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Application of Modified SXB Method for Hydrogen to Zeeman-splitted Hα Line Shape in ITER Main Chamber

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ABSTRACT: The modified SXB method for hydrogen is applied to the case of high-resolution spectroscopy of the H_α line shape in a strong magnetic field. The SXB method, originally designed for evaluating the impurity atoms/ions flux from the tokamak's first wall into the plasma using the observed wavelength-integrated spectral line intensity, was recently modified to estimate – in real-time measurements – the fluxes of atomic and molecular hydrogen without measuring the molecular spectra. Instead, the asymmetry of the atomic spectral line shape was used to solve the inverse problem of recovering the flux density. The proposed modification was motivated by the fact that the hydrogen molecular spectra will not be used for ITER operation diagnostics because of difficulties of their interpretation. The results of modified SXB method for scrape-of-layer plasma in ITER main chamber show good agreement with the results of the Ballistic Model, which has previously been validated by comparison with the EIRENE code Monte-Carlo simulations of hydrogen recycling, but is still not applicable to real-time measurements.

Keywords: plasma diagnostics, hydrogen recycling, ITER, SXB method, high resolution spectroscopy.

1. INTRODUCTION

The influx of hydrogen isotopes from the first wall (FW) into the plasma is of practical interest for the controlled nuclear fusion in hydrogenic (D, T) plasmas. The recycling of hydrogen between the FW and the plasma directly influences the profiles of plasma parameters in the peripheral regions and has an impact on the operation of a fusion reactor [1, 2]. The complexity of the kinetic recycling of hydrogen between the plasma and the first wall, as well as the presence of a strong radiation background, the divertor stray light (DSL) in the main chamber [3], require highresolution spectroscopy (HRS) and solving the multiparametric inverse problems for recovering ("measuring") the requested parameters [3].

The calculation of plasma kinetics is a complex task that cannot be solved analytically. The currently most accurate prediction of plasma parameters in the tokamak scrape-off layer (SOL) can be obtained using numerical simulations. In the ITER case, the SOLPS4.3 (B2-EIRENE) numerical code [4, 5] is often used. Also, it requires using the OEDGE code [6] to extend the plasma parameters from the original SOLPS4.3 numerical grid up to the first wall. These codes perform complicated numerical modeling, so that it is impossible in real time measurements (i.e. in the time interval of about 100 ms in the ITER case) to recover the flux of hydrogen from the wall using the observation data and SOLPS simulations.

The semi-analytic Ballistic Model (BM) [7, 8, 9] has been created to make fast calculation of the penetration of molecules and hydrogen neutral atoms into the plasma, taking into account the primary source in the form of slow neutral atoms produced by the dissociation of molecules, and the sequential generation of faster and faster neutral atoms produced by the charge exchange of neutral atoms on plasma ions. Using as input data the density and temperature profiles of ions and electrons in the SOL, and wall temperature, the Ballistic Model allows to obtain, in

the slab geometry approximation applicable to the SOL in the most part of the main chamber, the velocity distribution functions (VDFs) of neutral atoms and molecules. These VDFs are the one-dimensional distributions in the space coordinate and one-dimensional distributions in the velocity projection on the direction transverse to the wall. Such VDFs allow one to calculate the flux density of molecules and atoms from the wall into the plasma. The Ballistic Model has the following free parameters:

- the density and temperature of neutral molecules on the wall (the temperature of molecules on the wall can be taken equal to the known wall temperature),
- the density and the characteristic temperature (namely, mean energy of a non-Maxwellian VDF) of atoms formed via direct conversion of the flow of ions from the plasma to the wall into the flow of neutral atoms into plasma, without formation of molecules on the wall.

These parameters in real experiments can be found by solving an inverse problem via fitting the experimentally measured high-resolution spectra of hydrogen lines, for example, the Balmer-alpha lines. The required theoretical prediction of spectral intensity of the lines of hydrogen (and its isotopes) may be calculated using the following data:

- VDF of neutral atoms from Ballistic Model,
- electron density and temperature profiles from experimental data or predictive modeling data, and
- the so-called photon emission coefficients (PEC) from the ADAS database [10].

