Bayesian inference of particle source and sink in a closed-divertor using Balmer line spectroscopy

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Abstract

A new analysis technique for Balmer line spectroscopy that enables recombination rate (particle sink) and ionization rate (particle source) inference in a closed divertor configuration is reported. Bayesian inference is employed to systematically utilize all available information from multiple Balmer lines and constrain parameter ranges by using prior knowledge about plasmas. While a closed-divertor facilitates detachment, neutral plugging typically leads to large spatial variations in plasma parameters. A forward model is developed to take into account non-uniformity in the plasma parameters and applied to test data generated by divertor plasma simulations. It is shown that the forward model robustly provides particle source and sink inference over a wide parameter range. In addition, the precision improves as more Balmer lines are resolved simultaneously. The new analysis technique is also applied to an L-mode ASDEX Upgrade plasma in the high-recycling regime. The inferred quantities and their profiles are consistent with the expectations of a high-recycling divertor plasma. The further insight into the detachment physics will be provided by using this new analysis technique.

Keywords: detachment, spectroscopy, Bayesian inference

1. Introduction

Mitigating heat load on a divertor target is considered as one of the critical challenges in achieving a commercial fusion reactor. If no counter measures are taken, a peak heat flux on the divertor target in ITER \([1]\) will largely exceed the heat load limit of present-day materials. Fortunately, the divertor heat load can be reduced significantly through a process called ‘detachment’, leading to a tolerable heat flux \([2, 3]\). When detachment takes place, both electron temperature \(T_e\) and density \(n_e\) drop near the strike point and the plasma ‘detaches’ from the divertor target. However, the current understanding of the detachment process is mostly based on empirical laws and qualitative descriptions and the extrapolation of the detachment behavior to ITER and future reactors is not reliable. To this end, further study of the detachment processes through experiments, modeling and simulations is crucial for successful operations of ITER and future commercial fusion reactors.

Balmer line spectroscopy is a non-intrusive diagnostic technique and often used for characterizing divertor plasmas. Balmer lines are a spectral series of deuterium or its isotopes with wavelengths in the visible range, for which implementation of diagnostics is relatively easy. Since many magnetic fusion experiments use mostly deuterium or its
isotopes for the main gas, Balmer line spectroscopy is often run routinely and a large set of atomic data is available. One of the plasma parameters Balmer line spectroscopy provides is $n_e$. When $n_e$ is high ($\gtrsim 4 \times 10^{20} \text{ m}^{-3}$), the broadening of a $D_\alpha (n=7 \to 2)$ line ($H_\alpha$ for hydrogen) is dominated by Stark-broadening for a relatively cold divertor plasma. Fitting a $D_\alpha$ spectrum by using a proper line-shape model provides $n_e$ measurements [4, 5]. When other processes such as Zee- man effect and fine ion and neutral temperature are taken into account, $n_e$ can also be measured from a $D_\alpha (n=6 \to 2)$ line, or $D_\beta (n=5 \to 2)$ line [4, 6, 7]. Another use of Balmer line spectroscopy is the detection of volume recombination [5, 8]. When recombination is present, the ratio of two Balmer line intensities changes. Recently, even quantitative measurements of ionization and recombination rates are reported by using the line-ratios and absolute emission intensities [9, 10].

While Balmer line spectroscopy has provided useful information, this diagnostic technique intrinsically measures line-integrated signals. When the plasma inside the emission volume along a line of sight cannot be treated as uniform, quantitative measurements are challenging. A closed-divertor plasma is one of those examples where spatial variations in plasma parameters are not negligible. However, accurate determination of parameters in this type of plasma is critical in understanding detachment in reactor-relevant conditions since it is widely accepted that the closed-divertor configuration facilitates detachment and will be the standard design for tokamak-based fusion reactors [1, 11].

In this paper, a new analysis technique for Balmer line spectroscopy that enables particle source and sink inference in a closed-divertor plasma is introduced. Instead of evaluating line-shapes or line ratios individually, the proposed analysis technique formulates a single inference problem by using a PEC that enables particle source and sink inference in a closed-divertor plasma. This diagnostic technique intrinsically measures line-shapes or line ratios individually, the proposed analysis technique formulates a single inference problem by using a PEC on $n_e$, $n_i$, and $n_0$ the electron density, ion density and neutral density, respectively. The first and second terms on the right hand side are recombination emission and excitation emission. In addition to these emission processes, molecular reactions can also contribute to the Balmer line spectrum [13]. The influence of the molecular reactions generally becomes larger for longer wavelengths [14]. Thus, $D_\alpha (n=5 \to 2)$ is excluded from the analysis in this paper. Lines with the upper state over $n=7$ are also excluded since measuring these lines is often difficult due to their weak emission intensities. While included in the analysis, care has to be taken when interpreting the discussion of $D_\beta (n=4 \to 2)$ since this line may also be affected by the molecular reactions under some circumstances. Equation (1) holds more rigorously for $D_\alpha (n=7 \to 2)$, $D_\alpha (n=6 \to 2)$ and $D_\alpha (n=5 \to 2)$ [9, 10]. Another important effect, opacity, is also neglected in this analysis. Considering photon trapping may be critical especially for high-density divertors [14–16]. Including this effect remains future work. For the rest of the paper, it is assumed that the plasma is made solely of deuterium, i.e. $n_e = n_i$ as is done in Ref [9, 10]. This is a fair assumption for AUG since nitrogen ion concentration is typically less than a few percent in the outer divertor.

Figure 1 shows photon emissivity coefficients for each line. As the upper state increases from $n = 4$ to 7 ($\beta$ to $\epsilon$), both PEC$_{ex}$ and PEC$_{re}$ decrease. It is important to note that the relative intensity between PEC$_{ex}$ and PEC$_{re}$ also varies. The crossing point between PEC$_{ex}$ and PEC$_{re}$ shifts to higher $T_e$ as the energy of the upper state increases, indicating that $D_\beta$ tends to be dominated by excitation emission while $D_\alpha$ tends to have a dominant contribution from recombination emission. The dominant radiation process also depends strongly on $T_e$. As can be seen in figure 1, PEC$_{ex}$ drops sharply below 10 eV while PEC$_{re}$ increases as $T_e$ decreases. The dependencies of PECs on $n_e$ are moderate and the trends seen in figure 1 hold in the range of $n_e$ relevant to divertor plasmas $\sim [10^{19} - 10^{21}] \text{ m}^{-3}$. As equation (1) shows, PEC for recombination emission is multiplied by $n_i^2$ ($n_e = n_i$ is assumed) and PEC for excitation emission is multiplied by $n_i n_0$. Thus, $n_i$ also contributes to the ratio of recombination to excitation emission.

