Overview of the RENATE beam emission spectroscopy simulation package

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Abstract

One of the main diagnostic tools for measuring electron density profiles and the characteristics of long wavelength turbulent fluctuations in fusion plasmas is Beam Emission Spectroscopy (BES) [1] which in turn created a high demand for such systems. To facilitate the design of new systems along with the evaluation of measured data the RENATE (Rate Equations for Neutral Alkali-Beam Technique) simulation code was developed that can model lithium, sodium and hydrogen isotope beam. It possesses its own atomic physics kernels, allowing the calculation of the beam evolution utilizing the latest atomic cross sections. Unlike most beam evolution codes, RENATE is developed to model the three-dimensional features of the measurement in detail, including the inner structure of the beam and the optical setup, thus allowing the modeling of complete BES systems, in particular heating beam measurements. RENATE also has a set of tools aimed at simulating and designing fluctuation measurements: visualization of the spatial resolution and calculation of the fluctuation response matrix. The results of the rate equation solver module of RENATE has been benchmarked for hydrogenic beam species and lithium. Meanwhile validation of the code is in progress by detailed comparisons to a heating beam BES measurement at the KSTAR tokamak.

Keywords:
Beam emission spectroscopy, simulation, rate equations, RENATE, fluctuation measurements, diagnostics

1. Introduction

Beam Emission Spectroscopy (BES) is one of the key diagnostics used in the study of plasma turbulence. BES is an active plasma diagnostic which uses either a nonintrusive Diagnostic Neutral Beam (DNB) probe or in some cases a Neural Beam Injection (NBI) heating beam injected into the plasma and analyzes the collisionally induced emission [1]. The distribution of this emission provides information about the distribution of density in the plasma.

The development of new BES systems and the evaluation of current measurements required a detailed simulation which takes all geometrical effects, including observation, beam structure and plasma parameter distributions into account, allowing it to directly simulate measured signals. This motivated the development of the RENATE simulation code. The aim of the current paper is to introduce the RENATE BES code by providing information about its main features in part following [2].

2. The RENATE simulation code

The RENATE (Rate Equations for Neutral Alkali-beam Technique) BES simulation code, has a modular structure and is written in the IDL language [3]. As the name suggests, the original purpose of RENATE was the modeling of alkali atomic beams (lithium and sodium) [4], but during the course of its development support for the more common hydrogen isotopes was also implemented. RENATE has two different atomic physics kernels, both allowing the modeling of the beam evolution in plasmas with mixed isotope content and arbitrary impurity composition.

RENATE is capable of calculating beam evolution by using a collisional-radiative model [5, 6], taking collisional excitation and de-excitation (*exc*), ionization (*ion*), charge exchange (*CX*) reactions and spontaneous de-excitation into account. In this model the recombination of ionized beam material and the interaction with the background electromagnetic field are neglected as these are considered to be negligible in this aspect. This leads to the following time dependent rate equations in the frame moving with the atoms of the beam:

$$\frac{dN_i}{dt} = \sum_I n_I \left[-N_i \left(\sum_{j=1}^{m} R_I^{exc}(i \to j) + R_I^{ion}(i) + R_I^{CX}(i) \right) + \sum_{j=1}^{m} N_j R_I^{exc}(j \to i) \right] - N_i \sum_{j=1}^{i-1} A(i \to j) + \sum_{j=i+1}^{m} N_j A(j \to i), \tag{1}$$

where N_i is the population of the atomic level i ($i = 1$ denotes the ground state and m is the number of considered levels), n_I is the density of species I, R denotes the rate coefficients and A denotes the Einstein coefficients. The rate coefficients are calculated from the cross sections of individual atomic processes by assuming that the plasma species have a Maxwellian population while the beam is assumed to be monoenergetic. The rate equations are solved either directly or by employing a quasi-steady approximation [6].

