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HOW RELIABLE ARE LINE INTENSITIES FOR TEMPERATURE CALCULATION USING THE BOLTZMANN PLOT METHOD

M. Henkel*, D. Gonzalez

Leibniz Institute for Plasma Science and Technology (INP), Felix-Hausdorff-Straße 2, 17489 Greifswald, Germany

* marion.henkel@inp-greifswald.de

Abstract. This study investigates the reliability of electron temperature calculations for plasmas using line intensities, specifically through the Boltzmann plot method. Simulated spectra of a copper plasma reveal that while using line intensities may be sufficient under certain conditions, significant deviations arise under high-pressure and low-temperature scenarios. Our findings emphasize the need for caution, as inaccuracies can occur when the optical depth reaches a relevant magnitude.

Keywords: Boltzmann plot method, electron temperature, spectral lines, accuracy.

1. Introduction

The determination of plasma temperature through atomic lines from an measured spectrum has long been a valuable technique in plasma physics. This method allows researchers to infer temperature from the spectral characteristics of emitted light, providing critical insights into the properties of various plasma states. Two primary approaches are commonly employed: the single-line analysis, which necessitates absolute calibration, and the Boltzmann plot method, where relative calibration suffices by utilizing the ratios of lines corresponding to different energy levels. Despite the differences in their calibration requirements, both methods hinge on the accurate knowledge of the emission coefficient, which must be derived from the measured line intensities.

Recent advancements have seen the increasing prevalence of fiber-based compact spectrometers in experimental setups, highlighting a trend towards more portable and user-friendly instrumentation. However, it is noteworthy that temperature calculations derived from these spectroscopic measurements frequently do not employ the emission coefficient ϵ; instead, they rely on directly measured line intensities from the spectral radiation density L. For optically thin plasmas, the approximation ($L \sim \epsilon$) may yield sufficient results. Nonetheless, prior studies have not conclusively addressed the parameter ranges over which this simplification is valid and where the temperature calculations may be falsified by using line intensity instead of the emission coefficient.

This paper focuses on plasmas in local thermodynamic equilibrium (LTE) and aims to investigate the reliability of the Boltzmann plot method, concentrating on the parameter ranges where the simplification of the temperature calculation can be sufficiently deemed while identifying the physical parameters that influence its applicability. Diverse effects, such as non-local thermodynamic equilibrium (non-LTE) and non-thermal ionization, can significantly distort temperature calculations. However, these factors will not be examined in this manuscript to investigate its distortion effect for plasmas in equilibrium. In this paper, spectroscopic data will be simulated with known temperature and density (or pressure) conditions. Subsequently, these simulated spectra will be analyzed using line intensities and the Boltzmann plot method, and the calculated temperatures will be compared to the actual temperatures to assess the accuracy and reliability of this approach.

2. Theoretical background

For this purpose, the atomic data for the relevant transitions of the involved elements were taken from the atomic data bases from NIST [1] and Kurucz/Bell [2]. A detailed description of the radiation transport can be found in [3], whereas a brief introduction to the calculation of emission and radiation density is further presented in this chapter.

2.1. Description of radiation transport

The partition function Z according to the Planck-Larkin relation [4], as an element-specific weighting factor, depends on the ionization energy E_i of the respective element and on the electron temperature T_e of the plasma. All possible transitions of the element are summed up using the respective upper level energy E_k and the respective statistical weights g_k:

$$Z(T) = \sum_k g_k \cdot \exp\left(-\frac{e_0 E_k}{k_B T_e}\right) \quad (1)$$

effects of scattering

$$+ g_k \cdot \exp\left(-\frac{e_0 E_i}{k_B T_e}\right) \cdot \left(\frac{e_0 (E_k - E_i)}{k_B T_e} - 1\right)$$

effects of thermodynamic potential.

In the next step, the particle density of the ions n_i depending on the density of the previous ionization level n_{i-1} can be calculated by solving the Saha

equation for each species [3]. The required thermal or de-Broglie wavelength can be calculated as in equation 3. From that, the plasma composition (e electrons, i ions, n neutrals and t all particles) can be calculated:

$$\frac{n_e n_i}{n_n} = \frac{Z_e Z_i}{Z_n} \frac{1}{\lambda^3_{\text{de Broglie}}} \exp\left(-\frac{e_0 E_i}{k_B T_e}\right) \quad (2)$$

$$\lambda_{\text{de Broglie}} = \sqrt{\frac{h^2}{2\pi m_e k_B T_e}}. \quad (3)$$

where the partition function of the electrons is $Z_e = 2$ and the total particle density $n_t = n_n + n_i$ is given by the plasma pressure ($n \sim p/T$).

In the next step, the emission and absorption coefficients for a plasma in LTE is calculated. While the associated radiation transfer equations can be found in [3] in more detail, the most important equations are summarized in the following.

The emission coefficients ϵ of the atomic and, if needed, of the ionic lines were calculated using the transition probability A_{ul} between upper and lower energy level, the emitted wavelength λ and the particle density at the upper energy level n_u, which depends on the electron temperature T_e and the total particle density of the corresponding species n_k:

$$\epsilon_k = \frac{c_0 h}{4\pi\lambda_k} A_{ul,k} n_{u,k}, \quad (4)$$

$$n_{u,k} = \frac{g_{u,k} n_k}{Z_k} \exp\left(-\frac{e_0 E_{u,k}}{k_B T_e}\right). \quad (5)$$

It should be noted that the atomic data from various databases naturally also have inaccuracies (e.g., NIST $\pm$ 12% for A_{ul}), which influence the accuracy of the temperature calculation. However, since these values are used for both the simulation and the analysis of the spectrum, this should not affect the following results, which are intended to show basic behavior in temperature calculation using the line intensities.