The Ballistic Model makes it possible to calculate, with satisfactory accuracy, the required parameters thousands of times faster than the SOLPS code.

Unfortunately, the BM does not allow us to make the real time measurements that assumes getting the values of requested parameters within time interval, <100 ms, of interest for ITER operation control services. To calculate the flux density of atoms and molecules from the wall to plasma in real time, using only the spectroscopy data and the density and temperature profiles data, one may apply the SXB method [11, 12] for atoms (the data for the so called ionization per photon coefficients may be found in [10], for ITER case, in [13]), and its extension to molecules, DXB method, to the case of hydrogen (see e.g. Sec. 3.3 in [14]). The SXB method was suggested for diagnostics of impurities influx and is based on the approximate relationship between the flux density Γ of atoms (or ions) from the wall and the spectral intensity I_{jk} of atomic line radiation collected in a detector on the line of sight (LoS) targeted at the respective area on the wall,

$$\Gamma = 4\pi \left\langle \frac{S}{XB} \right\rangle I_{jk}, \tag{1}$$

where the ionization per photon coefficient is expressed in terms of the ionization rate S, the excitation rate X and the branching factor B which is the ratio between the probabilities of spontaneous radiative decay, per unit time, from the level with the principal quantum number $n = j$ to, respectively, the level $n = k$ and all lower levels.

Eq. (1) is valid if the density of atoms (or ions) in the region near the wall on the LoS may be described by the balance between the influx of atoms from the wall and their ionization by electron impact (otherwise the balance takes a more complicated form). Eq. (1) is valid for a weak dependence of the SXB factor on the coordinate along the line of sight in the SOL (the latter is often true due to the close dependencies of S and X on the electron temperature). The combined SXB+DXB approach would make it possible to estimate the flux of atoms and molecules from the tokamak wall, however this would require the molecular emission spectra, which in ITER will not be used for ITER operation diagnostics because of well-known difficulties of interpreting these spectra.

The use of the DXB method for molecular spectra in the ITER case can be replaced with using the modified SXB method [15], which uses the asymmetry of the spectral line shape of atomic radiation. In Section 2, all equations used in modified SXB method and their extension on the case of a Zeeman-splitted line are presented. The verification of the extended model is given in section 3. Finally, the results are briefly discussed in section 4.

2. SOLVING SYSTEM OF EQUATIONS

We solve the system of linear equations, obtained in [15]. The system requires the atomic spectral line shape as an input data. The first equation uses the well-known SXB method [11] and the second one takes into account the asymmetry of the spectral line shape.

$$\begin{cases} j_{wall\_rec}(0)f_1(0) + j_{mol}(0)(\alpha + f_2(0)) = 4\pi \left\langle \frac{S}{XB} \right\rangle I_{32}, \\ j_{wall\_rec}(0)F_1 + j_{mol}(0)F_2 = \int I_{32}(\omega)\frac{\omega-\omega_s}{\omega_s}d\omega. \end{cases} \tag{2}$$

Here ω_s is the frequency of the Balmer-alpha line of the hydrogen isotope of the type s.

The atomic flux is a sum of two fluxes:

$$j_{atom}(x) = j_{wall\_rec}(0)f_1(x) + j_{mol}(0)f_2(x), \tag{3}$$

where $j_{wall\_rec}(0)$ is the flux of atoms from the wall, formed by the reflection of plasma ions from the wall with their immediate recombination, without converting the formed atoms into molecules on the wall. In the EIRENE code [4], for describing such a flux, the reflection coefficient of atoms from the wall are used), $j_{mol}(0)$ is the flux of hydrogen molecules from the wall. The functions $f_1(x)$ and $f_2(x)$ describe, respectively, the contributions of the wall-recombination flux of atoms and molecular flux from the wall to the atomic flux in the volume (these functions may be calculated using the Ballistic Model).