In case of hydrogen isotope beams the transition cross sections between atomic states for $(n, l) \rightarrow (n, l \pm 1)$ processes are often so high, that a statistical population between the subshells can be assumed, this is called the bundled-n approximation [7] that we adopt (here n and l denote the principal and azimuthal quantum numbers, respectively). Due to the fact that only a finite number of atomic levels can be taken into account, RENATE solves Eq. (1) by considering only the first 9 levels in case of lithium, 8 levels in case of sodium and 6 levels (shells) in case of hydrogenic species. This approximation is based on the fact that higher levels tend to be only lightly populated (see Fig. 1a and Fig. 1b) due to the small cross sections and high rate of spontaneous de-excitement. Numerical calculations have shown that increasing the number of considered levels above the number considered by RENATE only negligibly affects the emission distribution (e.g. less than 1% in case of hydrogen beams).

The rate coefficients - corresponding to the individual transitions - are calculated by the atomic physics kernel of RENATE, using atomic physics data from several sources. The cross sections for lithium were taken from Schweinzer et al. [8], while data for sodium were obtained from Igenbergs et al. [9]. Cross section data for hydrogenic species were obtained from the IAEA ALADDIN[10] and the Open ADAS[11] databases with the corrections from E. Delabie and O. Marchuk [12].

The rate equation solver of RENATE has been benchmarked against the code developed by O. Marchuk [13] for hydrogenic beams (Fig. 1a), and against the SIMULA code [14] for lithium beams (Fig. 1b), yielding identical results within the numerical accuracy of the calculations.

RENATE calculates the beam evolution along the beamline in three dimensions, while the plasma parameters (density, temperature and impurity composition) are considered to be flux functions, which are distributed according to the provided profiles and magnetic geometry of the configuration.

As it was previously mentioned, BES diagnostic measurements are performed not only on thin diagnostic beams but on heating beams as well. The latter are in general not localized to a poloidal plane, hence the need for a full 3D simulation. Heating beams require large and complex ion sources, thus the 3D structure of the neutral beam is not necessarily trivial, which in turn could have a significant effect on the measured signal. To account for this, the neutral beam itself is modeled as a set of infinitesimally thin virtual beams, for which the beam evolution is calculated individually in the 3D model of the tokamak. After the emission distribution along each virtual beam is calculated, their contributions to the individual observation channels are summed up by the optical modules of RENATE. Currently there are two possible choices for the observation modeling, representing different levels of sophistication. The simpler module utilizes a pinhole optics approximation which assumes that each channel of the optical system can only detect light that was emitted within a pyramid whose apex is the observation point, see Fig. 3.

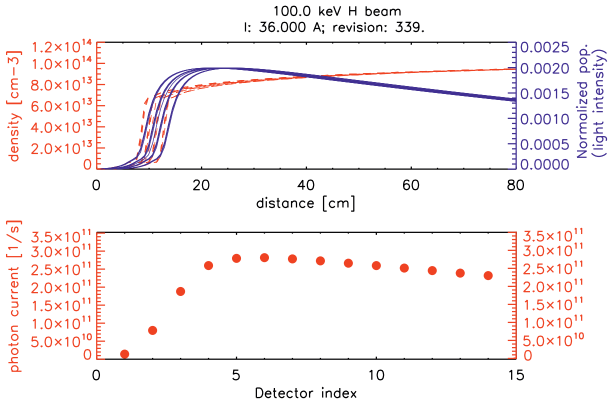


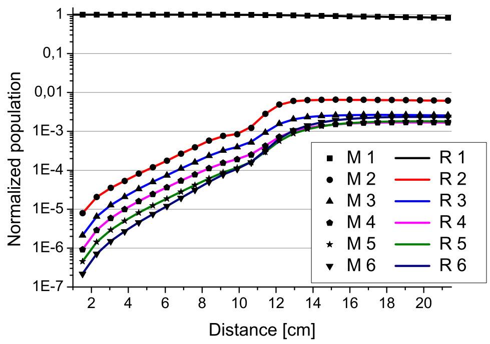
Figure 2: Graphical output of RENATE showing the density along the beamlets (top-red), light profiles (top-blue) and the photon currents reaching the detector surfaces (bottom)