The divertor plasma in a closed-divertor can have plasma parameters with significant spatial variations. Figure 2 shows the lines of sight in the outer divertor of AUG. To investigate how a line-integrated Balmer line emission intensity is related to the line-integrated ionization $F_{io}$ and the line-integrated recombination rate $F_{re}$, a set of test data is generated from 17 different equilibria of AUG simulated by SOLPS [17]. 15 of them are H-mode [18] (drift included) and the rest are L-mode discharges (drift not included). For each equilibrium, test data corresponding to each line of sight shown in figure 2 is calculated. Typical parameter profiles along the red line of sight in figure 2 are shown in figure 3(a) (H-mode). In general, $n_i$ and $n_0$ tend to be higher in the private flux region (PFR) than in the scrape-off layer (SOL) while $T_e$ is typically higher in the SOL than in the PFR. The excitation and recombination emission

\begin{equation}
\tilde{I}_X(n_e, T_e, n_0) = n_e n_i \text{PEC}_{ex}(n_e, T_e) + n_e n_0 \text{PEC}_{re}(n_e, T_e), \tag{1}
\end{equation}

where $X = \epsilon(n=7 \to 2)$, $\delta(n=6 \to 2)$, $\gamma(n=5 \to 2)$ and $\beta(n=4 \to 2)$. PEC$_{ex}$ and PEC$_{re}$ are photon emissivity coefficients for recombination emission and excitation emission, provided by ADAS [12], while $n_e$, $n_i$, and $n_0$ are the electron density, ion density and neutral density, respectively. The first and second terms on the right hand side are recombination emission and excitation emission. In addition to these emission processes, molecular reactions can also contribute to the Balmer line spectrum [13]. The influence of the molecular reactions generally becomes larger for longer wavelengths [14]. Thus, $D_\alpha (n=5 \to 2)$ is excluded from the analysis in this paper. Lines with the upper state over $n=7$ are also excluded since measuring these lines is often difficult due to their weak emission intensities. While included in the analysis, care has to be taken when interpreting the discussion of $D_\beta (n=4 \to 2)$ since this line may also be affected by the molecular reactions under some circumstances. Equation (1) holds more rigorously for $D_\alpha (n=7 \to 2)$, $D_\alpha (n=6 \to 2)$ and $D_\alpha (n=5 \to 2)$ [9, 10]. Another important effect, opacity, is also neglected in this analysis. Considering photon trapping may be critical especially for high-density divertors [14–16]. Including this effect remains future work. For the rest of the paper, it is assumed that the plasma is made solely of deuterium, i.e. $n_e = n_i$ as is done in Ref [9, 10]. This is a fair assumption for AUG since nitrogen ion concentration is typically less than a few percent in the outer divertor.
profiles for each Balmer line are shown in figures 3(b), (c), (e) and (f). The recombination emission mostly comes from the PFR whereas the SOL provides the majority of excitation emission. As the principle quantum number of the upper state increases, the line-integrated emission intensity is more dominated by the recombination emission than by the excitation emission as expected from figure 1.

The spatial profiles of the ionization and recombination rates are shown in figure 3(d). Similar to the relation between the excitation and recombination emissions, the ionization rate is large in the SOL while the recombination rate peaks in the PFR. Figure 4(a) shows the relation between $F_{\text{re}}$ and $I_e$ (the line-integrated emission intensity of $D_e$), which tends to be dominated by recombination emission. The color of each point is a ratio of $I_e$ to $I_{\beta}$ (the line-integrated emission intensity of $D_{\beta}$). This ratio is often used for characterizing which emission process dominates $I_e$ and $I_{\beta}$[5]. The higher $I_e/I_{\beta}$, the more the recombination emission dominates compared to the excitation emission. The black dashed line is proportional to $I_e$. Roughly linear relation between $I_e$ and $F_{\text{re}}$ is seen except $I_e/I_{\beta} < 0.35$, where the excitation emission is non-negligible in $I_e$. This scaling can be understood through figure 5(a) that shows an effective recombination coefficient ACD over $\text{PEC}_{e}^\text{re}$. This quantity represents a number of recombination events per photon due to the recombination emission in $D_e$. The black dashed line in figure 4(a) is $F_{\text{re}} = 1.81 \times 10^2 I_e$, indicating that about 181 recombination events happen for each photon in the $D_e$ emission. This proportional relation is also seen in Figs 3(b) and (d). The profile shape of the recombination emission in $D_e$ looks quite similar to that of the recombination rate. The combination of $n_e$ and $T_e$ corresponding to $F_{\text{re}} = 1.81 \times 10^2 I_e$ is shown by the thick red line in figure 5(a). The dependency of ACD/PEC$_e^\text{re}$ on $T_e$ and $n_e$ is moderate for $T_e > 1$ eV. While PEC$_e^\text{re}$ increases as $T_e$ decreases for $T_e < 1$ eV, $I_e$ is rarely dominated by the emission coming from regions with $T_e < 1$ eV since $n_e$ there is significantly lower than near the separatrix due to frequent recombination. Therefore, $F_{\text{re}}$ roughly scales linearly with $I_e$ for $I_e/I_{\beta} > 0.35$.

Contrary to $I_e$, $I_{\beta}$ tends to be dominated by excitation emission. Figure 4(b) shows the relation between $F_{\text{io}}$ and $I_{\beta}$. While a correlation can be seen, the data points scatter more widely compared with figure 4(a). In some cases, $F_{\text{io}}$ differs by a factor of $\sim 2$ for the same $I_{\beta}$. The ratio of an effective ionization coefficient SCD to $\text{PEC}_{\beta}^\text{io}$ (the number of ionization events per photon due to excitation emission in $D_{\beta}$) is shown in figure 5(b). SCD/PEC$_{\beta}^\text{io}$ depends strongly on $n_e$. Below $T_e < 10$ eV, the $T_e$ dependence on SCD/PEC$_{\beta}^\text{io}$ is also strong, indicating that proportionality between $I_{\beta}$ and $F_{\text{io}}$ is not expected. While educated guesses may be made by using empirical formulae that relate $I_{\beta}$ to $F_{\text{io}}$ from the SOLPS simulation results, the focus of this paper is to infer ionization and recombination rates based on a physics model, which will be discussed in the following sections.