The α parameter can be written in following terms:

$$\alpha = \frac{\int n^{(H_2)}(x)n_e(x)\left[2\langle\sigma_d v_e\rangle(x) + \langle\sigma_{mi}v_e\rangle(x) + \langle\sigma_{di}v_e\rangle(x)\right]dx}{\int n^{(H_2)}(x)n_e(x)\left[\langle\sigma_d v_e\rangle(x) + \langle\sigma_{mi}v_e\rangle(x) + \langle\sigma_{di}v_e\rangle(x)\right]dx}, \tag{4}$$

where $n^{(H_2)}(x)$ and $n_e(x)$ are the densities of hydrogen molecules and electrons, $\langle\sigma_d v_e\rangle$, $\langle\sigma_{mi}v_e\rangle$ and $\langle\sigma_{di}v_e\rangle$ are rates of the dissociation, the ionization and the dissociation with ionization of hydrogen molecule respectively, caused by their collisions with electrons.

Although the right hand side in the second equation in the system (2) was obtained without taking into account the Zeeman splitting, it turns out that the system (2) can be used in the case of the normal Zeeman effect. Indeed, if we write the spectral line shape observed in direction perpendicular to the magnetic field:

$$I_Z(\omega) = \frac{1}{4}\left[I(\omega+\Omega) + I(\omega-\Omega)\right] + \frac{1}{2}I(\omega), \tag{5}$$

where $I_Z(\omega)$ and $I(\omega)$ are the spectral intensities with and without account of the Zeeman splitting, respectively, Ω is the Larmor frequency. Substituting the line shape (5) in the right hand side of the second equation in the system (2), we obtain the following equation:

$$\int I_Z(\omega)\frac{\omega-\omega_s}{\omega_s}d\omega \equiv \int I(\omega)\frac{\omega-\omega_s}{\omega_s}d\omega. \tag{6}$$

Although the H_α Zeeman-splitted line shape has a multiplet structure, for the Doppler-Zeeman line shape it is similar to Paschen-Back Doppler-broadened triplet [16].

3. SOLUTION AND COMPARISON WITH BALLISTIC MODEL

The results of the modified SXB method and their comparison with the Ballistic Model are presented here for the observation of plasma on the line of sight shown in figure 1.

We are solving an inverse problem to recover the atomic and molecular fluxes of neutral deuterium using

Doppler-Zeeman Balmer-alpha spectral line shape. The spectral intensity used as a synthetic experimental data was calculated using the atomic VDF (see e.g. eq. (20-24) in [9]) obtained running EIRENE for plasma parameters in the SOL (figures 4 and 7) taken from the SOLPS4.3 run #2252 (the same run has been used in [9]) and extrapolated to the wall by a constant value.

The atomic and molecular fluxes (and atomic and molecular VDFs) can be obtained by solving the inverse problem of fitting the spectral line shape using the Ballistic Model [9] and recovering its free parameters. But since the BM cannot be used in real time measurements we use the modified SXB method. The recovery of the fluxes from the FW is an ill-posed problem that tends to overfitting, so it requires Tikhonov regularization. Besides, we introduce to the inverse problem a condition, which states that fluxes in (3) should be equal within the order of magnitude. So we obtained an optimization problem:

$$\|\mathbf{Ax}-\mathbf{b}\| \underset{\mathbf{x}}{\to} 0, \tag{7}$$

where:

$$\mathbf{A}=\begin{pmatrix} f_1(0) & \alpha+f_2(0) \\ F_1 & F_2 \\ C_{reg} & -C_{reg} \end{pmatrix}, \qquad \mathbf{x}=\begin{pmatrix} j_{wall\_rec}(0) \\ j_{mol}(0) \end{pmatrix}, \qquad \mathbf{b}=\begin{pmatrix} 4\pi\left\langle\frac{S}{XB}\right\rangle I_{32} \\ \int I_{32}(\omega)\frac{\omega-\omega_s}{\omega_s}d\omega \\ 0 \end{pmatrix}. \tag{8}$$

There C_{reg} is a regularisation parameter which describes the contribution of the residual caused by the inequality of the fluxes in (3) to the total residual in the inverse problem (7).