The second, more sophisticated optical module uses ray-tracing through the Zemax [15] model of the optical system to calculate the observation efficiency for every point in space, thus the transfer matrix of the optical system. This involves a Monte Carlo simulation - carried out by Zemax - that creates a large number of randomly generated rays originating from a point-like source.Although ray-tracing provides more accurate results, since it takes all the optical elements of the system into account, it requires detailed optical plans which are not available before the final design phase of BES system development. Meanwhile the pinhole optics module is much more flexible allowing the tryout of a multitude of different configurations without the computationally demanding calculation of transfer matrices.

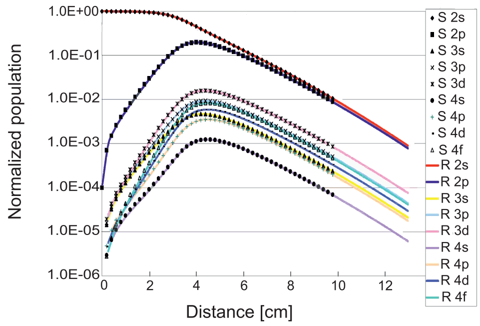
It should be noted that while RENATE can calculate the Doppler-shifted spectrum and thus take filtering into account, it is currently unable to take other wavelength shifting effects (e.g. motional Stark-effect) into account, which means that filtering efficiency for each channel has to be provided externally (e.g. by another simulation code, like Simulation of Spectra [16]).

The final result of these RENATE calculations is the expected absolute photon currents (1/s) reaching the surface of the individual detector segments (Fig. 2).

To give a complete account of the capabilities of RENATE, we note that it can compute the density perturbation response matrices. This calculation involves placing small amplitude quasi delta-function like plasma density perturbations along the beam, and computing the change in detected photon currents for each detector segment. The results are organized into a matrix that gives the response of a chosen detector's signal to a quasi Dirac-delta perturbation at a given position (thus the matrix has 4 indices: 3 coordinate and 1 detector index). Given a sufficiently high resolution perturbation response matrix, the BES system response to an arbitrary shaped small amplitude density perturbation can be easily calculated. A visualization of the perturbation response matrix is shown on Fig. 3.



(a) Hydrogenic benchmark



(b) Lithium benchmark

Figure 1: Evolution of the population of atomic levels along the beam normalized to the initial particle number. Figure (a) shows the evolution of a hydrogen beam calculated by RENATE (R) and the code of O. Marchuk (M). Figure (b) shows the evolution of a lithium beam calculated by RENATE (R) and Simula (S)

3. Application to KSTAR trial measurement

Using measured data simulations have been run with the parameters of KSTAR discharge #6123 at 1744 ms, and its results have been compared against experimental results from the KSTAR BES trial measurement [17]. The magnetic geometry was reconstructed using EFIT [18] while the temperature profile was obtained from Electron Cyclotron Emission (ECE) measurements, assuming $T_i = T_e$ (Fig. 4). Unfortunately during the time of the measurements KSTAR had only a single interferometry channel for plasma density measurement, so it was not possible to obtain localized density data from the experiment. Instead an arbitrary density profile was fitted to the line integrated data. This density profile is flat in the core plasma, while follows the shape of the relative BES emission in the edge as shown in Fig. 4. Impurity data were also unavailable thus a homogeneous 1% carbon impurity was assumed, leading to to $Z_{eff} = 1.35$.

During the experiment a single deuterium beam (13 A, 90 keV) with known current distribution was injected into the plasma (only the central beam source was active). A detector array of 4 x 8 with spatial resolution of 1 cm was used during the measurement. To be able to compare the experimental and simulation results the background light was subtracted from the measured data and the various factors originating from the transmittance of the optical system along with the effect of the filtering and detector amplification were also taken into account. These operations yielded the absolute photon current reaching the aperture for each individual channel. Since only a relative calibration of the detector amplification was possible from gas shots, the results of this method carry a significant relative error. By estimating this error term to be roughly 30% and assuming the other terms to be independent, the measured data have a total 33% relative error. Fig. 5 shows these data compared against RENATE results. Also, the density profile of this simulation was highly arbitrary and a basic pinhole optics module was used to model the observation, which represent error terms of 40% and 20% respectively. This means an estimated relative error of 44% for the the simulation results.