3. $D_e$ and $D_{\beta}$ spectroscopy for a uniform plasma slab using Bayesian inference

The diagnostic techniques discussed in the rest of the paper employ Bayesian inference to extract maximum available

Figure 1. Recombination photon emissivity coefficients and excitation photon emissivity coefficients for $n_e = 1 \times 10^{20}$ m$^{-3}$ from the ADAS data base [12]

Figure 2. Lines of sight in the outer divertor of ASDEX Upgrade (Green and red lines). The lines of sight shown in solid lines are used for measurements discussed in section 5. The blue solid line is the separatrix and the blue dotted lines show flux surfaces. The black dots show the measurement points of Langmuir probes.
Figure 3. (a) Typical plasma parameter profiles ($n_e$, $n_0$ and $T_e$) along the line of sight shown in red in figure 2. Profiles of recombination emission $i_{re}$ and excitation emission $i_{ex}$ for each Balmer line are shown in (b), (c), (e) and (f). (d) Profiles of the recombination rate $f_{re}$ and ionization rate $f_{io}$. The x axis ranges from the PFR to the SOL. The separatrix is near 3 cm.

Figure 4. Relations between the line-integrated $D_\epsilon$ emission intensity $I_\epsilon$ and line-integrated recombination rate $F_{re}$ (a) and between the line-integrated $D_\beta$ emission intensity $I_\beta$ and line-integrated ionization rate $F_{io}$ (b). The black dotted lines show the proportional relations.

information from limited data. In this section, basic framework of Bayesian inference for Balmer line spectroscopy is described before the technique is applied to the plasma in a closed-divertor.

Since Balmer line emission depends on multiple plasma parameters in a complex fashion, available measurements often fail to provide sufficient information to uniquely determine each plasma parameter, i.e., the problem is underdetermined. However, within the framework of Bayesian inference, possible ranges of unknown parameters can be inferred. For demonstration purposes, measurements of a uniform plasma slab using two Balmer lines $D_\epsilon$ and $D_\delta$ are discussed. As mentioned in the introduction, when $n_e \geq 4 \times 10^{19} \text{ m}^{-3}$, $n_e$ can be reliably measured by fitting a Stark-broadened $D_\epsilon$ line. Due to the proximity of $D_\delta$ to $D_\epsilon$ in wavelength, these two Balmer lines are often measured simultaneously with high wavelength resolution using a single spectrometer [5, 9, 10]. For a uniform plasma, the measured emission intensity of $D_\epsilon$ and $D_\delta$ are:

$$I_\epsilon = \delta l [n_e^2 \text{PEC}_{e}^{\epsilon}(n_e, T_e) + n_e n_0 \text{PEC}_{e}^{\delta}(n_e, T_e)],$$

$$I_\beta = \delta l [n_e^2 \text{PEC}_{e}^{\beta}(n_e, T_e) + n_e n_0 \text{PEC}_{e}^{\delta}(n_e, T_e)],$$

where $\delta l$ is the length of the emission volume along a line of sight, which is unknown this case. Note that the plasma is assumed to be made of pure deuterium, i.e., $n_i = n_e$. In Balmer line spectroscopy for divertor plasmas, the ratio $I_\epsilon/I_\beta$ is often
evaluated [5, 9, 10]. While \( I_e/I_s \) is independent of \( \delta l \), there are still two undetermined plasma parameters, \( n_0 \) and \( T_e \). Therefore, neither of them can be determined without assuming the other. Figure 6 shows the ratios of PEC_{r, e} to PEC_{r, \beta}. Those plots imply that \( I_e/I_s \) is low when excitation emission is dominant (or high when recombination emission is dominant).

From the line ratio \( I_e/I_s \), possible combinations of \( n_0 \) and \( T_e \) are determined for a given \( n_e \). While they produce the same \( I_e/I_s \) ratio, the absolute light intensities vary. The possible range of \( \delta l \) can be estimated from the viewing geometry and knowledge about the plasma, e.g., \( \delta l \) is shorter than a line of sight. Therefore, the ranges of \( n_0 \) and \( T_e \) can be constrained by calculating \( \delta l \) corresponding to each combination of \( n_0 \) and \( T_e \). To investigate the relation between \( \delta l, n_0 \) and \( T_e \), three cases with different \( I_e/I_s \) ratios given in table 1 are considered. In the Bayesian framework, a forward model calculates synthetic data in a parameter space defined by a prior. Since a likelihood evaluates how much the synthetic data is close to the experimentally measured data, the absolute intensities of \( D_e \) and \( D_0 \) are automatically taken into account as well as the line ratio. The probability distributions of the parameters given that data \( D \) is observed are given by Bayes’ Rule [19]:

\[
p(I_4 | D, I) = \frac{p(D | I_4 I) p(I_4 | I)}{p(D | I)}
\]

(4)

where \( I \) is prior information and \( \theta \) is the parameters in the forward model. In this case, \( D = [ I_e, I_s ] \) and \( \theta = [ \delta l, n_0, T_e ] \). In this analysis, each element of \( \theta \) is allowed to vary many orders of magnitude. To avoid biasing distribution toward higher orders of magnitude [19, 20], the following prior distributions are used:

\[
T_e = 10^6 \text{ eV}, \quad a \in [-1.0, 2.3], \\
n_0 = 10^6 \text{ m}^{-3}, \quad b \in [15.0, 24.0], \\
\delta l = 10^6 \text{ m}, \quad c \in [-4.0, 2.0],
\]

(5)

where \( a, b \) and \( c \) have uniform distributions within the specified ranges. The likelihood is given by:

\[
p[I_e,I_s] | [T_e, n_0, \delta l], I = \prod_{x=e,\delta} \frac{1}{\sqrt{2\pi \sigma_{I_x}^2}} \exp \left( -\frac{(I_x - I_x^{\text{FWM}})^2}{2\sigma_{I_x}^2} \right)
\]

