge neither in the modelling nor in the plasma reconstruction, while most of the present integrated modelling tools solve time-dependent transport equations. In the present paper we are extending our concept of automated comparison to dynamic simulations and simultaneous reconstruction of multiple profiles (namely electron density, electron and ion temperatures). We will first include time dependence in the prediction of temperature profiles, i.e. the reconstruction part still remains time independent, but we aim at validating 1D heat transport models which implies solving the time-dependent transport equations. In addition to the heat transport model validation, data consistency is checked by a simultaneous reconstruction of the electron density, electron and ion temperature profiles and comparison to the measured diamagnetic energy content. The analysis was done for 21 Tore Supra and 14 JET shots.

In the second application presented in this paper the analysis will become completely time dependent, i.e. the reconstruction of the electron temperature profiles will be done throughout the whole shot and used as an input to a current diffusion simulation. The statistics obtained by the Bayesian reconstruction of the electron temperature profiles is used to quantify the resulting uncertainties on current diffusion. Data consistency checks on the flux consumption and comparison to experimental MHD markers are then carried out in the frame of these uncertainties. This application is demonstrated for one Tore Supra and one JET pulse.

Section II includes a brief introduction to Bayesian profile reconstruction of plasma profiles. Section III describes the integrated analysis tools used in the comparison. Section IV describes the temperature profile reconstruction and validation of heat transport models. Section V presents the application of the developed system to the quantification of uncertainty on current diffusion. Conclusions are presented in the section VI.

2. RECONSTRUCTION OF PLASMA PROFILES

2.1 PROFILES INVOLVED IN THE ANALYSIS

We carried out a reconstruction of three profiles: electron density and electron and ion temperatures. Electron density profile reconstruction is done using interferometry and Thomson scattering measurements and was discussed in a previous work [12], whereas the electron and ion temperature profiles are discussed below. All the three profiles are then used in the current diffusion model validation procedure and calculation of the diamagnetic energy discussed in this paper.

2.2 RADIAL PROFILE PARAMETERIZATION

To parameterize a temperature profile, we used 3rd order splines on the grid of normalized flux coordinate (ϱ). Such parameterization gives us $N+2$ coefficients where N is the number of grid

points (N values of splines in grid points, derivative values in the core and at the edge of the plasma). Given a toroidal geometry, the first derivative in the center is fixed to be 0. Thus we have N+1 parameters to describe the radial profile at a given time slice. The grid is automatically chosen consistently with the experimental data so that each grid bin included sufficiently experimental points for reconstruction.

2.3 PRINCIPLES OF BAYESIAN ANALYSIS

All the basic principles remain the same as was described in our previous paper [12] in the corresponding chapter.

To recall, we shall say that we are looking for the posterior distribution of parameters (the spline coefficients described in the previous paragraph) given experimental data. Such distribution is defined by the following formula:

$$P\left(\left\{Params_j\right\}_{j=1}^{N+1} \mid \left\{Data_k\right\}_{k=1}^M\right) \propto \prod_{i=1}^M P\left(Data_i \mid \left\{Params_j\right\}_{j=1}^{N+1}\right) \cdot \prod_{j=1}^{N+1} P\left(Params_j\right) \quad 2.1$$

where *Params* are N+1 parameters described in the previous paragraph, *Data* are M experimental data points.

The right hand side of the equation consists of two parts (a product over *i* and a product over *j*), the former is called likelihood, and the latter is a prior distribution.

2.4 DIAGNOSTICS INVOLVED IN THE PROFILE RECONSTRUCTION

Two main diagnostics are used in the electron density profile reconstruction, namely interferometry and Thomson Scattering. Since the quality of the measurements is different in Tore Supra and JET, different relative weights between diagnostics are applied in the Profile Reconstruction (related to the likelihood in the section below).

Interferometry [7] provides measurements of electron density integrated along lines of sight, while Thomson Scattering provides local measurements [3].

We considered the Thomson scattering and the Electron Cyclotron Emission (ECE) diagnostics for the electron temperature reconstruction. The ECE was used for the Tore Supra dataset only since its measurements are consistent with the Thomson scattering data, while for the JET dataset the diagnostic gives two branches of measurements for low-field side and high-field side parts and features some consistency issues with Thomson scattering. Since the quality of the measurements is different in Tore Supra and JET, different relative weights between diagnostics are applied in the Profile Reconstruction (related to the likelihood in the section below).

To reconstruct the ion temperature profile an active charge exchange diagnostic was used.

2.5 ASSUMPTIONS OF THE BAYESIAN ANALYSIS

To calculate posterior distribution of the parameters defined by (2.1), we need to make some

assumptions. We described the diagnostics involved in the analysis and the parameters used. Now we should make assumptions about the prior probability distribution and the likelihood.

We assume that the prior probability distributions for the $N+1$ parameters of spline interpolation (described in II.a) are uniform, since we do not have a strong prior knowledge of the solution. As we have a number of local measurements (Thomson scattering and ECE for the electron temperature and charge exchange for the ion temperature profiles), we can determine boundaries of the prior distribution for each parameter based on these measurements. To be prudent about the outliers we define the center of the uniform distribution for a parameter as a median of the local measurements in the corresponding grid interval and then define the boundaries of the distribution as $[0.5*\text{median}; 1.5*\text{median}]$.

The likelihood used in our analysis was normal as we assumed the normality of the errors distribution for all the diagnostics. The error bars for electron temperature profile reconstruction are presented in the Table 2.1 below. All the error bars include but not necessarily equal to the instrumental error bars. They were chosen by comparing models with different values of error bars using Bayesian methods and choosing among them the values of error bars that describe the experimental data in the best way (it is so called model selection task in Bayesian analysis theory).

For the ion temperature profile reconstruction instrumental error bars specified in the database were used as the data are relatively accurate. They were typically of the order of 50–100eV, representing less than 10%.

Then using Monte Carlo Markov Chain algorithms implemented in a Python module pymc (Pymc) which make sampling from the posterior distribution according to the equation (2.1) we get the samples for all the parameters. Based on the samples obtained, we can calculate statistics on any quantities of our interest (for example, peaking and line-average temperature). The statistics also gives us 95% highest probability density intervals which are used in the comparison with the temperature profile predictions. Further in the paper we will discuss the model used for the prediction of electron temperature profile and current diffusion.

3. INTEGRATED MODELLING TOOLS

The novelty of the developed expert system lays in the systematic and automated comparison of plasma reconstruction results with models. In this work, models involving solving the transport equations are applied. To predict the reconstructed quantities we used METIS [1], a fast integrated modeling transport code. It is a simplified integrated modeling tool and its speed and robustness are the key advantages in view of automated analysis of a large amount of data. Nonetheless any other integrated modelling code may be easily plugged-in for the analysis.

The expert system that is discussed in this analysis was implemented within the framework of the European Integrated Tokamak Modeling Task Force (ITM-TF) [6]. Correspondingly all the results discussed were obtained using this framework. The two main motivations for this choice are i) the ITM-TF Data Model is tokamak-generic [11], thus the methods can then be applied to any

experiment ii) the link with Integrated Modelling tools, namely equilibrium identification codes and METIS for this particular application. Moreover, the ITM-TF Framework provides also methods for accessing data from various experiments, Tore Supra and JET in this application.

4. TEMPERATURE PROFILE RECONSTRUCTION AND VALIDATION OF HEAT TRANSPORT MODELS

In this section we develop automated comparison criteria between reconstruction and modelling for the detailed shape of temperature profiles. One of the simple heat transport models used in METIS, with three variations of one of its parameters, is tested against a chosen experimental dataset. This illustrates an application of the method to model validation.