While on average the simulated results are 60% higher than the measurement, the standard deviation of the error is rather small (20%) so the dominant term is caused by a systematic error which can originate from a number of effects:

- No localized density data were available while the density profile is the primary input of RENATE simulations, making it the primary source of error. The shape of used the density profile in the non-BES region is highly arbitrary which could cause a systematic error. Using a parabolic profile for the plasma center instead of the flat one shown in Fig. 4 could mitigate this effect. It was found that a 40% reduction of the BES region density eliminates the systematic error term leaving only an error of only 20%, which could easily be attributed to other uncertainties.
- The RENATE simulation utilized a simple pinhole optical model which could have easily neglected a portion of the real observed area.
- The cross sections of most hydrogenic transitions have a relative error of 10-20% [10, 11].

Although the results are promising as experimental results for the KSTAR BES trial measurement agree with the simulated results well within the estimated error, further experimental validation is needed on better diagnosed discharges to reduce possible systematic errors. Thus in the future RENATE is to be compared against other experimental results and is to be upgraded to be able to take more wavelength shifting effects (e.g. motional Stark-effect) into account.

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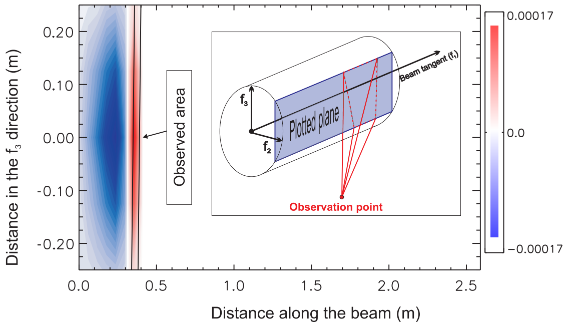

Figure 3: Segment of a perturbation response matrix, showing the normalized absolute response of the detector for perturbations in the given plane. The rectangular box indicates observed area of the beam slice.

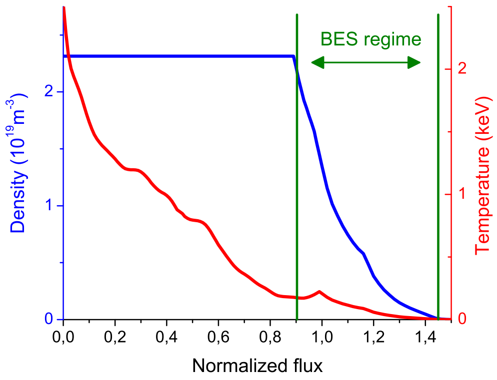

Figure 4: Density (blue) and temperature (red) profiles used in the BES modeling of the KSTAR BES trial measurement.

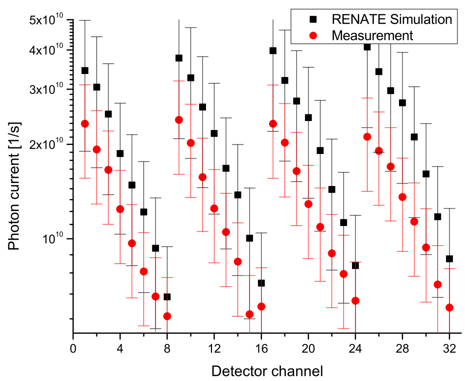

Figure 5: Measured and simulated photon currents for individual detector channels for KSTAR #6123 at 1744 ms. The detectors are sorted into a 4 x 8 matrix, indexing start from the detector of the first row observing the innermost part of the plasma.