(6)

where \( I_x^{\text{FWM}} \) is the forward-modeled Balmer line intensity, which is calculated by inserting \( T_e, n_0 \) and \( \delta l \) into equations (2) and (3). Note that \( n_e \) is independently measured and not an element of \( \theta \). The measurements of \( I_e \) and \( I_s \) are assumed to have a relative uncertainty of 3%, i.e., \( \sigma_{I_e, I_s} = 0.03 \times I_e, I_s \). The evidence \( p(D | I) \) is neglected since the absolute probability is not of interest. Due to the low dimensionality, a brute force algorithm is employed and an unnormalized posterior is calculated for each point in the three dimensional space \([T_e, n_0, \delta l]\). Figures 7, 8 and 9 show the posterior distributions and the marginalized distributions in terms of one of the thee parameters for each case: \( I_e/I_s = 0.46, 0.32 \) and 0.25. The contour line 0.46 corresponding to Case 1 is indicated in figure 6(a). \( I_e/I_s = 0.46 \) can also be realized by mixing recombination emission with PEC_{e, \delta} > 0.46 and excitation emission with PEC_{e, \beta} < 0.46. Note that PEC_{e, \delta} > PEC_{e, \beta} below 1 eV as shown in figure 1. Therefore, excitation emission is negligible with respect to recombination emission for \( T_e < 1 \) eV unless \( n_0 \) is greater than \( n_e \) by many orders of magnitude. Below 1 eV, a band of high probability range is seen along the \( n_0 \) axis in figures 7(a), (b) and (c). This structure corresponds to the parameter range that reproduces the observed \( I_e \) and \( I_s \) with recombination emission only. Since excitation emission does not contribute to the total light intensity, the probability distribution of \( n_0 \) is flat, i.e., \( n_0 \) is undetermined. The other high probability structure that depends on
all $T_e$, $n_0$ and $\delta l$ reproduces $I_e$ and $I_\delta$ with both recombination and excitation emissions. While there are two ways of achieving the ratio $I_e/I_\delta$ of 0.46, the required size of the plasma $\delta l$ that reproduces the observed absolute light intensities is different. If it is known that $\delta l$ is less than a few cm, the observed ratio can be realized by only recombination. In this case, there are only two unknowns, $T_e$ and $n_e$, for two equations (2) and (3). Therefore, the problem is not under-determined and $T_e$ and $n_e$ are uniquely determined. In this case, $T_e \approx 0.3$ eV where the vertical band peaks in figure 7(b) and $\delta l \approx 8 \times 10^{-3}$ m where the horizontal band peaks in figure 7(c). It is not possible to constrain the range of $n_0$ more than what the prior does. When $\delta l > 0.8 \times 10^{-2}$ m, both recombination and ionization contribute to the total light intensity. If one of $T_e$, $n_0$ and $\delta l$ is given, the other two that reproduce $I_e$ and $I_\delta$ are determined. It is important to note that figure 7(b) is dependent only on the ratio $I_e/I_\delta$ and independent of the absolute light intensities. When the absolute emission intensities vary with $I_e/I_\delta$ fixed, the probability distributions shown in figure 7 move along the $\delta l$ direction, but the shapes of them do not change. This is also true for Case 2 and Case 3.

In Case 2 shown figure 8, the $I_e/I_\delta$ ratio is 0.32. This $I_e/I_\delta$ cannot be realized by only recombination as can be seen from figure 6. Therefore, the band of high probability range along the $n_0$ direction observed in figure 7 is absent in figure 8. While the exact values of $I_e$ and $I_\delta$ can never be reproduced without ionization emission, the likelihood given by equation (6) becomes large near $[T_e, \delta l] = [0.1$ eV, $10^{-3}$ m]. This effect accumulates when marginalized in terms of $n_0$ and leads to a spot of high probability near the y axis in figure 8(d). The absence of high probability region below $\delta l = 4 \times 10^{-2}$ m and $T_e = 8 \times 10^{-1}$ eV is due to the prior of $n_0$.

In Case 3 ($I_e/I_\delta = 0.25$), excitation emission dominates $I_e$ and $I_\delta$. The high probability range traces out a surface instead of a curve in figure 9(a). In principle, when recombination emission is negligible, $T_e$ is uniquely determined by the $I_e/I_\delta$ ratio based on equations (2) and (3). However, it is difficult to infer $T_e$ from figure 9(b) or (d). When the excitation emission is negligible, $T_e$ also uniquely determines the absolute intensities of $I_e$ and $I_\delta$ as well as the $I_e/I_\delta$ ratio for given $n_e$ and $\delta l$. In contrast, the intensity of excitation emission depends also on $n_0$, which is not known. Therefore, the absolute intensities do not provide a strong constraint. The assumed 3% uncertainty in the $I_e$ and $I_\delta$ measurements translates to about the uncertainty of 0.1 in the $I_e/I_\delta$ ratio. The $T_e$ range corresponding to $I_e/I_\delta = 0.24$ to 0.26 shown in figure 6(b) is rather

![Figure 6. Ratios of PEC$^{re}$ to PEC$^{\delta}$ (a) and PEC$^{ex}$ to PEC$^{\delta}$ (b) as a function of $n_e$ and $T_e$.](image)

![Table 1. Emission intensities of $D_e$ and $D_\delta$ and their ratio for each case.](table)}
Figure 7. Case 1 for $I_\epsilon/I_\delta = 0.46$. A posterior distribution (a) and marginalized posterior distributions (b), (c) and (d). A volume where $2\pi\sigma_{\ell}\sigma_{\delta}p(D|\theta, I) > 1/e$ is shown in (a).

Figure 8. Case 2 for $I_\epsilon/I_\delta = 0.32$. A posterior distribution (a) and marginalized posterior distributions (b), (c) and (d). A volume where $2\pi\sigma_{\ell}\sigma_{\delta}p(D|\theta, I) > 1/e$ is shown in (a).

Figure 9. Case 3 for $I_\epsilon/I_\delta = 0.25$. A posterior distribution (a) and marginalized posterior distributions (b), (c) and (d). A volume where $2\pi\sigma_{\ell}\sigma_{\delta}p(D|\theta, I) > 1/e$ is shown in (a).