4.1 HEAT TRANSPORT AND PREDICTION OF TEMPERATURE PROFILES IN METIS

The METIS code implements a simplified treatment of the heat transport equation in order to be a faster-than-real-time transport solver (an ITER pulse is simulated in about 1 minute of CPU time). To achieve this performance, METIS treats separately the time and radial dimensions of the transport equation [1] The time dimension is treated by solving a simple 0D equation for the plasma thermal energy content W_{th} :

$$\frac{dW_{th}}{dt} = -\frac{W_{th}}{\tau_E} + P_{loss} \quad 3.1$$

where τ_E is energy confinement time, and P_{loss} is the total power transported through the plasma separatrix by diffusion or convection mechanisms.

The radial dimension is treated by solving a 1D time independent transport equation for the electron and ion temperature profiles:

$$\begin{aligned} \frac{\partial T_e}{\partial x} &= \frac{-\int_0^x V' Q_e}{n_e \chi_e V' \langle |\nabla \rho|^2 \rangle} \\ \frac{\partial T_i}{\partial x} &= \frac{-\int_0^x V' Q_i}{n_i \chi_i V' \langle |\nabla \rho|^2 \rangle} \end{aligned} \quad 3.2$$

where Q_e and Q_i are the sums of all the electron and ion heat source terms, including the equipartition term Q_{ei} that is proportional to $(T_e - T_i)$; $\frac{\partial}{\partial x}$ is derivative of the plasma volume enclosed in a magnetic surface with respect to the normalised minor radius x , while $\langle |\nabla \rho|^2 \rangle$ is the surface average of the squared gradient of the toroidal flux coordinate. The diffusion coefficients χ_e and χ_i are assumed to be as follows:

$$\begin{aligned} \chi_e &= \kappa_0 \cdot (1 + K_E \cdot x^2) \text{ if } K_E > 0 \\ \chi_e &= \kappa_0 \cdot B g B \text{ if } K_E = 0 \\ \chi_e &= \kappa_0 \cdot q^{abs(K_E)} \text{ if } K_E < 0 \\ \chi_i &= \mu_{e,i} \cdot \chi_e \end{aligned} \quad 3.3$$

where $\mu_{e,i}$ is a scalar that is prescribed to be constant. Three different values of the parameter K_E are used in this work in order to test the automated comparison with three different heat transport model assumptions. The constant κ_0 is found by solving the following equation, which allows a normalization of the temperature profiles to the thermal energy content of the experiment:

$$\frac{3}{2} \int_{x=0}^1 (n_e \int_1^x \frac{\partial T_e}{\partial x} dx + n_i \int_1^x \frac{\partial T_i}{\partial x} dx) V' dx = W_{th} - W_0 \quad 3.4$$

Where W_0 is an offset related to the pressure boundary condition at the LCFS.

The electron density profile is calculated from simple scaling expressions for its edge value and peaking factor (using the model that assumes dependence of peaking factor on the ratio between saturation density and average density, i.e. model 1 of reference [12], while being constrained to follow the experimental line averaged density.

Although METIS is predicting both the electron and ion temperatures, we focus the comparison on the electron temperature since it is measured during the whole pulse while we have very few T_i measurements from charge exchange in our L-mode/ohmic data set.

4.2 STEPS OF THE ANALYSIS

The analysis was done in the following steps:

1. we first run the METIS code for the whole duration of the pulse to get predictions of electron and ion temperature profiles for three models of electron diffusion coefficient (ref. Formula 3.3)
2. we run an equilibrium identification code (Equinox [4] in this application) to have a description of plasma equilibrium
3. map experimental measurements on the equilibrium
4. run Bayesian analysis
5. Run comparison of predicted (step 1) and reconstructed (step 4) temperature profiles

4.3 DATABASE FOR THE ANALYSIS

A database of 21 Tore Supra and 14 JET shots has been selected to establish the automated comparison criteria. We chose one time slice per shot to perform the analysis in a stationary phase (i.e. plasma pressure does not evolve over several characteristic transport times). This is the same dataset as used in [12], where all analyzed time slices were taken in ohmic or L-mode phases of the discharge. Summary tables for the Tore Supra and JET databases are presented below.

4.4 DEVELOPMENT OF AUTOMATED COMPARISON FOR TORE SUPRA AND JET

To compare the reconstructed and the predicted profiles, we marked the agreement quality as “acceptable” or “not acceptable”. The “acceptable” agreement means that the predicted profile lies within or very close to the 95% Highest Probability Density (HPD) interval provided by the

Bayesian analysis. It also confirms that the gradients of the experimental profile are in agreement with the METIS predictions. An “acceptable” agreement provides a sort of mutual validation of the models used in the simulation and the Bayesian profile reconstruction, since it would be quite fortuitous that both would be “wrong” in the same way. The agreement is considered to be “not acceptable” if the simulation profile is strongly outside the 95 % HPD interval.

The discrepancy estimators used for the automated comparison involve the local temperature values but also the slope of the profiles via a “gradient” and peaking factor discrepancy estimators: relative gradient discrepancy: a ratio between minimal distance of profile gradient predicted by METIS and one of its 95% HPD boundaries (the “gradient” is calculated as $T(0.3) - T(0.7) / \rho(0.3) - \rho(0.7)$ between $\rho = 0.3$ and $\rho = 0.7$)

- relative peaking discrepancy: a ratio between minimal distance of predicted peaking factor (a ratio between central temperature and the average one) and one of its 95% HPD boundaries
- relative integral discrepancy: a ratio between minimal distance of METIS line-average integral and one of its 95% HPD boundaries
- relative squared profile discrepancy on the interval [0; 0.8] for the normalized flux coordinate r : a sum of squares of ratios between predicted profile and the closest boundary of 95% HPD interval (0 if the predicted profile is within the HPD interval boundaries)
- These discrepancy estimators are equal to zero when the related quantity predicted by METIS is within the 95% boundaries of the reconstructed experimental profile. A small tolerance has been added in the “comparison acceptance” criteria from the consideration of a few Tore Supra cases which were marginally outside of the 95 % HPD and would have been accepted in a “by the eyes” comparison.

In addition to these comparison discrepancy estimators, the quality of the experimental profile reconstruction is judged from the width of the 95% HPD interval for gradient of the reconstructed profile: a ratio between upper and lower bound of the 95% HPD for gradient. If it is too high, it may point to the troubles in the experimental data.

The exact value of the criteria used to consider the agreement as acceptable in each case, have been derived from the Tore Supra database only (see Table 3). Then they have been applied as such to the JET dataset. They also provided a satisfying classification of the various pulses for the JET case, which emphasizes the tokamak-generic character of the analysis.

Examples of acceptable and not acceptable quality agreement are shown correspondingly on Figures 1 and 2. Figure 1 illustrates a case where the predicted electron temperature profile lies on almost all radial points within 95% highest probability range or is very close to it and therefore the analysis concludes that the predictions and experimental data are in agreement. Conversely, on Figure 2 is shown an example of not acceptable agreement. The predicted electron temperature profile is visibly significantly outside of the 95% HPD range and the profile slope is also strongly outside its 95% HPD range.

4.5 APPLICATION OF THE METHOD FOR MODEL VALIDATION

Using the criteria derived in the previous part, we applied the analysis for the diffusion coefficient model validation. We used three models as per Formula 3.3 with K_E equals to 3, 0, and -1.5 . The results of our analysis are presented in the Tables 4 and 5 for Tore Supra and JET correspondingly.

A summary on the results of our analysis is presented in the Table 6. We may see that all three models for diffusion coefficient as per Formula 3.3 with K_E equals to 3, 0, and -1.5 give not acceptable agreement in most of cases.

