Integrated Bayesian Estimation of Z_{eff} in the TEXTOR Tokamak from Bremsstrahlung and CX Impurity Density Measurements

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Abstract. The validation of diagnostic data from a nuclear fusion experiment is an important issue. The concept of an Integrated Data Analysis (IDA) allows the consistent estimation of plasma parameters from heterogeneous data sets. Here, the determination of the ion effective charge (Z_{eff}) is considered. Several diagnostic methods exist for the determination of Z_{eff}, but the results are in general not in agreement. In this work, the problem of Z_{eff} estimation on the TEXTOR tokamak is approached from the perspective of IDA, in the framework of Bayesian probability theory. The ultimate goal is the estimation of a full Z_{eff} profile that is consistent both with measured bremsstrahlung emissivities, as well as individual impurity spectral line intensities obtained from Charge Exchange Recombination Spectroscopy (CXRS). We present an overview of the various uncertainties that enter the calculation of a Z_{eff} profile from bremsstrahlung data on the one hand, and line intensity data on the other hand. We discuss a simple linear and nonlinear Bayesian model permitting the estimation of a central value for Z_{eff} and the electron density n_{e} on TEXTOR from bremsstrahlung emissivity measurements in the visible, and carbon densities derived from CXRS. Both the central Z_{eff} and n_{e} are sampled using an MCMC algorithm. An outlook is given towards possible model improvements.

Keywords: tokamak, plasma impurities, Z_{eff}, bremsstrahlung, CXRS, Bayesian estimation, MCMC
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INTRODUCTION

With the recent decision on the construction of the International Thermonuclear Experimental Reactor (ITER) with a definite schedule, the research on Controlled Nuclear Fusion has received a new boost. Reliable diagnostic information will be of primary importance for the success of the ITER experiment. On the one hand, this is essential to allow the observation of the new physics inside the ITER plasma. On the other hand, plasma diagnosis is vital for the real-time control of various plasma parameters (burn control). This is required for the raising and managing of the plasma conditions in order to reach the ITER objectives. To obtain the highest possible accuracy of measurements in the hostile plasma environment of ITER, advanced diagnostic techniques need to be developed.

The development of new diagnostic methods is one step, but a large part of the work remains in the subsequent analysis of acquired data. In particular, validation of data with regards to underlying physical models and complementary measurements is a crucial aspect of experimental methodology. Moreover, the combined analysis of data from heterogeneous sources of information can substantially increase the reliability and robustness of inferred physical quantities, and can identify critical diagnostic uncertainties. In addition, the available space for diagnostic setups at ITER will be restricted, and physical quantities will need to be determined from a limited data set. As such, any type of available information will have to be exploited. The concept of a Bayesian Integrated Data Analysis (BIDA) [1] provides an outstanding framework that can accomplish these various tasks, with the possibility to include expert prior knowledge. Through its statistical nature, BIDA properly takes into account all uncertainties in the information at hand.

This paper is concerned with the Bayesian integrated determination of the ion effective charge Z_{eff}, a critical local measure of plasma impurity concentration, from bremsstrahlung spectroscopy on the one hand, and Charge Exchange Recombination Spectroscopy (CXRS) on the other hand. The characterization of the behaviour of plasma impurities is vital for the control of impurity levels in ITER and reactor grade plasmas. Impurities, released by various processes from the plasma facing surfaces, can deteriorate the reactor efficiency through radiated power loss, while increasing fuel dilution, and transport barriers can lead to impurity accumulation. Study of impurity transport is also of key importance to the exhaust of helium, which would otherwise suffocate the nuclear reactions.

We start with a short overview of the calculation of Z_{eff} from visible bremsstrahlung and CXRS measurements. We next mention the main uncertainties that enter the calculation of Z_{eff} via both methods. We then present a simple linear model for the integrated estimation of Z_{eff}, consistent with both measurement sets, and discuss extensions towards a nonlinear model. The ultimate goal of this work is the formulation of a detailed Bayesian model of Z_{eff} as a function of the raw measurements, taking into account all major uncertainties in the forward calculation.

Z_{eff} IN MAGNETICALLY CONFINED PLASMAS

In the context of magnetically confined plasmas, the ion effective charge Z_{eff} is a measure for the contamination of the plasma by impurities (the non-fuel components of the plasma). It is a weighted average of the individual impurity concentrations:

$$Z_{\mathrm{eff}} \equiv \frac{\sum_i Z_i^2 n_i}{\sum_i Z_i n_i} = \frac{\sum_i Z_i^2 n_i}{n_{\mathrm{e}}} = 1 + \sum_i Z_i (Z_i - 1) \frac{n_i}{n_{\mathrm{e}}}, \tag{1}$$

where Z_i and n_i are the charge number and density of impurity species i, respectively, n_{e} is the electron density, and the sum is over all impurity species. Clearly, $Z_{\mathrm{eff}} = 1$ for a pure hydrogen isotope plasma, imposing a minimum value on Z_{eff}.