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Figure 9. Case 3 for $I_\epsilon/I_\delta = 0.25$. A posterior distribution (a) and marginalized posterior distributions (b), (c) and (d). A volume where $2\pi\sigma_{\ell}\sigma_{\delta}p(D|\theta, I) > 1/e$ is shown in (a).

4. Inferring line-integrated recombination and ionization rates in a closed-divertor using a simplified profile model

In the previous section, the methodology for inferring the plasma parameters of a uniform plasma is discussed. As figure 3(a) shows, spatial variations of plasma parameters are not negligible in a closed-divertor plasma and the discussion for a uniform plasma slab is not necessarily applicable. Inferring local plasma parameters is challenging by only using line-integrated measurements through the lines of sight shown in figure 2. However, as can be seen in figure 4, line-integrated recombination and ionization rates are correlated to measurable quantities such as $I_\ell$, or $I_\beta$, suggesting that line-integrated plasma parameters can still be inferred. In this section, the analysis technique for line-integrated recombination and ionization rates ($F_{re}$ and $F_{io}$) in a closed-divertor geometry is discussed.
The plasma parameter profiles shown in figure 3 (a) represent general features of outer-divertor plasmas in AUG. The peak of \( n_\epsilon \) is near the separatrix. There are typically large differences in \( T_e \) and \( n_0 \) between the PFR and the SOL. In general, complex forward models with many parameters lead to wide probability distributions of individual parameters when marginalized. However, if a forward model is too simple and fails to capture important features of true physical processes, significant mismatches between the true values and inferred values occur. Therefore, a forward model for the \( F_{\text{re}} \) and \( F_{\text{io}} \) inference needs to have sufficient flexibilities to match real plasma parameter profiles while keeping the number of parameters in the model to a minimum. A simplified profile model (SPM) shown in figure 10 is employed for the forward model in this analysis. SPM has six parameters: \( \theta = [l, \hat{n}_e, T_{e,l}, T_{e,b}, \hat{n}_0] \). The FWHM of the \( n_e \) profile is \( \hat{l} \). The triangular shape of \( n_e \) profile can be asymmetric. The peak position of \( n_e \) is specified by a parameter \( \alpha \in [0, 2] \). The \( n_e \) value at the half-maximum is \( \hat{n}_e \). The \( T_e \) profile has a step at the peak of \( n_e \). The lower value corresponding to the PFR is \( T_{e,l} \) and the higher value corresponding to the SOL is \( T_{e,b} \). Even though there is typically a large difference in \( n_0 \) between the PFR and the SOL, the \( n_0 \) profile is uniform in SPM. Practically, \( n_0 \) represents \( n_0 \) in the SOL. The emission profiles shown in figures 3(b), (c), (e) and (f) indicate that the majority of excitation emission occurs in the SOL. Since \( P_{\text{EC}} \) decreases by many orders of magnitude as \( T_e \) drops from 10 to 1 eV (shown in figure 1), excitation emission in the PFR is small despite the higher \( n_0 \). In addition, ionization, which also depends on \( n_0 \), occurs mostly in the SOL. Therefore, the calculation of synthetic data and the inference of \( F_{\text{re}} \) are relatively insensitive to the underestimation of \( n_0 \) in the PFR.

In the previous section, the data are \( D = [I_e, I_b] \) (intensities of \( D_e \) and \( D_b \) lines). However, Balmer line spectroscopy originally measures intensities of wavelength channels and \( n_e \) is inferred by the Stark-broadened line shape. Thus, \( D \) should be the intensities of wavelength channels. The synthetic data based on SPM is given by:

\[
F_{\text{SPM}}^X = \int d\lambda H_\lambda^X(\lambda) \int_0^{\hat{l}} dl \cdot i_X(\theta) L_X(\lambda, \theta),
\]

where \( X = \varepsilon, \delta, \gamma, \) and \( \beta \). The line emissivity coefficient \( i_X \) is already defined by equation (1). The normalized line shape of a Balmer line \( X \) is given by \( L_X \) and \( H_\lambda^X \) is an instrument broadening function. There are many line shape models with different complexities for Balmer lines \([4, 6, 7]\). This analysis uses a relatively simple model provided by Ref \([7]\):

\[
L_X(\lambda, n_e, T_e) \propto \frac{1}{(\lambda - \lambda_0)^{5/2} + (c_X n_e)^{5/2}}.
\]

where \( \lambda_0 \) is the central wavelength of a Balmer line \( X \). Each Balmer line has different values for coefficients, \( a_X, b_X \) and \( c_X \). Many processes cause broadening. Here, only Stark-broadening, from which \( n_e \) is measured and the instrument function of a spectrometer are considered. These two are typically dominant for \( D_e \) and \( D_b \) measurements of conduction-limited divertor plasmas at AUG. The instrument function of a wavelength channel \( \lambda_X \) is:

\[
H_{\lambda_X} = \frac{1}{\sqrt{2\pi\sigma_X^2}} \exp\left(-\frac{(\lambda - \lambda_0)^2}{2\sigma_X^2}\right).
\]

where \( \sigma_X \) is the wavelength resolution of a spectrometer, \( \sigma_X \approx 35 \text{ pm} \) (\( \sigma_X \) is slightly different for each \( \lambda_X \)). For \( D_e \) and \( D_b \) lines, the instrument broadening is dominant and practically only absolute intensities provide constraints. Local emission as a function of wavelength \( \hat{l} \) is integrated along the line of sight \( l \). Then, instrumental effects are taken into account by integrating in terms of \( \hat{l} \).