The conclusion of this analysis is the following: first no pulse/time slice has been rejected from too large width of the gradient HPD interval, which indicates that all experimental temperature profile reconstructions could be done in a successful way. Second, all three options tested for the transport model poorly fail to adequately reproduce the experimental profiles in most cases, although the first option ($K_E = 3$, i.e. as per Formula (3.3)), has slightly better statistics than the others (20% of successful cases on the Tore Supra dataset, 14% on the JET data set). This is not surprising, since the heat transport models used in METIS are rather simplistic while our comparison criteria were rather demanding in terms of agreement quality on the value and shape of the temperature profiles. While such simplified, scaling-based models are usually sufficient for fast scenario simulation (the main purpose of the METIS code), more sophisticated and first-principles based models are necessary for a detailed prediction of the temperature profile shape. Although it would require a longer computation time, it would be possible to apply the same automated comparison method and criteria replacing METIS with a classical Integrated Modelling suite such as CRONOS [2]. The CRONOS suite of codes for integrated tokamak modelling, (2010) enabling solving rigorously the heat transport equations with advanced heat transport models.

4.6 DATA CONSISTENCY CHECK OF MULTI-PROFILES RECONSTRUCTION WITH THE ENERGY CONTENT

The Bayesian reconstruction of the T_e , T_i and N_e profiles already allowed for consistency checks for each profile. An interesting further check is to verify their overall consistency at a global level, namely by checking the plasma energy content. From these profiles and assumptions on the ion species densities, one can reconstruct with Bayesian statistics the thermal energy content

$$W_{th} = \frac{3}{2} 2\pi \int (n_e(\rho) \cdot T_e(\rho) + n_i(\rho) \cdot T_i(\rho)) \cdot \frac{dV}{d\rho} \cdot d\rho \quad 7.1$$

where ρ is the normalized toroidal coordinate, V is the volume enclosed within the surface of coordinate ρ , n_e , T_e , n_i , T_i are electron density, electron temperature, ion density and ion temperature profiles respectively.

The ion densities are calculated by METIS assuming the proportionality to the electron densities profiles, the coefficient of proportionality is calculated from the condition of electroneutrality which takes into account the effective charge (experimental one for the Tore Supra shots and the one

calculated using the scaling law from [5]), composition of the plasma (Deuterium in all cases) and the impurity accumulation (calculated using neoclassical simplified formula depending on density peaking and temperature peaking from [9]).

The thermal energy is not measured directly but can be compared to the diamagnetic energy content measurement, provided an assumption (or a modelling) of the fast particle contribution to the diamagnetic energy. This can again be estimated by METIS (or any other integrated modelling code). The comparison can be used or interpreted in two ways, either as a data consistency check if the models have been validated for the conditions of the pulse or as a model validation check. Summary table for the Tore Supra and JET shots used for the calculation of the diamagnetic energy content is presented below.

To calculate the probability distribution of the thermal energy we used the statistics obtained in the profile reconstruction part for all the coefficients of electron density, electron and ion temperature profiles. We then approximated the statistics of every coefficient with the continuous distribution functions using kernel density estimation technique. Using the Metropolis-Hastings algorithm we sampled from the continuous distribution functions to obtain the probability distribution for thermal energy. We calculated 95% highest probability ranges and compared them to the measured diamagnetic energy content minus the modelled fast particle energy. The quality of the agreement is determined. When this quantity is within the Bayesian range or when the discrepancy with respect to its closest bound does not exceed the uncertainty of the diamagnetic energy (typically 10%), the quality of the agreement is judged to be acceptable. If the discrepancy is between 10 and 20%, the agreement is judged marginally acceptable, while it is “not acceptable” if the discrepancy exceeds 20%.

This procedure has been applied to selected time slices from four Tore Supra shots and three time slices of a JET shot. The results of the comparison are presented in the Table 8.

The six analyzed time slices indicate a good agreement, thus confirming the consistency of the profile reconstructions.

5. QUANTIFICATION OF UNCERTAINTY ON CURRENT DIFFUSION

Simulations of current diffusion using prescribed temperature and density profiles obtained from experimental measurements is the basic kind of analysis carried out for a tokamak pulse. It allows in particular obtaining details of the current profile that are not always measured with enough details in some experiments. Current diffusion results strongly depend, among other parameters, on the electron temperature profile through the neoclassical resistivity. Therefore uncertainties in the electron temperature profile reconstruction (which is fed as an input to such “interpretive” simulations) have a large impact on the results of the current diffusion. In this paragraph, we present an application of our automated analysis ideas to the quantification of the uncertainties on current diffusion.

5.1 STEPS OF THE ANALYSIS

To validate current diffusion models we continued our analysis in the following way (for a given plasma discharge):

1. we reconstruct the electron temperature and density profiles from Bayesian analysis for multiple time slices of the discharge, covering its full duration with a time slice every 0.1s. Time slices are analyzed independently and no attempt is made to correlate measurements in time.
2. we made three METIS simulations of the whole plasma discharge using the following types of electron temperature profiles: the mean profiles, the upper bound of 95% highest probability density interval profiles (i.e. “the highest possible profiles”), and the lower bound of 95% highest probability density interval profiles (i.e. “the lowest possible profiles”) For all the simulations we use the mean electron density profiles. At every time slice, the simulation with the highest temperature will also have the lowest flux consumption (lowest resistivity and highest non-inductive current drive efficiencies) and the slowest current diffusion, therefore representing the lowest/slowest possible result given the uncertainty on the electron temperature profile.
3. we made a comparison of the poloidal flux consumption trends and MHD activity markers obtained from three runs with the experimental one. Here the comparison is made on the appearance time of sawteeth on the ECE diagnostic and the occurrence time of the $q = 1$ surface in the simulation.

5.2 PREDICTION OF CURRENT DIFFUSION

The current diffusion model in METIS is the same as was implemented in CRONOS 1.5D code ([2] The CRONOS suite of codes for integrated tokamak modelling, 2010) [10]. It solves the following equation for the poloidal flux Ψ on a uniform normalized toroidal flux coordinate Ψ grid (which consists of 21 nodes and does not depend on time):

$$\left. \frac{\partial \Psi}{\partial t} \right|_{\rho_{norm}} = \frac{\langle \frac{|\nabla \rho|^2}{R^2} \rangle}{\mu_0 \sigma_{||} \rho_m^2 \langle \frac{1}{R^2} \rangle} \frac{\partial^2 \Psi}{\partial \rho_{norm}^2} + \left\{ \frac{\langle \frac{|\nabla \rho|^2}{R^2} \rangle}{\mu_0 \sigma_{||} \rho_m^2 \langle \frac{1}{R^2} \rangle} \frac{\partial}{\partial \rho_{norm}} \left[\ln \left(\frac{\partial v}{\partial \rho_{norm}} \langle \frac{|\nabla \rho|^2}{R^2} \rangle \right) \right] + \frac{\rho_{norm}}{\rho_m} \frac{d\rho_m}{dt} + \frac{\rho_{norm}}{2B_0} \frac{dB_0}{dt} \right\} \frac{\partial \Psi}{\partial \rho_{norm}} + \frac{B_0}{\sigma_{||} F \langle \frac{1}{R^2} \rangle} j_{ni} \quad 3.5$$

where $\left. \frac{\partial \Psi}{\partial t} \right|_{\rho_{norm}}$ is a time derivative of the poloidal flux at a given radial position ρ_{norm} , $\sigma_{||}$ denotes the parallel conductivity (calculated according to the Sauter model [15]), F is the diamagnetic function, j_{ni} is the current density driven by the non-inductive sources, R is the major radius, μ_0 is the magnetic permeability of free space, ρ_m the value of ρ at the last closed flux surface, and the normalised toroidal flux coordinate $\rho_{norm} = \frac{\rho}{\rho_m}$. The notation $\langle \rangle$ indicates a magnetic flux surface

average, defined as the volume average of a quantity around a flux surface of radial coordinate ρ , i.e. in an elementary volume dV enclosed between two magnetic surfaces distant of $d\rho$.