Accurate knowledge of the local ion effective charge Z_{eff} is of key importance in a tokamak reactor, since the value of Z_{eff} is related to bremsstrahlung radiation losses, loop voltage, neutron yield, etc. For ITER, the next-step tokamak device, a Z_{eff} value of 1.8

is foreseen. Depending on the discharge scenario, this number may only vary by ± 0.2. However, the determination of Z_{eff} relies on the absolute measurement of several plasma quantities, and is therefore inherently difficult. Several diagnostic methods have been proposed for the derivation of Z_{eff}, but the results have large error bars, and are often both quantitatively and qualitatively not in agreement. We here consider the calculation of Z_{eff} from bremsstrahlung measurements in the visible, and from the weighted summation of individual impurity concentrations from CXRS, according to (1).

Z_{eff} from bremsstrahlung measurements

Z_{eff} can be determined via the measurement of the line-integrated bremsstrahlung emissivity from the plasma, typically along multiple chords through the plasma. If the observations are performed from a single location, the local bremsstrahlung emissivity ϵ_{ff} is assumed to be constant on magnetic flux surfaces. In many cases, this is a reasonable assumption, since the transport along the magnetic field lines is much larger than the cross-field transport. However, especially when the edge plasma on TEXTOR is ergodized with the Dynamic Ergodic Divertor, poloidal asymmetries may become important. A profile for ϵ_{ff} as a function of the torus minor radius r can be reconstructed from the line-integrated data. ϵ_{ff} is proportional to Z_{eff}, according to

$$\epsilon_{\mathrm{ff}}(r, \lambda, Z_{\mathrm{i}}) = \frac{C_{\mathrm{b}}}{\lambda^2} \bar{g}_{\mathrm{ff}}(\lambda, Z_{\mathrm{i}}, T_{\mathrm{e}}) \frac{{n_{\mathrm{e}}}^2(r) Z_{\mathrm{eff}}(r)}{\sqrt{T_{\mathrm{e}}(r)}} \quad \left(\frac{\mathrm{W}}{\mathrm{cm^3 sr \AA}}\right), \tag{2}$$

with C_{b} a calibration factor, λ the measuring wavelength, T_{e} the electron temperature and $\bar{g}_{\mathrm{ff}}$ the Maxwell-averaged Gaunt factor, which includes all quantum effects. In this work, measurements from interferometry were used for the determination of n_{e}, and measurements from Electron Cyclotron Emission for T_{e}. The dependence of ϵ_{ff} on T_{e} is weak, since the various dependencies on T_{e} tend to cancel each other. On TEXTOR, ϵ_{ff} is measured in the visible along 24 lines of sight [2] in a single poloidal cross-section of the plasma. An interference filter selects a narrow wavelength band that is known to be relatively free of line emission on TEXTOR and the light is collected by a cooled CCD. An emissivity profile is reconstructed by Abel inversion, while recently also Tikhonov and Maximum Entropy regularization have been tested.

The main sources of error on the Z_{eff} profile derived from bremsstrahlung emissivity measurements are listed below in descending order of importance:

- emissivity profile reconstruction: inversion procedure (error propagation), poloidal asymmetries, knowledge of magnetic equilibrium,
- inaccuracy in n_{e} and T_{e} profiles, especially near plasma boundary,
- contribution of non-bremsstrahlung continua and atomic line radiation,
- absolute calibration,
- overall diagnostic design,
- in-vessel reflections,
- Gaunt factor approximation,

- measurement noise.

The determination of Z_{eff} near the plasma boundary is particularly difficult using this method.

Z_{eff} from CXRS measurements

The energies in the core plasma of a magnetically confined plasma are sufficient to fully ionize impurities, rendering direct spectroscopic observation of these ions impossible. However, fully stripped impurity ions in the plasma core can undergo a charge exchange reaction with atoms from a neutral beam that is injected into the plasma. Since the charge exchange reaction leaves the impurity ion in an excited state, the associated atomic line radiation can be observed. From the line intensity, the impurity ion density can be derived [3]. CXRS is a local spectroscopic measurement, because the CX light is emitted only in the path of the neutral beam. Therefore, no inversion procedure is required for the reconstruction of impurity density profiles. Although in principle the light from multiple impurity species can be observed at the same time via CXRS, in practice only the most abundant species are monitored. On TEXTOR, carbon is in many cases the dominant impurity, and in this work so far only the contribution of fully stripped C^{6+} was considered.