A probability distribution of \( \theta \) given the experimental measurements is calculated, again, by using the Bayes’ theorem. Assuming that errors in the measurements follow a Gaussian distribution, the likelihood is given by:

\[
p(D|\theta, I) = \prod_X \prod_{\lambda_X} \frac{1}{\sqrt{2\pi\sigma_X^2}} \exp\left(-\frac{(I_{X,\lambda_X} - I_{\text{SPM}}^{X,\lambda_X})^2}{2\sigma_X^2}\right).
\]

where \( I_{X,\lambda_X} \) is the experimentally measured intensity of the wavelength channel \( \lambda_X \) and \( \sigma_X \) is the uncertainty of \( I_{X,\lambda_X} \). The product over \( \lambda_X \) includes wavelength channels near a Balmer line \( X \). Once a probability distribution is calculated in the \( \theta \) space, the distribution can be mapped onto probability distributions of \( F_{\text{re}} \) and \( F_{\text{io}} \) using an effective recombination rate ACD and an effective ionization rate SCD discussed in section 2. The validity of SPM is tested by using the same set of SOLPS simulation data used for figure 4. The uncertainties \( \sigma_{\lambda_X} \) are set to be 3% of the maximum intensity of the line \( X \), i.e., \( \sigma_{\lambda_X} = 0.03 \times \max(I_{X,\lambda_X}) \). While \( \sigma_{\lambda_X} \) depends on the diagnostic setup, this analysis is underdetermined. Thus, as is discussed in section 3, some degree of uncertainties are expected to entail even when \( \sigma_{\lambda_X} \) is infinitesimally small. In the real measurements discussed in the next section,

\[
\sigma_{\lambda_X} = \sqrt{\sigma_{\lambda_X,\text{ph}}^2 + \sigma_{\lambda_X,\text{int}}^2},
\]

where \( \sigma_{\lambda_X,\text{ph}}^2 \) is the photon counting noise (Poisson noise) \([22]\) and \( \sigma_{\lambda_X,\text{int}}^2 \) is the intrinsic noise in the data acquisition.
Figure 11. Comparison between line-integrated recombination rates calculated by the Bayesian inference and true values. (a) Line integrated ionization rates inferred by SPM when $D_{e}$ and $D_{\delta}$ are measured. (b) Line integrated recombination rates inferred by the uniform slab model when $D_{e}$ and $D_{\delta}$ are measured. The y axes are the true line-integrated recombination rates calculated directly from the SOLPS simulations. The color represents the emission intensity ratio of $D_{e}$ to $D_{\delta}$. The data points are the 50th percentiles of the probability distributions of recombination rates. The errors show the range between the 16th and the 84th percentiles.

Figure 12. Comparison between line-integrated ionization rates calculated by the Bayesian inference and true values. Line integrated ionization rates inferred by SPM: (a) $D_{e}$ and $D_{\delta}$ measurement, (b) $D_{e}$, $D_{\delta}$ and $D_{\gamma}$ measurement and (c) $D_{e}$, $D_{\delta}$, $D_{\gamma}$ and $D_{\beta}$ measurement. Line integrated ionization rates inferred by the uniform slab model: (d) $D_{e}$ and $D_{\delta}$ measurement, (e) $D_{e}$, $D_{\delta}$ and $D_{\gamma}$ measurement and (f) $D_{e}$, $D_{\delta}$, $D_{\gamma}$ and $D_{\beta}$ measurement. The y axes are the true line-integrated ionization rates calculated directly from the SOLPS simulations. The color represents the emission intensity ratio of $D_{e}$ to $D_{\delta}$. The data points are the 50th percentiles of the probability distributions of ionization rates. The errors show the range between the 16th and the 84th percentiles.
system. The uncertainties in absolute intensity calibration is absorbed into the prior of ̂l. See appendix A for the details. Priors are given by:

\[ ̂l = 10^4 \text{ cm}, \quad A \in [\log_{10} 1, \log_{10} 5], \]
\[ \hat{\alpha} \in [0, 2], \]
\[ \hat{n}_e \in [1 \times 10^{19} \text{ m}^{-3}, 9 \times 10^{20} \text{ m}^{-3}], \]
\[ \hat{T}_{e,j} = 10^6 \text{ eV}, \quad B \in [\log_{10} 0.1, \log_{10} 100], \]
\[ \hat{T}_{e,h} = 10^6 \text{ eV}, \quad C \in [\log_{10} 0.1, \log_{10} 100], \]
\[ \hat{n}_0 = 10^9 \text{ m}^{-3}, \quad D \in [17, 20], \] (12)

where A, B, C, D, ̂α and ̂n_e have uniform distributions within the specified ranges. A linear prior is chosen for ̂n_e since, due to the strong constraint given by the Stark broadening of D_e, the marginalized probability distribution for ̂n_e is strongly peaked and biasing toward higher magnitudes is not observed. In order to properly sample a non-monomodal posterior probability distribution, the parallel tempering algorithm [23] in the emcee library is employed [24]. The integral over ̂l is calculated by using ten steps along the line of sight. Five of them are in the PFR, the other five in the SOL. The difference in the inferred values is marginal when finer steps are used. The inferred line integrated recombination rate ̂F_{e,SPM} and line integrated ionization rate ̂F_{io,SPM} are compared with true values directly calculated from the SOLPS simulation profiles. Figures. 11(a) and 12(b) show the relation between the inferred values and true values when ̂D_e and ̂D_δ are measured. While ̂F_{re} is inferred with reasonable precision, the ̂F_{io} inference suffers from large uncertainties especially when ̂I_e/̂I_δ > 0.45. The result of the ̂F_{io} inference when ̂D_e is included in the measurement is shown in figure 12(b). The uncertainties are significantly reduced compared with figure 12(a). Further improvement is seen in figure 12(c) which shows the results when ̂D_e, ̂D_δ, ̂D_e, and ̂D_δ are measured. The reason for this improvement can be seen in the correlations between the parameters in SPM. Figure 13 shows marginalized probability distributions corresponding to the plasma parameter profiles shown in figure 3 (I_e/I_δ = 0.47). A strong correlation between ̂T_{e,j} and ̂l is seen in figure 13(a). For the data points with ̂I_e/̂I_δ > 0.45, recombination emission dominates the D_e and D_δ emission. As ̂T_{e} increases, ̂PEC_{io} decreases. Therefore, a larger emission volume is required to keep the emission intensities constant for lower ̂T_{e,j}. On the other hand, the correlation between ̂T_{e,h} and ̂l is weak (not shown). Excitation emission provides ‘fine adjustment’ to realize the observed line ratio. The strong correlations between ̂T_{e,j} and ̂n_0 shown in figures 13(b) and (c) are expected since excitation emission depends on both ̂T_{e,h} and ̂n_0. However, the probability distribution in figure 13(b) has relatively high amplitude below the high amplitude band. In this range, excitation emission is negligible in ̂I_e and ̂I_δ and the observed data can be reproduced with only recombination emission. Since the information on ̂n_0, which the ionization rate is proportional to, is contained only in excitation emission, ‘recombination only solutions’ lead to large uncertainties in the ̂F_{io} inference. In contrast, figure 13(c) shows much lower amplitude below the high amplitude band. Due to high sensitivities of ̂D_e and ̂D_δ to excitation emission, recombination emission alone cannot reproduce the observed ̂D_e and ̂D_δ emission. The relation between the size of error bars and the ̂I_e/̂I_δ ratio can be understood through the contribution of the excitation emission. In figure 12(a), the data points with high ̂I_e/̂I_δ, which are dominated by recombination emission, tend to have larger error bars. When ̂I_e/̂I_δ > 0.54, excitation emission becomes negligible even in the ̂D_e and ̂D_δ emission, leading to large error bars shown in Fig2. (b) and (c). For ̂I_e/̂I_δ < 0.54, the 50th percentile of ̂F_{io,SPM} systematically overestimates ̂F_{io}. It is thought to originate from the triangular shape of the ̂n_e profile in SPM. SPM approximates the ̂n_e profiles in the SOL, which looks more like exponential in figure 3, by using a linear function. Figure 5(b) shows that SCD/PEC_{io} is relatively insensitive to ̂T_e above 10 eV, which is a typical ̂T_e in the SOL. However, SCD/PEC_{io} depends strongly on ̂n_e, indicating that assigning proper ̂n_e is more important then ̂T_e for inferring ̂F_{io}. Due to the limited flexibility, SPM tends to reproduce the excitation emission by using higher ̂n_e than the true ̂n_e, leading to the overestimation of ̂F_{io}.  