The line-average effective charge measurement from bremsstrahlung is used to prescribe the effective charge, assuming a flat profile.

Non-inductive current drive external sources (NBI for the JET shot, LHCD for the Tore Supra one) are calculated self-consistently by the models included in METIS. The model for LHCD efficiency is the empirical model described in [8].

METIS also implements a sawtooth model that accounts for the time-averaged effects of sawteeth. Applied here to the current diffusion, it prevents the q -profile from going below 1 by clamping it to the $q = 1$ surface.

5.3 RESULTS

First we analyse Tore Supra Pulse No: 47658, an L-mode pulse featuring two plateaus of LHCD power, ($\sim 4.5\text{MW}$ from $t = 5$ to 10s , then $\sim 3.3\text{MW}$ from $t = 10$ to 12s).

A first global analysis of the flux consumption is shown on the Figure 4. The flux consumption of the simulation using the mean temperature profiles are in excellent agreement with the experimental measurement, which provides a simultaneous validation of the current diffusion model used (including the LH current drive efficiency) and the reconstructed T_e profiles during the various phases of the pulse. The two other simulations with highest and lowest profiles in the 95% HPD interval introduce a confidence interval around the simulation with mean profiles. Nonetheless such a global view is integrating the instantaneous flux consumption over the whole pulse. There can be cases where the flux consumption is overestimated during a particular phase of the pulse, then this overestimation is later on compensated by an underestimation of the flux consumption in another phase, always staying within the confidence interval. Therefore the global analysis should be supplemented by an instantaneous analysis of whether the modelled flux consumption is consistent with the confidence interval of the electron temperature at a given time slice. To do this, we have calculated the time derivative of the consumed flux and smoothed it using Savitzky-Golay filtering procedure implemented in MATLAB [13]. The results are presented on Figure 5.

To develop an automated method for the comparison of derivatives of consumed flux we calculated the discrepancy between i) the experimental values and the closest boundary of the highest probability density range and ii) the experimental values and the mean temperature simulation. The discrepancy then was normalized to the maximum loop voltage that would be obtained in a steady state where the current would be fully inductively driven, which is equal to the plasma current times plasma resistivity (estimated using the mean electron temperature). The results are presented on the Figure 6. The first discrepancy estimator is zero when the flux time derivative within the confidence interval and therefore allows determining whether the experimental flux consumption is within or outside the T_e errorbars. The second one allows the relevance of a single simulation, done with the mean T_e . The normalized discrepancy is chosen instead of the relative discrepancy, for two reasons. First, in

phases with large non-inductive current drive, the flux consumption tends towards zero, making the relative discrepancy very large. Moreover, in such a case, the discrepancy would be due essentially to the non-inductive current models, for which the temperature dependence is weaker than for the resistive flux consumption in ohmic phases, i.e. the discrepancy has less probability to arise from the electron temperature uncertainties.

A threshold of ± 0.3 is chosen to define an acceptable agreement in the automated comparison process. This value is chosen so that the system would detect the flux consumption deviation between the experiment and the simulation with mean T_e occurring around $t = 12$ s on this Tore Supra case. Indeed, a human judgment of figure 4 would conclude that this is the only time where a significant deviation is observed. The idea is that the comparison criterion value provides the same conclusion, in a quantified way so that it can be automatized.

For the Tore Supra case, the discrepancy with the confidence interval (red curve on Figure 6) is almost always within the acceptability threshold, indicating that the experimental flux consumption is consistent with the electron temperature uncertainties. It does not imply that the T_e uncertainties are necessarily the cause of the discrepancy between experiment and the mean T_e simulation, but they could potentially explain it.

When the discrepancy with the confidence interval is within the acceptability threshold, one can use the two HPD simulations to determine the confidence interval on the safety factor profile. This is illustrated for the Tore Supra case at $t = 2$ s in figure 7.

We can also verify that MHD markers dynamics, e.g. the time of appearance of sawteeth, are consistent with the confidence interval.

We now apply the same analysis to the carbon wall JET Pulse No: 75225 (hybrid scenario). An overview of its scenario is shown on the Figure 9. A high level of NBI power is injected just after a plasma current overshoot in order to optimize the current profile and freeze it as long as possible during the H-mode phase (from $t \sim 5$ s to 10.5s). The flux consumption in this phase is close to 0, owing to almost fully non-inductive current drive. It is even negative (transformer recharge) during the reduction of the plasma current after the overshoot.

Applying the same procedure as in the Tore Supra case, a set of three simulations is carried out using the recommended Z_{eff} processing that can be found in the JET database, namely the values in PPF/KS3/ZEFV, corresponding to a vertical line of sight of bremsstrahlung measurement. The results are indicated on the Figures 10-12 (the consumed flux, the time derivative, and the absolute discrepancy).

In this case, the discrepancy between the experimental values and the HPD range simulations (the blue line on the Figure 12) stays within the acceptable threshold throughout the whole pulse except for the transitional phases where the neutral beam injection was switched on and off (around $t = 5$ s and $t = 11$ s) and a few time slices in between where the discrepancy is explainable by the noise in the effective charge measurements.

Figure 12 illustrates the confidence interval on the q-profiles obtained at $t = 7.0$ s.

CONCLUSION

The present work was devoted to the development of an automated comparison method between Bayesian reconstruction of plasma profiles and time dependent solutions of the transport equations. Two major applications have been shown: the former is aimed at comparing electron and ion temperature profiles to heat transport modelling. This quite classical type of analysis has been fully automated and the highest probability density intervals coming from the Bayesian reconstruction have been used to define various comparison criteria on the temperature profile shape (average gradient, peaking factor,..). This method can be applied to model validation of a simple heat transport model with three radial shape options. It has been tested on a database of 21 Tore Supra and 14 JET shots. All three choices of the radial shape parameter have been found not to meet the “acceptable agreement” criteria, indicating that more sophisticated, physics based transport models should be used for such detailed comparison of the temperature profile shape. Another application of the multi-profile reconstruction which has been carried out (n_e , T_e and T_i) is a data consistency check on the plasma energy content.

The second application aims at quantifying uncertainties due to the electron temperature profile in current diffusion simulations. A systematic reconstruction of the T_e profiles is first carried out for all time slices of the pulse. The Bayesian 95% highest probability density intervals on the T_e profile reconstruction are then used for i) data consistency check of the flux consumption and ii) defining a confidence interval for the current profile simulation. The latter can be further used to compare with possible MHD markers such as the onset time of sawteeth. The method has been applied to one Tore Supra pulse and one JET pulse.

The implementation of both applications is tokamak-generic as was performed using the ITM-TF Framework. The proposed method therefore provides a combination of automated comparison between simulation and experiment, data consistency checks and uncertainty quantification in simulations, all based on the highest probability density intervals arising from Bayesian profile reconstruction.

Although Bayesian analysis is an attractive and rigorous method to calculate error bars, it is not employed in a routine way in present fusion experiments. Our hope is that our work will help to spread its usage. The idea of a unique integrated modelling platform for deploying both plasma reconstruction and predictive tools provides the opportunity of using a whole range of predictive models and even to integrate some of them directly in the reconstruction if some measurements are missing. It also allows a variety of high order data consistency checks, such as the diamagnetic energy content which involves three profile reconstructions and assumptions on the impurity and fast particles content, and the verification of the consistency of the flux consumption. Our work provides a prototype implementation of this idea, resulting in a tokamak generic and automated tool to deal with the massive amount of data to be produced by long pulse plasma experiments.