The line-integrated CX line intensity I_{CX} depends on the impurity density n_i and the charge exchange emission rate q_{CX}, which again depends on n_{e}, T_{e}, the beam energy E_{b} and weakly on the impurity density:

$$I_{\mathrm{CX}} = \frac{C_{\mathrm{CX}}}{4\pi} q_{\mathrm{CX}}(E_{\mathrm{b}}, n_{\mathrm{e}}, T_{\mathrm{e}}, n_i) \int_{\mathrm{l.o.s.}} n_{\mathrm{b}} \mathrm{d}s,$$

where C_{CX} is a calibration factor, n_{b} is the beam density and the integral is over the (relatively short) part of the line of sight that crosses the beam. The diagnostic on TEXTOR features 20 channels and three spectrometers for the simultaneous monitoring of three different impurity species [4]. The spectrometers are equipped with CCD cameras. The CVI carbon line $n = 8 \rightarrow 7$ is routinely observed for the determination of the carbon density.

If only carbon is taken into account, then Z_{eff} can be approximated by

$$Z_{\mathrm{eff}} \approx 1 + Z_{\mathrm{C}}(Z_{\mathrm{C}} - 1)\frac{n_{\mathrm{C}}}{n_{\mathrm{e}}}. \tag{3}$$

The main sources of error on the thus calculated Z_{eff} profile are listed here in descending order of importance:

- spectral line fit,
- knowledge of magnetic equilibrium,
- contribution from additional impurities,
- n_{e} and T_{e} profiles (for beam attenuation),
- absolute calibration,

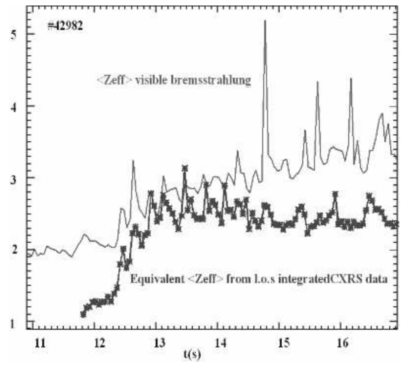


FIGURE 1. Comparison of the line averaged Z_{eff} from visible bremsstrahlung and its equivalent CX line integral reconstructed from contributions of C^{6+}, Be^{4+} and He^{2+} on the JET tokamak.

- overall diagnostic design,
- measurement noise,
- atomic data.

INTEGRATED Z_{eff} ESTIMATION

As a result of the aforementioned sources of error, the Z_{eff} values obtained from visible bremsstrahlung emissivity and from CX spectroscopy in general do not agree. Figure 1 gives an example, showing a substantial discrepancy between the two Z_{eff} signals. The situation is much worse for local Z_{eff} values near the plasma boundary. Moreover, so far none of the available methods for the determination of Z_{eff} has provided a reliable profile over the entire plasma cross-section, which is at present a real challenge. However, the two techniques for the determination of Z_{eff} described in the previous sections, are based on very different principles, and the corresponding sources of error can be very different in nature as well. Therefore, the integrated estimation of Z_{eff} from both data sets is expected to greatly improve the accuracy of Z_{eff} profiles. In a first stage, we will start from a series of ϵ_{ff}, T_{e} and n_{C} measurements, and calculate Z_{eff} from (2) on the one hand, and (3) on the other. We simultaneously estimate both the local Z_{eff} and n_{e}, the latter being used as a measure for the accuracy of the Z_{eff} estimates, by comparison with interferometric measurements. In a Bayesian framework, we will estimate Z_{eff} and n_{e} through their posterior means. The temperature T_{e} is assumed to be known exactly, an assumption that has little influence on the estimation results because of the weak dependence of ϵ_{ff} on T_{e}.

Linear Bayesian model

We now formulate a simple linear Bayesian model for the integrated estimation of Z_{eff} from local measurements of bremsstrahlung emissivity and CXRS carbon density. The details of Z_{eff} estimation from this model can be found in Ref. [5]. Taking the logarithm of (2) and (3), we arrive at the following equations:

$$\begin{cases} \log\epsilon = 2\log n_\mathrm{e} + \log Z_\mathrm{eff} + \nu_1, & \epsilon \equiv \epsilon_\mathrm{ff}\dfrac{\sqrt{T_\mathrm{e}}\lambda^2}{C_\mathrm{b}\bar{g}_\mathrm{ff}} \\ \log\delta = \log n_\mathrm{e} + \log(Z_\mathrm{eff}-1) + \nu_2, & \delta \equiv Z_\mathrm{C}(Z_\mathrm{C}-1)n_\mathrm{C} \end{cases}. \quad (4)$$