Figure 13. (a) Correlation between ̂T_{e,j} and ̂l when ̂D_e and ̂D_δ are measured. (b) Correlation between ̂T_{e,h} and ̂n_0 when ̂D_e and ̂D_δ are measured. (c) Correlation between ̂T_{e,j} and ̂l when ̂D_e, ̂D_δ, ̂D_e, and ̂D_δ are measured. The input data for the Balmer line measurements are generated from the plasma parameter profiles shown in figure 3.
For comparison, \( F_{\text{re}} \) and \( F_{\text{io}} \) are also inferred by using a uniform plasma slab model. The only difference from the SPM case is that \( n_e \) and \( T_e \) are constant and the same procedure discussed for SPM is followed to calculate wavelength channel intensities. Figure 11(b) shows the relation between the inferred line-integrated recombination rates from the uniform slab model \( F_{\text{re,slab}} \) and the true values. Interestingly, good agreement is obtained even though the uniform slab model does not take into account the spatial variations of the plasma parameters. As discussed in section 2, recombination events per number photons due to recombination emission of the \( D_e \) line are relatively insensitive to \( T_e \) and \( n_e \) in the ranges relevant to a divertor plasma. Hence, as long as the forward model reproduces the observed absolute intensity of \( D_e \), the inferred \( F_{\text{re,slab}} \) is reasonably close to the true value. On the other hand, figure 12(d) shows that the uniform slab model significantly underestimate \( F_{\text{re}} \) for data points with \( I_e/I_s < 0.45 \). In the cases shown in figure 12(e) and (f) where more lines are measured, \( F_{\text{io}} \) is systematically underestimated for \( I_e/I_s > 0.45 \). Moreover, \( F_{\text{io,slab}} \) has larger error bars than the corresponding \( F_{\text{io,SPM}} \). These results indicate that it is critical to model the spatial variations in the \( F_{\text{io}} \) inference.

5. Particle source and sink inference in an L-mode plasma

In this section, the analysis technique for particle source and sink inference is applied to an AUG L-mode discharge with \( N_2 \) seeding and a density ramp. Basic discharge parameters are shown in figures 14(a) and (b). This discharge has a lower single null configuration with the ion \( \nabla B \) drift in the favorable direction. The edge safety factor \( q_{95} \) is 4 and the toroidal magnetic field \( B_t \) is 2.5 T. At \( t = 1.6 \) s, \( N_2 \) seeding starts and the \( D_2 \) puff amount increases at \( t = 2.5 \) and 3.5 s stepwise, leading to a gradual increase both in the core and edge \( n_e \). The external heating is only through electron cyclotron resonance heating (ECRH). The profiles of \( T_e \), \( n_e \) and ion flux \( \Gamma_i \) on the outer divertor target are shown in figures 14(c), 14(d) and 14(e), respectively. Even with \( N_2 \) puffing and incremental \( D_2 \) fueling, the strong drops in \( n_e \) and \( \Gamma_i \) reported in Ref [5] are not observed. Thus, the outer divertor stays attached. However, after \( t = 1.8 \) s, \( T_e \) decreases and \( n_e \) increases significantly, indicating that the outer divertor plasma has entered the conduction-limited regime.

For this discharge, the line shapes of \( D_e \) and \( D_3 \) are measured by using the lines of sight depicted in solid lines in figure 2. The line-integrated recombination and ionization rates \( (F_{\text{re}} \) and \( F_{\text{io}}) \) are inferred by using SPM. The analysis based on SPM is not applicable for \( t < 2.3 \) s due to insufficient \( D_e \) and \( D_3 \) emission intensities. The profiles of \( I_e \) and the \( I_e/I_s \) ratio along the outer divertor leg are shown in figures 15(a) and (b). The intersections between the lines of sight and the separatrix are assigned for each line of sight. Figures 15(c) and (d) show \( F_{\text{io,SPM}} \) and \( F_{\text{re,SPM}} \) along the divertor leg. The ionization rate increases as one moves away from the target. A large amount of ionization is expected in the upstream region, which is outside the coverage of lines of sight. It is important to note that the \( I_e/I_s \) ratio is above 0.45 for all points in time. Thus, as figure 12(b) indicates, \( F_{\text{io}} \) inference has relatively large uncertainties for those \( I_e/I_s \) values while not shown. Recombination is localized near the strike point. The strong correlation between \( F_{\text{re,SPM}} \) and \( I_e \), which is expected from figure 4(a), is also observed. The profile of \( \dot{n}_e \) (the average \( n_e \) in SPM) shown in figure 15(e) indicates that \( n_e \) monotonically increases as one approaches the strike point. Such \( n_e \) profiles are a feature of the conduction-limited regime.