ACKNOWLEDGEMENTS

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	Tore Supra	JET
Thomson Scattering	20% + 0.1keV	20% + 0.1keV
ECE	5% + 0.05keV	Not used

Table 2.1: Error bars used in the Bayesian analysis.

Shot	Time, s	Toroidal field, T	Plasma current, MA	Central electron temperature, keV	Central density, $\times 10^{19}, \text{m}^{-3}$	NBI power, MW	LH power, MW	ICRH power, MW	Ohmic heating power, MW
45175	9.5	3.84	1.00	1.32	7.47	0.00	1.47	0.00	1.42
45552	9.5	3.84	1.00	1.82	3.79	0.00	0.59	0.00	0.84
46982	11.1	3.83	0.61	1.64	2.75	0.00	1.82	0.00	0.28
47011	10.0	3.84	1.00	1.69	4.94	0.00	0.00	0.72	1.20
47067	10.0	3.79	0.71	1.94	3.12	0.00	3.05	0.00	0.16
47092	10.0	3.74	1.00	1.78	4.81	0.00	0.00	0.83	1.10
47096	4.0	3.74	1.00	1.47	4.49	0.00	0.00	0.00	1.41
47160	3.3	3.84	1.00	1.53	4.06	0.00	0.00	0.00	1.17
47170	8.6	3.69	1.00	2.37	3.78	0.00	0.00	0.00	0.75
47171	9.7	3.69	1.00	2.23	3.46	0.40	0.00	0.00	0.73
47310	27.6	3.77	0.70	1.97	3.13	0.56	0.13	0.00	0.44
47324	10.5	3.81	1.06	2.70	5.82	0.62	1.44	0.00	0.61
47327	10.5	3.81	1.07	2.87	5.80	0.00	1.69	0.00	0.50
47654	12.1	3.78	0.91	2.93	3.96	0.60	3.77	0.00	0.23
47657	10.0	3.78	1.50	2.06	5.90	0.00	0.83	0.00	1.30
47658	4.0	3.77	1.30	2.48	5.27	0.00	2.34	0.00	0.75
47659	5.0	3.78	1.30	2.33	5.51	0.00	2.74	0.00	0.57
47663	7.9	3.78	1.21	3.24	5.28	0.59	4.28	0.00	0.45
47666	11.0	3.78	1.50	1.40	5.23	0.00	4.06	0.00	0.58
48102	3.1	3.68	1.00	2.45	2.82	0.00	0.00	0.00	0.75
48317	10.2	3.74	0.71	2.93	3.86	0.00	3.76	1.48	0.17

Table 1: Summary of the shots characteristics for the Tore Supra dataset: the data are taken from the METIS code, which in turn takes it from the Tore Supra database (the central density is estimated based on the peaking factor scaling laws, the central temperature is estimated based on the solution of time-independent transport equation).

Shot	Time, s	Toroidal field, T	Plasma current, MA	Central electron temperature, keV	Central density, $\times 10^{19}, \text{m}^{-3}$	NBI power, MW	Ohmic heating power, MW
75225	47.5	2.03	1.69	4.55	3.87	7.34	0.61
77895	43.0	2.69	1.47	1.05	1.88	0.00	0.92
77914	45.0	2.32	2.43	1.94	2.12	0.00	1.33
77922	45.4	2.32	2.25	1.45	2.14	0.00	1.46
77933	45.8	2.34	2.65	1.52	2.38	0.00	1.99
82120	47.9	2.20	1.97	1.39	3.62	0.00	1.61
82536	52.9	2.69	2.45	1.81	4.32	0.00	2.06
82541	52.0	2.64	2.46	1.51	5.05	0.00	4.23
84541	43.5	1.73	1.57	1.11	2.11	0.00	1.23
84543	43.5	1.73	1.57	1.10	2.08	0.00	1.21
84545	43.5	1.73	1.57	1.12	2.10	0.00	1.20
84792	43.5	1.73	1.58	1.06	2.09	0.00	1.19
84795	43.5	1.72	1.59	1.04	2.08	0.00	1.19
84796	43.5	1.72	1.58	1.11	2.08	0.00	1.17

Table 2: Summary of the shots characteristics for the JET dataset: the data are taken from the METIS code (the central density is estimated based on the peaking factor scaling laws; the central temperature is estimated based on the solution of time-independent transport equation). The Pulse No's: 75225–77933 are the ones with carbon wall and the Pulse No's: 82120–84796 are the ones with ITER-like wall.

Quantity	Value
relative gradient discrepancy	$\leq 3\%$
relative peaking discrepancy	$\leq 2\%$
relative integral discrepancy	$\leq 8\%$
relative squared profile discrepancy on the interval [0; 0.8]	≤ 0.06
width of the HPD interval for gradient	≤ 3

Table 3: Summary of the analysis criteria to classify the agreement as “acceptable”

Shot	K_E		
	3	0	-1.5
45175	OK	NO	NO
45552	NO	NO	NO
46982	NO	NO	NO
47011	NO	NO	NO
47067	NO	NO	NO
47092	OK	NO	NO
47096	OK	NO	NO
47160	NO	NO	NO
47170	NO	NO	NO
47171	OK	NO	NO
47310	NO	NO	NO
47324	NO	NO	NO
47327	NO	NO	NO
47654	NO	NO	NO
47657	NO	OK	NO
47658	NO	NO	NO
47659	NO	NO	NO
47663	NO	NO	NO
47666	NO	NO	NO
48102	NO	NO	NO
48317	NO	NO	NO

Table 4: Results of the automated comparison for Tore Supra database with three METIS runs: with K_E equals to 3, 0, and -1.5. “OK” means that the agreement is acceptable, “NO” corresponds to not acceptable agreement.

Shot	K_E		
	3	0	-1.5
75225	NO	NO	NO
77895	NO	NO	NO
77914	NO	NO	NO
77922	NO	NO	NO
77933	NO	NO	NO
82120	NO	NO	NO
82536	NO	NO	NO
82541	OK	NO	OK
84541	OK	OK	NO
84543	NO	NO	NO
84545	NO	NO	NO
84792	NO	NO	NO
84795	NO	NO	NO
84796	NO	NO	NO

Table 5: Results of the automated comparison for JET database with three METIS runs: with K_E equals to 3, 0, and -1.5 . “OK” means that the agreement is acceptable, “NO” corresponds to not acceptable agreement.

Tokamak	Agreement	K_E		
		3	0	-1.5
Tore Supra	Acceptable	4	1	0
	Not acceptable	17	20	21
Total		21	21	21
JET	Acceptable	2	1	1
	Not acceptable	12	13	13
Total		14	14	14

Table 6: Summary table on results of the automated comparison for Tore Supra and JET databases with three METIS runs: with K_E equals to 3, 0, and -1.5 .

Tokamak	Shot	Time, s	Toroidal field, T	Plasma current, MA	Central electron temperature keV	Central density, $\times 10^{19}, \text{m}^{-3}$	NBI power MW	LH power, MW	Ohmic heating power, MW
Tore Supra	47655	10.3	3.77	0.61	2.37	3.39	0.41	4.59	0.02
Tore Supra	47656	10.4	3.78	1.21	3.75	4.82	0.62	4.48	0.42
Tore Supra	47176	8.1	3.38	1.30	1.91	5.38	0.59	0.00	1.16
JET	75225	5.0	2.04	1.75	3.65	2.36	7.08	0.00	0.60
JET	75225	7.5	2.03	1.69	5.40	3.85	7.35	0.00	0.44
JET	75225	10.0	2.02	1.68	5.51	3.63	7.18	0.00	0.24

Table 7: Summary of the shots characteristics for the dataset for the calculation of the diamagnetic energy content: the data are taken from the METIS code (the central density is estimated based on the peaking factor scaling laws, the central temperature is estimated based on the solution of time-independent transport equation). The JET Pulse No: 75225 is one with carbon wall.