The **x** is the unknown vector of that optimization problem which is solved by using the non-negative least squares (NNLS) method. Here α, $f_1(x)$, $f_2(x)$, F_1 and F_2 are the precalculated parameters.

The system of equations (7) was solved for each of two regimes, characterized by the low and high density in the far SOL, for each section on the line of sight: on the high-field side (HFS) and low-field side (LFS). The respective profiles of electron and ion densities and temperatures are shown on figures 2 and 3. The comparison of solutions with the results obtained using the solution of the inverse problem [9] is given in the Table 1.

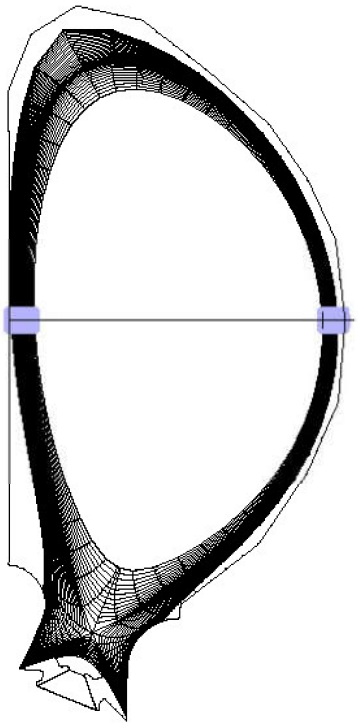

Figure 1: SOLPS 4.3 computational grid. The horizontal LoS is shown.

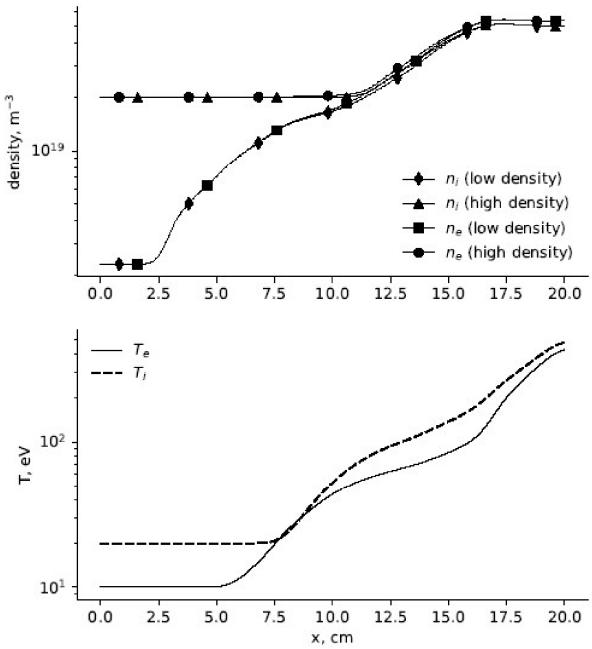

Figure 2: Electron and ion densities and temperatures in the HFS SOL on the horizontal LoS as functions of the distance along the LoS from the FW in the simulation cases with low and high plasma densities in the far SOL. The profiles of ion and electron temperature are equal in both cases.