The volume-integrated recombination rate and ionization rate are calculated by assigning the appropriate integration volumes for each line of sight. Figure 16 shows the volume-integrated recombination and ionization rates and the total ion flux on the outer divertor target. The particle source (volume integrated ionization) is reasonable for the high recycling regime given the expected additional contribution from the undiagnosed region. The particle sink (volume-integrated recombination) has a small contribution in the particle balance in this discharge. These observations are expected for the high-recycling regime where the particle influx from upstream is negligible in the particle balance.
Figure 15. Time evolutions of plasma parameter profiles along the outer-divertor leg. $d$ is the distance from the strike point in a poloidal cross-section. (a)$D_\epsilon$ emission intensity. (b)Ratio of $D_\epsilon$ emission intensity to $D_\delta$ emission intensity. (c)Line-integrated ionization rate inferred by the simplified profile model. (d)Line-integrated recombination rate inferred by the simplified profile model. (e)Average density $\hat{n}_e$ in the simplified profile model. These profiles are created by linearly interpolating 6 spatial data points.

With the current diagnostic capability of AUG, only $D_\epsilon$ and $D_\delta$ can be measured simultaneously using the same line of sight. However, if a signal from one optical fiber is split and fed to two different spectrometers, the four Balmer lines $D_\epsilon$, $D_\delta$, $D_\gamma$ and $D_\beta$ can be measured simultaneously without sacrificing wavelength resolution. Optical fiber splitters are now under development and the $F_{io}$ inference with higher precision will be possible in the near future at AUG.

6. Conclusions

A new analysis technique for Balmer line spectroscopy using Bayesian inference is presented. By comparing measured data and synthetic data calculated by a forward model, the new analysis technique utilizes all available information Balmer line spectroscopy provides: line broadening, line-ratios and absolute emission intensities. Moreover, the Bayesian framework allows for systematical inclusions of multiple Balmer lines in the analysis. This approach is especially useful for underdetermined problems, which Balmer line spectroscopy often encounters, since Bayesian inference provides constraints to the ranges of the parameters of interests by using prior knowledge about the plasma.

In order to measure line-integrated ionization and recombination rates in a closed divertor where spatial variations in the plasma parameters tend to be large, a simplified profile model (SPM) is developed as a forward model for the Bayesian inference. SPM is validated by using test data of $D_\epsilon$, $D_\delta$, $D_\gamma$ and $D_\beta$ spectra generated from SOLPS simulations. It is shown that SPM provides line-integrated ionization and recombination rates robustly over a wide parameter range. While line-integrated ionization rate inference using $D_\epsilon$ and $D_\delta$ lines have relatively large uncertainties especially when recombination emission dominates ($I_{\epsilon}/I_\delta > 0.45$), the precision improves significantly if $D_\gamma$ and $D_\beta$ are measured simultaneously.

SPM is also applied to $D_\epsilon$ and $D_\delta$ spectra obtained from an L-mode discharge in a high-recycling regime. The inferred ionization rate and recombination rate in the outer divertor volume is in a reasonable agreement with the expectations of the high recycling regime, providing further confidence in SPM.

Simultaneous four Balmer line ($D_\epsilon$, $D_\delta$, $D_\gamma$ and $D_\beta$) measurements using the same line of sight will be available in the near future at ASDEX Upgrade and more precise inference of particle sink and source in a closed-divertor will be possible. In addition, the Bayesian framework allows this analysis technique to evolve to integrated data analysis for divertor plasmas [21]. Currently, a two dimensional forward model that utilizes additional lines of sight for Balmer spectroscopy, divertor Thomson scattering and Langmuir probes is under development. Such a model will be able to probe detailed structures of the divertor plasma parameters more reliably.
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Appendix A. Uncertainties in the absolute intensity calibration

Since the wavelength channels in a spectrometer share the same optics, the errors in the absolute intensities typically have a strong correlation between them. For example, when the absolute intensity of one wavelength channel is overestimated by 10%, it is likely that the other wavelength channels also suffer from the overestimation of the absolute intensities by near 10%. The likelihood given by equation (10) does not hold when $\sigma_{\lambda_i}$s are correlated to each other. Therefore, the uncertainties in the absolute intensities cannot simply be included in $\sigma_{\lambda_i}$.

Assuming that all wavelength channels have the same relative error in the absolute intensities, equation (10) is rewritten:

$$
p(D|\theta, I) = \prod_{\lambda} \prod_{X} \exp \left( - \frac{(I_{X,\lambda_i} - \overline{I}_{SPM})^2}{2 \sigma_{\lambda_i}^2} \right)
$$

where $\epsilon$ represents the error in the absolute intensity, e.g., when $\epsilon = 1.1$, the absolute intensities of all wavelength channels $\lambda_i$s are overestimated by 10%. Note that $\sigma_{\lambda_i}$ is also divided by $\epsilon$ since $\sigma_{\lambda_i}$ is calculated by using the absolute intensity calibration. The leftmost $\epsilon$ in the second line of equation (A1) does not affect the ionization and recombination rate inference when the prior of $\epsilon$ is uniform. The second $\epsilon$ in the exponent modifies $I_{X,\lambda_i}^{SPM}$. This form is identical to that of equation (10) when $\hat{I}$ is replaced by $d$:

$$
I_{X,\lambda_i}^{SPM} = \int d\lambda H_{\lambda_i}(\lambda) \int_0^{2\pi} d\hat{\theta} \cdot i_X(\hat{\theta}) L_X(\theta)
$$

where $\theta' = [d, \hat{\alpha}, \hat{n}, \hat{T}_e, \hat{T}_i, \hat{T}_{e,h}, \hat{n}_0]$. Therefore, both the uncertainties in the width of the emission volume and in the absolute intensity calibration can be taken into account by $\hat{I}$ in SPM. When the prior of $\epsilon$ is not uniform, $\epsilon$ needs to be added to the elements of $\theta$ and the likelihood is given by equation (A1).

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