Tokamak	Shot	Time slice, s	W_{dia} (local database), kJ	W_{fast} (NEMO and SPOT codes), kJ	W_{th} ($W_{\text{dia}} - W_{\text{fast}}$), kJ	W_{th} (bayesian range), kJ		Discrepancy, %	Quality of agreement
A	B	C	D	E	F=D-E	from G	to H	F vs. closest G or H	
Tore Supra	47655	10.3	260.0	0.0	260.0	261.8	293.1	1%	OK
Tore Supra	47656	10.4	472.4	0.0	472.4	459.0	522.7	0%	OK
Tore Supra	47176	8.1	336.7	0.0	336.7	296.9	345.9	0%	OK
JET	75225	5.0	2309.7	1420.0	889.7	895.6	1037.0	1%	OK
JET	75225	7.5	4687.1	1450.0	3237.1	2984.9	3565.3	0%	OK
JET	75225	10.0	4851.8	1460.0	3391.8	3286.5	4056.3	0%	OK

Table 8: Summary table on results of the quantification of uncertainty on energy content. The columns G and H indicate the 95% highest probability range for W_{th} obtained by sampling from the reconstructed profiles. The column F presents the values of the thermal energy as difference between the measured diamagnetic energy (from local tokamak database) and fast particles energy calculated by the NEMO (Schneider & al, Simulation of the neutral beam deposition within integrated tokamak modelling frameworks, 2011) and the SPOT [17]. On alpha particle effects in tokamaks with a current hole, 2005) codes. The last column contains the discrepancy between the closest bound of the HPD range (columns G and H) and the column F (if the values from the column F are outside the range).

Shot	Te profiles used in METIS	Sawteeth onset time, s
JET@75225	HPD up	8.0
	mean	5.4
	HPD low	4.6
	Experiment	5.2

Table 9: Summary table on results of the comparison of sawteeth onset time for the Tore Supra shot Pulse No: 47658. The second column indicates what type of temperature profiles are used as an input to the METIS code. The experimental sawteeth onset time is determined from ECE measurements, while in METIS it is determined by the onset of the q-profile clamping to the $q = 1$ surface.

Shot	Te profiles used in METIS	Sawteeth onset time, s
JET@75225	HPD up	8.0
	mean	5.4
	HPD low	4.6
	Experiment	5.2

Table 10: Summary table on results of the comparison of sawteeth onset time for the JET Pulse No: 75225. The second column indicates what type of temperature profiles are used as an input to the METIS code. The experimental sawteeth onset time is determined from HRTS measurements, while in METIS it is determined by the onset of the q-profile clamping to the $q = 1$ surface.

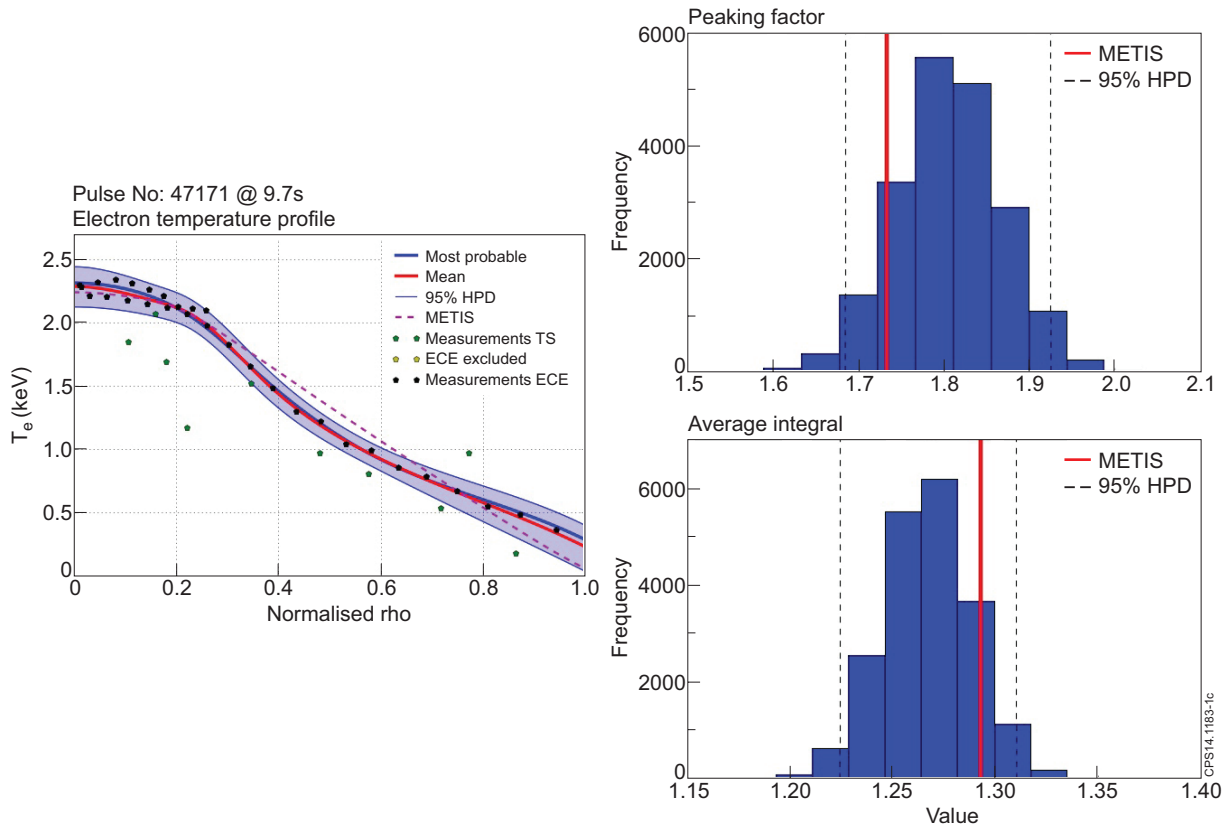


Figure 1: Example of acceptable agreement: electron temperature profile for the Pulse No: 47171. Left plot shows the mean (read) profiles and 95% HPD interval (blue area) obtained by Bayesian analysis and METIS result (dashed magenta line); right plots show distribution for the peaking factor and average integral, their 95% HPD interval (range between dashed lines) and the METIS values (red lines).