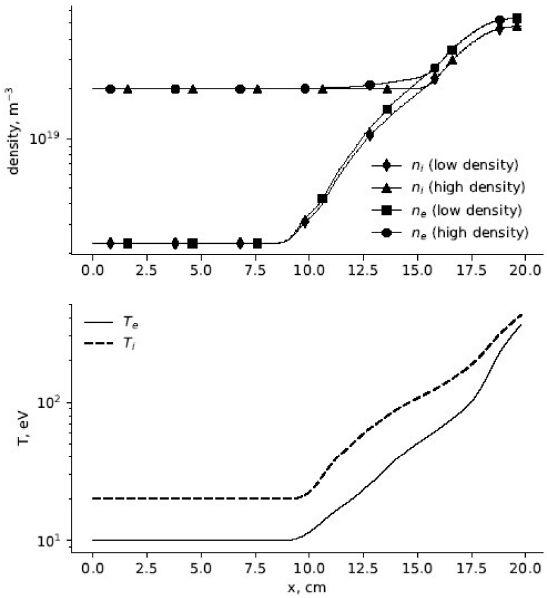

Figure 3: Electron and ion densities and temperatures in the LFS SOL on the horizontal LoS as functions of the distance along the LoS from the FW in the simulation cases with low and high plasma densities in the far SOL. The profiles of ion and electron temperature are equal in both cases.

Table 1: Comparison of $j_{wall\_rec}(0)$ and $j_{mol}(0)$, obtained from equation (7), with similar values from the Ballistic model

Case	$j_{wall\_rec}(0)$, atom s^{-1} m^{-2}	$j^{BM}_{wall\_rec}(0)$, atom s^{-1} m^{-2}	$j_{mol}(0)$, mol s^{-1} m^{-2}	$j^{BM}_{mol}(0)$, mol s^{-1} m^{-2}
Low density HFS	2.05×10^{19}	2.41×10^{19}	3.01×10^{19}	1.85×10^{19}
Low density LFS	4.70×10^{18}	3.81×10^{18}	6.65×10^{18}	7.30×10^{18}
High density HFS	2.22×10^{19}	2.18×10^{19}	3.09×10^{19}	2.48×10^{19}
High density LFS	5.68×10^{18}	3.44×10^{18}	1.24×10^{19}	1.40×10^{19}

The figures 4 and 7 show the spectral intensity on the LoS, respectively, on the HFS and LFS. An interesting fact that the signal on the HFS is higher in the case of low density, whereas on the LFS the situation is opposite. The comparison between the BM and the solution of eq. (7) for all cases is given at figures 5, 6, 8 and 9. The figures show a good recovering of the atomic and molecular flux profiles.

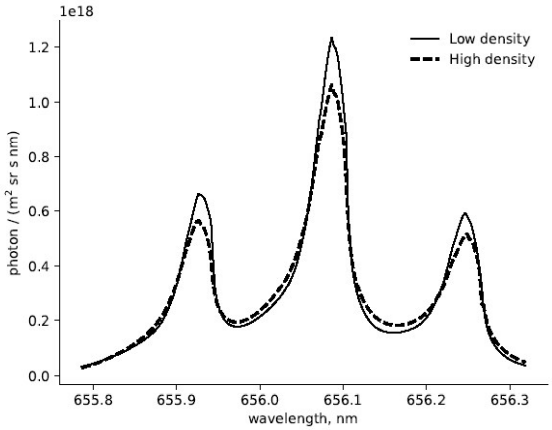

Figure 4: Spectral intensities of deuterium atoms radiation of the Balmer-alpha line in the HFS SOL on the horizontal LoS. The signal in the case of high density in the far SOL is shown as a dashed line, while the solid line corresponds to low density.

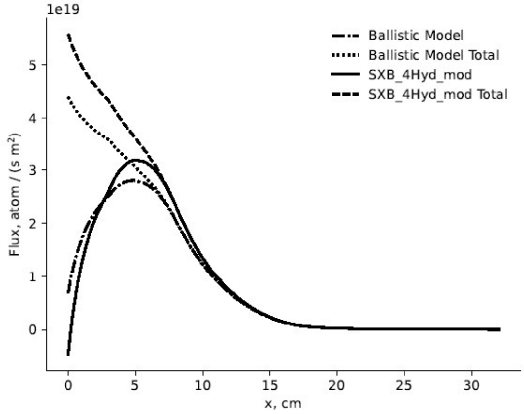

Figure 5: Atomic and total flux densities of neutral deuterium in the HFS SOL on the horizontal LoS in the case of low density in the far SOL. The solid line is the atomic flux profile obtained from the solution of eq. (7), while the dash-dotted line is the flux, modelled by the BM. The dashed and dotted lines show the total fluxes of hydrogen atoms, namely the sum of the purely atomic and doubled molecular fluxes, obtained from from the solution of eq. (7) and the BM, respectively.