In a first approximation, we have modelled all uncertainties that enter the derivation of Z_eff in the noise term $\nu = [\nu_1, \nu_2]^\mathrm{T}$, which we assume to be independently identically Gaussian distributed:

$$\nu \sim \mathcal{N}(0, \Sigma_\nu), \quad \Sigma_\nu \equiv \begin{bmatrix} \gamma_1 & 0 \\ 0 & \gamma_2 \end{bmatrix},$$

where γ_i denotes an inverse variance. This also defines the likelihood of the parameters of interest, Z_eff and n_e. The priors are established from the following prior information:

- Z_eff is always larger than unity and on TEXTOR has typical values in $]1,\ 4]$,
- both signals can not be negative.

For estimation convenience, we choose for both $\log(Z_\mathrm{eff})$ and $\log(n_\mathrm{e})$ (truncated) Gaussian priors. The posterior distribution for $\log(n_\mathrm{e})$ is again a Gaussian, while the posterior for $\log(Z_\mathrm{eff})$ is no standard distribution. Therefore, in order to sample from the posteriors, we perform Gibbs sampling for $\log(n_\mathrm{e})$ and Metropolis-Hastings sampling for $\log(Z_\mathrm{eff})$. For the latter, a proposal distribution is used based on the linearization of the $\log(Z_\mathrm{eff}-1)$ term in the second equation of (4).

To test the estimation algorithm, the central signals of ϵ_ff, T_e and n_C were taken from five consecutive TEXTOR pulses (#96152 – #96156), and these were used as input data. For these discharges, there is a moderate discrepancy between Z_eff from bremsstrahlung and Z_eff from CXRS, as can be seen in Figure 2(a). The central Z_eff and n_e were estimated and the results are shown in Figure 2. There is a reasonably good correspondence between the estimated n_e and the interferometric signal, indicating a satisfactory estimate of a consistent Z_eff as well.

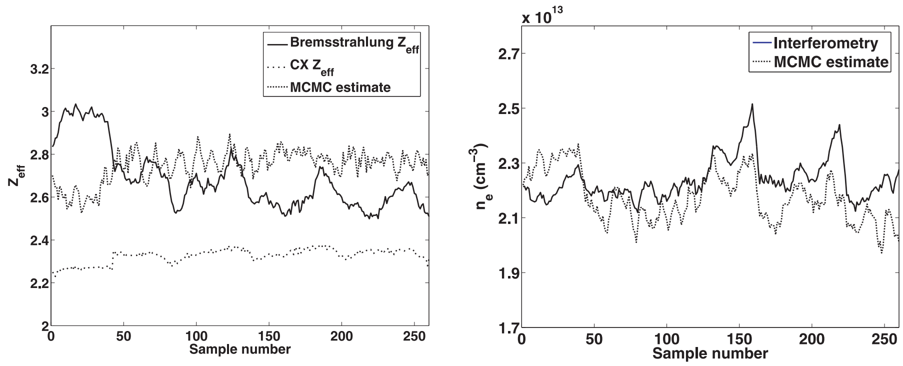
Nonlinear Bayesian model

Although the linear Bayesian model for Z_eff estimation, presented in the previous section, is very simple, it has some disadvantages. For instance, the linearization of $\log(Z_\mathrm{eff}-1)$ inevitably entails some loss of information, and the use of Gaussian priors on a log scale results in skewed distributions on a linear scale.

In order to improve the estimation the following nonlinear model was considered:

$$\begin{cases} \epsilon &=& {n_\mathrm{e}}^2 Z_\mathrm{eff} + \nu_1 \\ \delta &=& n_\mathrm{e}(Z_\mathrm{eff}-1) + \nu_2 \end{cases},$$

again incorporating all uncertainties in the independently identically Gaussian distributed noise term $\nu = [\nu_1, \nu_2]^\mathrm{T}$. The likelihood for the complete set of time points is then



(a) (b)

FIGURE 2. (a) Central line-averaged Z_{eff} determined from bremsstrahlung measurements in a series of TEXTOR discharges, central Z_{eff} from carbon density measurements by CXRS and the estimated Z_{eff}. (b) Central electron density from interferometry in a series of TEXTOR discharges, and its estimate by the MCMC sampling procedure.