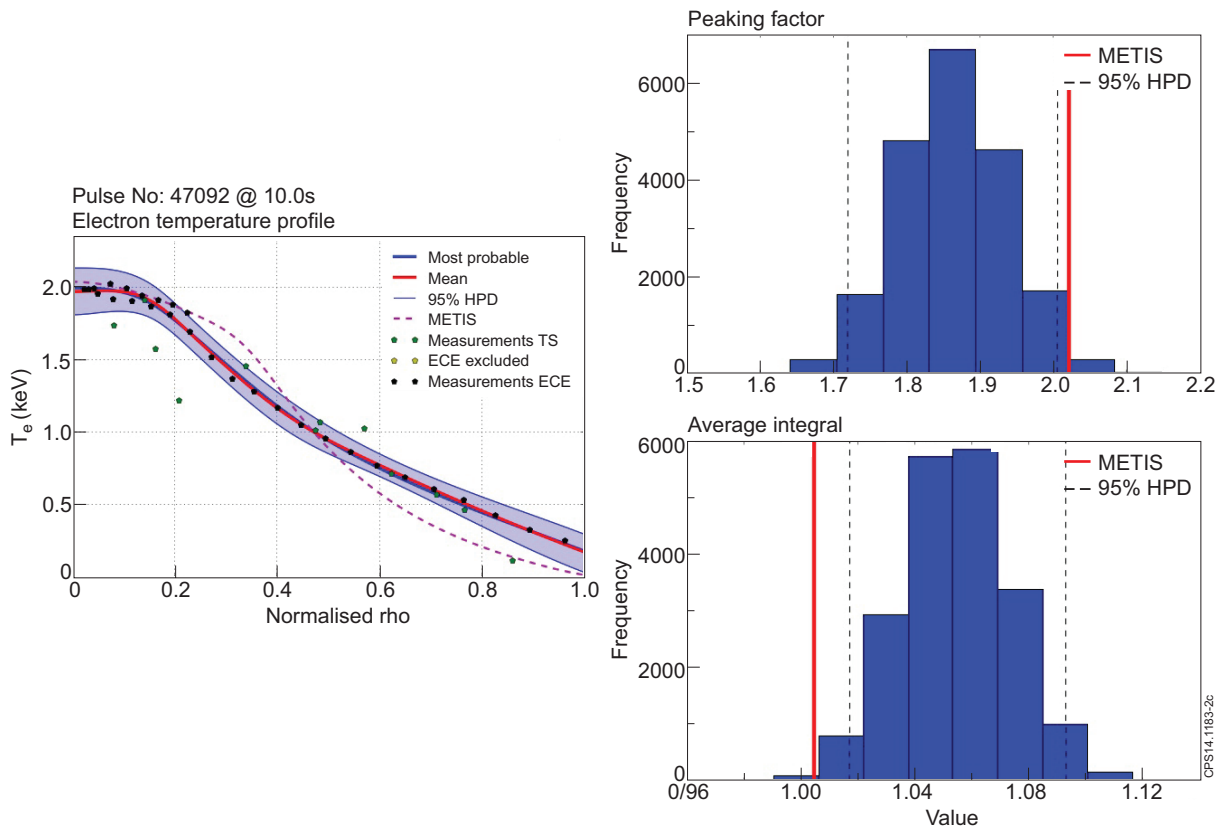


Figure 2: Example of not acceptable agreement: electron temperature profile for the Pulse No: 47092. Left plot shows the mean (read) profiles and 95% HPD interval (blue area) obtained by Bayesian analysis and METIS result (dashed magenta line); right plots show distribution for the peaking factor and average integral, their 95% HPD interval (range between dashed lines) and the METIS values (red lines).

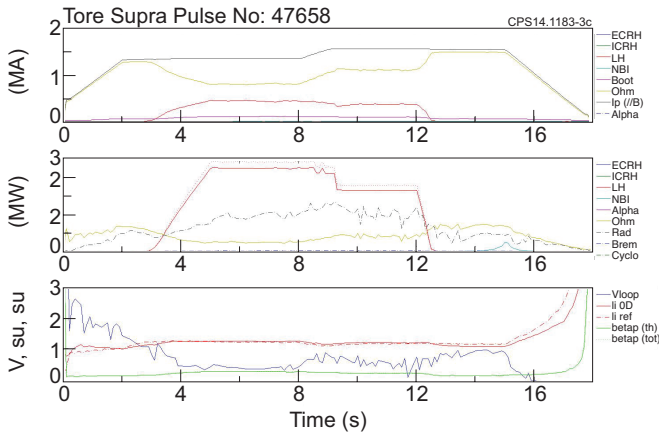


Figure 3: Overview of the Tore Supra Pulse No: 47658. The upper plot shows plasma current and its components throughout the length of the shot. The middle plot shows the heating scheme. The bottom plot shows other important parameters like loop voltage, li , β_p .

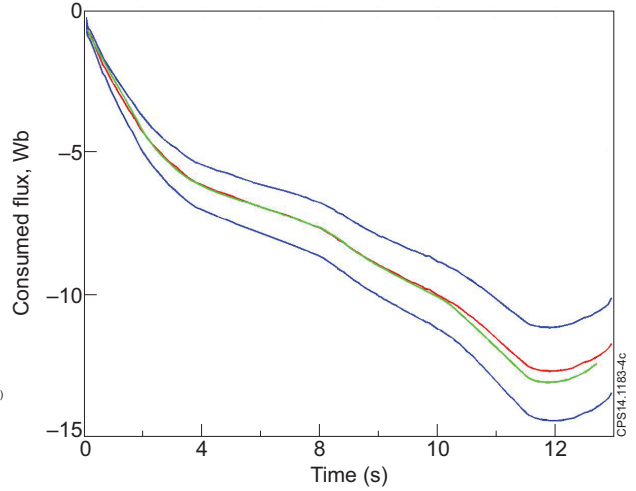


Figure 4: Consumed poloidal flux comparison for the Tore Supra Pulse No: 47658. The blue lines shows the results of the METIS run with HPD interval profiles as an input; the red line is the result of the METIS run with the mean profiles as an input. The green line is the experimental measurements. Note that the offset poloidal flux consumption is unknown thus it was determined as the difference between the mean METIS run and experimental trend in the beginning of the shot.

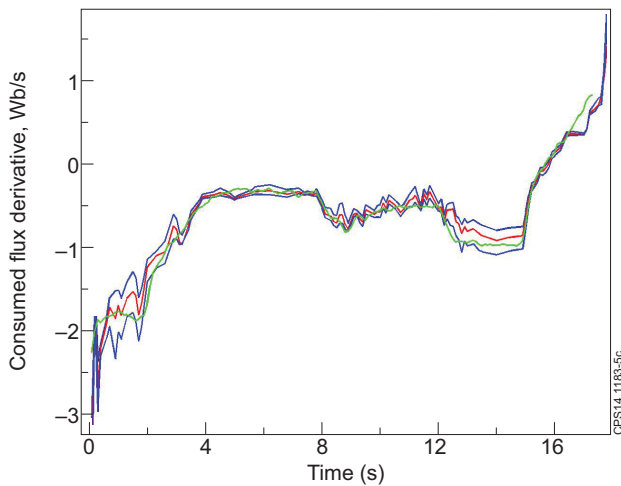


Figure 5: Comparison of filtered time derivatives of the consumed poloidal flux for the Tore Supra Pulse No: 47658. The blue lines shows the results of the METIS run with HPD interval profiles as an input; the red line is the result of the METIS run with the mean profiles as an input. The green line is the experimental measurements.

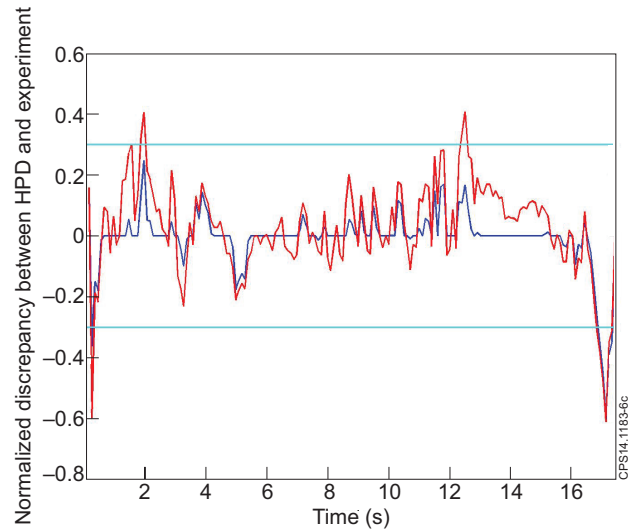


Figure 6: Normalized discrepancy between experimental values for the consumed flux derivative and the closest boundary of the highest probability density range simulations (in blue) and the normalized discrepancy between experimental values and the mean simulation (in red) for the Tore Supra Pulse No: 47658. The cyan lines show the boundaries of acceptable agreement (± 0.3).