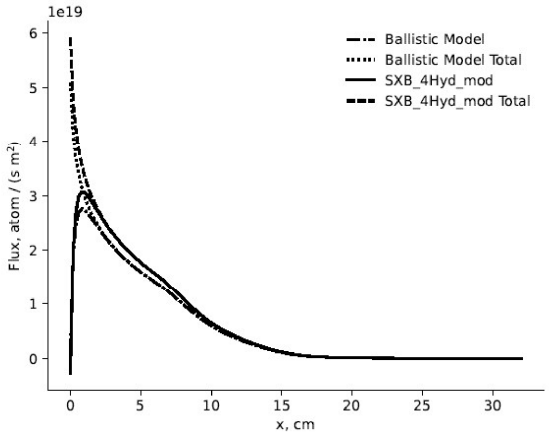

Figure 6: Atomic and total flux densities of neutral deuterium in the HFS SOL on the horizontal LoS in the case of high density in the far SOL. The solid line is the atomic flux profile obtained from the solution of eq. (7), while the dash-dotted line is the flux, modelled by the BM. The dashed and dotted lines show the total fluxes of hydrogen atoms, namely the sum of the purely atomic and doubled molecular fluxes, obtained from from the solution of eq. (7) and the BM, respectively.

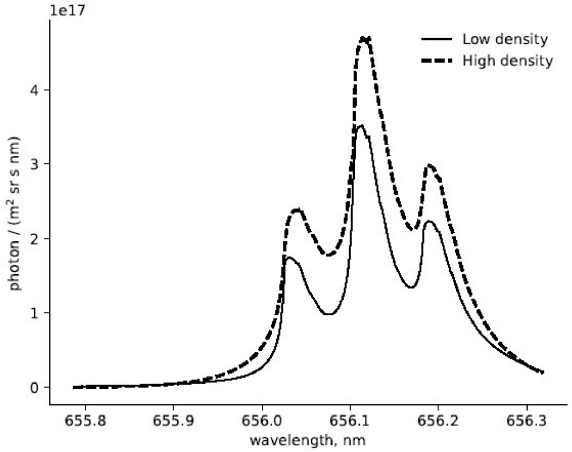

Figure 7: Spectral intensities of deuterium atoms radiation of the Balmer-alpha line in the LFS SOL on the horizontal LoS. The signal in the case of high density in the far SOL is shown as a dashed line, while the solid line corresponds to low density.

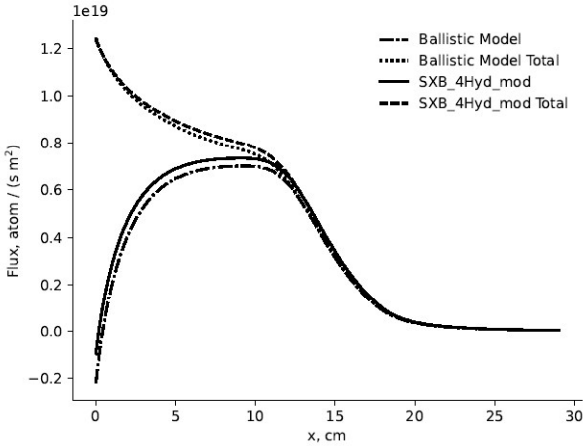

Figure 8: Atomic and total flux densities of neutral deuterium in the LFS SOL on the horizontal LoS in the case of low density in the far SOL. The solid line is the atomic flux profile obtained from the solution of eq. (7), while the dash-dotted line is the flux, modelled by the BM. The dashed and dotted lines show the total fluxes of hydrogen atoms, namely the sum of the purely atomic and doubled molecular fluxes, obtained from from the solution of eq. (7) and the BM, respectively.