given by

$$L\left(\epsilon,\delta|n_{\mathrm{e}},Z_{\mathrm{eff}},I\right)=\left(\frac{\gamma_1}{2\pi}\right)^{T/2}\exp\left[-\frac{\gamma_1}{2}\sum_t(\epsilon-{n_{\mathrm{e}}}^2Z_{\mathrm{eff}})^2\right]$$
$$\times\left(\frac{\gamma_2}{2\pi}\right)^{T/2}\exp\left[-\frac{\gamma_2}{2}\sum_t[\delta-n_{\mathrm{e}}(Z_{\mathrm{eff}}-1)]^2\right],$$

where T is the number of samples. The conditional posterior for n_{e} is

$$p(n_{\mathrm{e}}\|)\sim\prod\exp\left[-\frac{\gamma_1}{2}{Z_{\mathrm{eff}}}^2\left(\frac{\epsilon}{Z_{\mathrm{eff}}}-{n_{\mathrm{e}}}^2\right)^2\right.$$
$$\left.-\frac{\gamma_2}{2}(Z_{\mathrm{eff}}-1)^2\left(\frac{\delta}{Z_{\mathrm{eff}}-1}-n_{\mathrm{e}}\right)^2-\frac{\gamma_{n_{\mathrm{e}}}}{2}(\mu_{n_{\mathrm{e}}}-n_{\mathrm{e}})^2\right]\psi,$$

where we have taken a truncated Gaussian prior, and ψ is the indicator function on the positive half plane. The conditional posterior for Z_{eff} is

$$p(Z_{\mathrm{eff}}\|)\sim\prod\exp\left[-\frac{\gamma_1}{2}{n_{\mathrm{e}}}^4\left(\frac{\epsilon}{{n_{\mathrm{e}}}^2}-Z_{\mathrm{eff}}\right)^2-\frac{\gamma_2}{2}{n_{\mathrm{e}}}^2\left(\frac{\delta}{n_{\mathrm{e}}}+1-Z_{\mathrm{eff}}\right)^2\right.$$
$$\left.-\frac{\gamma_{Z_{\mathrm{eff}}}}{2}(\mu_{Z_{\mathrm{eff}}}-Z_{\mathrm{eff}})^2\right]\phi,$$

where we have again taken a truncated Gaussian as a prior, but now with ϕ the indicator function on the half plane $Z_{\mathrm{eff}}>1$. μ_θ and γ_θ, with $\theta=n_{\mathrm{e}},Z_{\mathrm{eff}}$ denote the prior mean and inverse variance, respectively. Again, a hybrid Gibbs-Metropolis-Hastings sampling algorithm was used, this time with Gibbs sampling of Z_{eff} and Metropolis-Hastings sampling of n_{e}. Up to now, some preliminary tests were run, but no definitive results are available as yet.

OUTLOOK

Whereas in many TEXTOR discharges, carbon is the dominant impurity, often there is a substantial contribution to Z_{eff} (and ϵ_{ff}) from the second most abundant impurity, namely oxygen. Taking into account also oxygen, the definition of δ becomes:

$$\delta \equiv Z_{\text{C}}(Z_{\text{C}} - 1)n_{\text{C}} + Z_{\text{O}}(Z_{\text{O}} - 1)n_{\text{O}}. \tag{5}$$

Up to now, oxygen has not been monitored routinely by CXRS on TEXTOR, but the ratio of oxygen to carbon abundances can be estimated from impurity fluxes determined from UV spectroscopy. The second term in (5) can then be modelled by a term μ_{O}, and incorporated in the definition of ν_2

$$\nu_2 \sim \mathcal{N}(-\mu_{\text{O}}, \gamma_2),$$

so that a systematic discrepancy between the bremsstrahlung Z_{eff} and the CX Z_{eff}, due to the contribution from oxygen, is also taken into account in the model.

The Bayesian model for integrated Z_{eff} estimation can be extended, through several stages of increased sophistication, by modelling increasingly more uncertainties by appropriate probability distributions. A sensitivity analysis then allows to quantify the impact of all uncertainties on the estimated Z_{eff}. This can be of great use for the optimization of a new pilot experiment on TEXTOR for the ITER charge exchange spectroscopy.

CONCLUSIONS

The determination by spectroscopic techniques of the ion effective charge Z_{eff} in a magnetically confined plasma was discussed. The main sources of uncertainty in the calculation of radial Z_{eff} profiles from bremsstrahlung and CXRS measurements, were mentioned, and the need for an integrated estimation of Z_{eff} was highlighted. A simple linear Bayesian model was presented, allowing the estimation of Z_{eff} and n_{e} via MCMC sampling. Improvements to the linear model were suggested through a nonlinear model, and the modelling of the oxygen density. The ultimate goal is the estimation of a consistent Z_{eff} profile over the whole plasma cross-section, by modelling of all major uncertainties in the forward model.

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