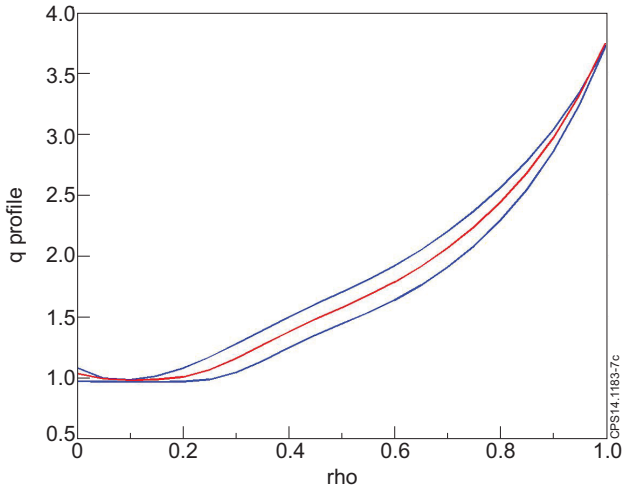


Figure 7: q -profiles at $t = 2s$ for the Tore Supra Pulse No: 47658. The red line corresponds to the METIS simulation with the mean T_e profiles. The two blue lines correspond to the METIS simulations with the highest and lowest possible T_e profiles.

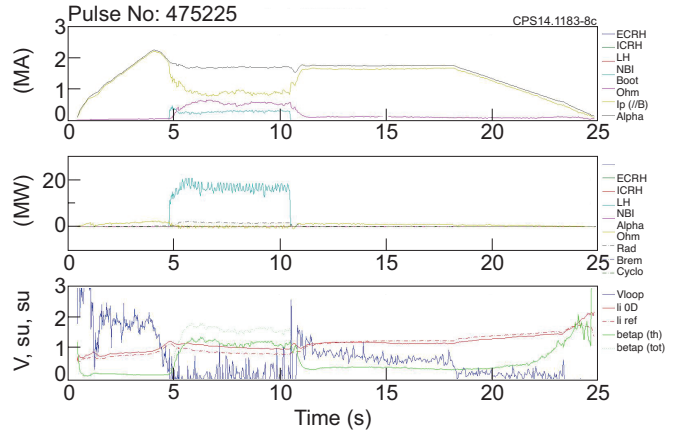


Figure 8: Overview of the JET Pulse No: 75225. The upper plot shows plasma current and its components throughout the length of the shot. The middle plot shows the heating scheme. The bottom plot shows other important parameters like loop voltage, l_i , β_p .

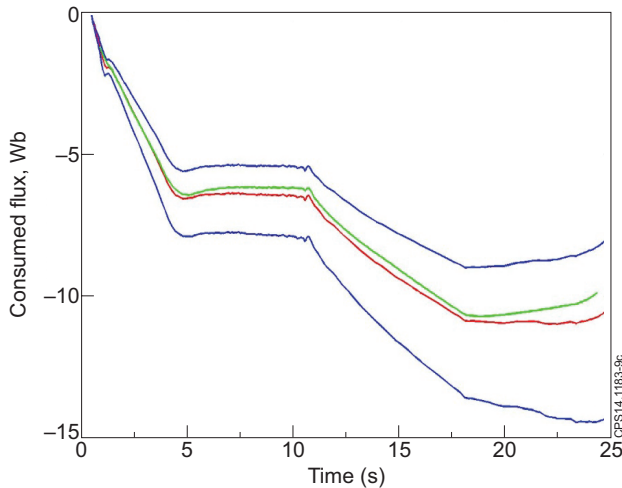


Figure 9: Consumed poloidal flux comparison for the JET Pulse No: 75225. The red line corresponds to the METIS simulation with the mean T_e profiles. The two blue lines correspond to the METIS simulations with the highest and lowest possible T_e profiles. The green line is the experimental flux consumption. Offset calculated at the initial time of the simulation and profile reconstruction.

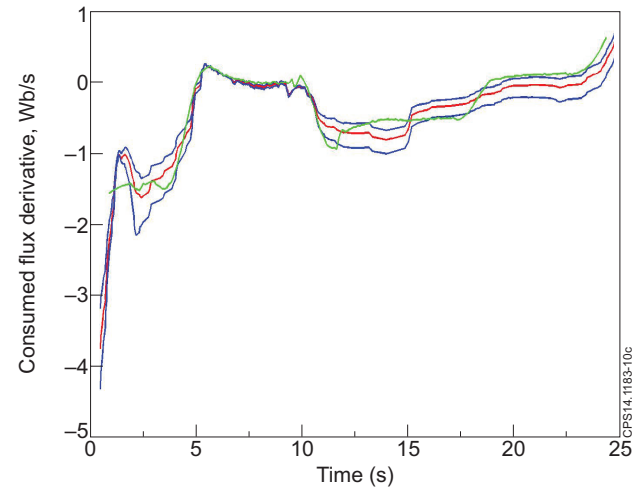


Figure 10: Comparison of filtered derivatives of consumed poloidal flux for the JET Pulse No: 75225. The blue lines shows the results of the METIS run with HPD interval profiles as an input; the red line is the result of the METIS run with the mean profiles as an input. The green line is the experimental measurements.

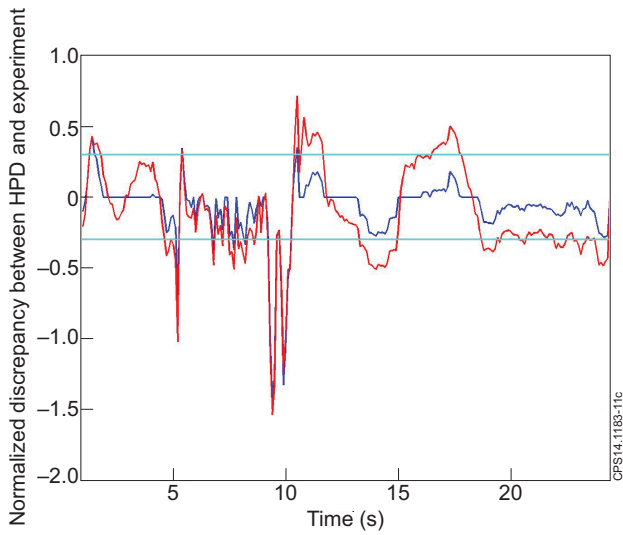


Figure 11: Normalized discrepancy between experimental values for the consumed flux derivative and the closest boundary of the highest probability density range simulations (in blue) and the relative discrepancy between experimental values and the mean simulation (in red) for the JET Pulse No: 75225. The cyan lines show the boundaries of acceptable agreement (± 0.3).

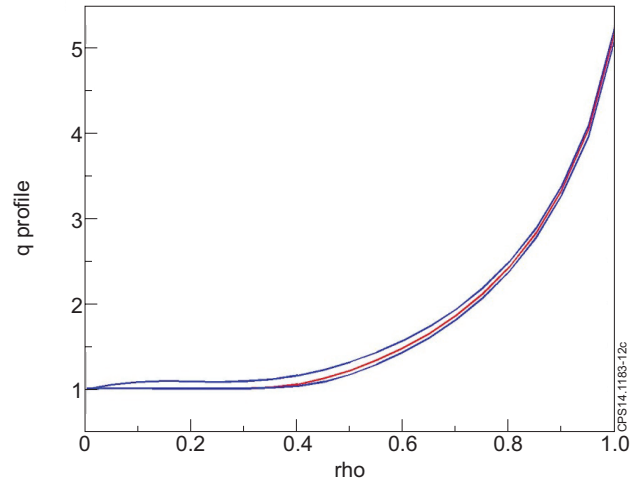


Figure 12: q -profiles at $t = 7.0s$ for the JET Pulse No: 75225. The red line corresponds to the METIS simulation with the mean T_e profiles. The two blue lines correspond to the METIS simulations with the highest and lowest possible T_e profiles.