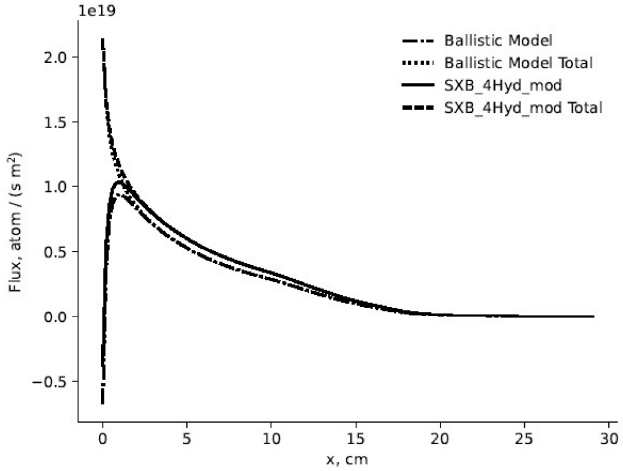

Figure 9: Atomic and total flux densities of neutral deuterium in the LFS SOL on the horizontal LoS in the case of high density in the far SOL. The solid line is the atomic flux profile obtained from the solution of eq. (7), while the dash-dotted line is the flux, modelled by the BM. The dashed and dotted lines show the total fluxes of hydrogen atoms, namely the sum of the purely atomic and doubled molecular fluxes, obtained from from the solution of eq. (7) and the BM, respectively.

4. DISCUSSION AND CONCLUSION

The problem of recovering the flux density of hydrogen atoms into the plasma from the first wall in a magnetic thermonuclear fusion reactor is considered. This problem is one of the main tasks of the ITER Main Chamber H-alpha and Visible Spectroscopy Diagnostics in ITER tokamak.

The analysis is carried out of the possibility of using the high-resolution spectroscopy data, specifically, the asymmetry of the Doppler-Zeeman spectral line shape of the radiation emitted in the Balmer-alpha lines of hydrogen isotopes, to recover the flux density of neutral hydrogen atoms and molecules from the wall to the plasma in real time measurements. The modified SXB method [15] is extended to the case of a Zeeman-splitted spectral line shape. It is shown that it does not require to change the system of equations (7), which allows us to recover two unknowns: the density of the wall-recombination flux of atoms (i.e., atoms formed by the reflection of ions, leaving the plasma, with their immediate recombination, without transformation of the formed atoms into molecules on the wall with the wall temperature) and the flux density of molecules from the wall.

The spectrum of the divertor stray light (DSL) is expected to possess much less spectral asymmetry than that of the light from the SOL, therefore the impact of the DSL on the second equation in the system (7) is not strong. However, the method is very sensitive to the DSL signal (the first equation of the system (7) is valid only for zero DSL) and the signal from the opposite side of the SOL on the line of sight in the main chamber because one should extract the signal from a certain side of the SOL in the main chamber from the total observed signal. This problem is complicated with the fact that the signals from opposite sides of the SOL in the main chamber have opposite signs of the asymmetry (see figures 4 and 7) because the asymmetry is caused by the net inward flux of atoms into plasma. The latter difficulty is mitigated by the fact that the influx of atoms in the region near the diagnostic port-plug is expected to be smaller than that on the opposite side on the SOL on the line of sight. Therefore, the proposed method is applicable for evaluating the influx of hydrogen atoms and molecules if, first, the DSL signal is comparable with the signal from the SOL and, second, the signal from the SOL on one side of the line of sight is substantially stronger than that from the other side.

The advantage of the proposed model with respect to the SXB+DXB approach is the use of atomic high-resolution spectroscopy data instead of difficult-to-interpret data of spectroscopy of hydrogen molecules in tokamaks. Indeed, the hydrogen molecular spectra will not be used for ITER operation diagnostics.

It is shown that the use of this approach allows one to estimate the fluxes of atoms and molecules from the wall into the plasma with an accuracy of the order of magnitude in real time measurements.

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