From this, the dependence of the absorption coefficient κ on the emission coefficient (e.g. [5]) and its ratio to the black body radiation B can be used. Further, the line broadening $\Delta\lambda$ will be taken into account, to calculate the absorption coefficient in the line center. This can be determined for each individual line in the spectrum:

$$\kappa_k = \frac{2/\pi}{\Delta\lambda} \frac{\epsilon_k}{B(\lambda_k, T_e)}. \quad (6)$$

Finally, the spectrum can be calculated by integrating over the line of sight using the emission and absorption coefficients of all involved transitions or lines and solving the differential radiation transport equation:

$$\mathrm{d}L(x,y) = (\epsilon(r) - \kappa(r) L(x,y))\, \mathrm{d}y. \quad (7)$$

For optically thin plasmas, it can be assumed that the absorption coefficient $\kappa \ll 1$ is negligible. The spatially resolved emission coefficient ϵ can then be determined from the spectral radiation density L using

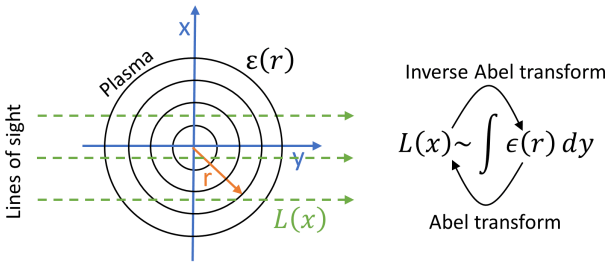

Figure 1. Sketch of the principle of Abel transformation.

a spatially resolved optical emission spectroscopy measurement and subsequent inverse Abel transformation. This exploits the fact that the spectral radiation density depends on the emission coefficient integrated over the line of sight, as stated in equation 7 and sketched in figure 1. Following, the electron temperature can be calculated using equation 4 and 5 or respectively the dependence between emission coefficient ϵ and particle density n_k and electron temperature T_e:

$$\ln\left(\frac{\epsilon\lambda}{g_u A_{ul}}\right) = -\frac{e_0}{k_B T_e} E_u + \ln\left(\frac{c_0 h}{4\pi}\frac{n_k}{Z_k}\right). \quad (8)$$

However, in some spectroscopic methods, e.g. fiber-based measurements, the plasma is not imaged onto the detector but is integrated and collected over a certain solid angle, as sketched in figure 2. Without the knowledge of the spatial profile, it is not possible to determine the emission coefficient from the spectral radiation density using inverse Abel transformation. Therefore, in such cases, $L \sim \epsilon$ is usually assumed for optically thin plasmas and the line intensity is used for further calculations, such as for electron temperature calculation using the Boltzmann plot method.

However, this approximation may become inadequate if the plasma has a non-homogeneous profile in density or temperature and thus a spatial profile in the emission coefficient or if the absorption coefficient can no longer be neglected.

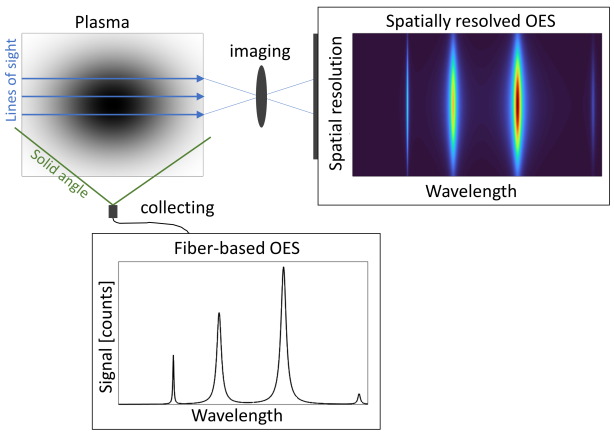

Figure 2. Sketch of difference between spatially resolved and fiber-based optical emission spectroscopy.

2.2. Boltzmann plot method

The evaluation methods described so far all require absolute calibration. This means that the emission of a calibration lamp with known spectral radiation density is measured with the spectroscopic setup in order to assign a spectral radiance density to the detector's signal strength. The Boltzmann plot method has the advantage, that the ratios of line intensities are used and thus a relative calibration is sufficient. In this case, calibration using a lamp is not necessary as long as the transmittance/reflectivity of the optical components and the spectral sensitivity of the detector are known. Often, the detector's sensitivity changes little over a certain spectral range, making lines with narrow wavelength difference particularly suitable for temperature calculation using this method.

For this, spectral lines with different energy levels of an element are used and the linear dependence between the left side of equation 8, which depends on the emission coefficient, and the energy of the upper level of the corresponding level transition is exploited. A frequently used variant is the so-called two-line method, in which equation 8 is defined for two different lines and then subtracted from each other and thus the density dependence is eliminated giving the equation 9 :

$$\frac{1}{T_e} = \ln\left(\frac{\epsilon_1\lambda_1}{g_{u,1}A_{ul,1}}\frac{g_{u,2}A_{ul,2}}{\epsilon_2\lambda_2}\right)\frac{k_B}{e_0\Delta E_u}. \quad (9)$$

This allows the electron temperature to be calculated from the ratio of the emission coefficients ϵ_k of two lines (i) of the same particle species. However, as already mentioned, no information about ϵ is available in fiber-based spectral measurements, but only about the spectral radiance L_k. Since a linear relationship is a sufficient approximation for optically thin plasmas, the spectral radiation density L can also be used in the Boltzmann plot method. The extent to which this approximation affects the accuracy of the temperature calculation has not yet been reliably tested and will therefore be further investigated below.

3. Results and discussion

To investigate the accuracy of temperature calculation using line intensities instead of the actual emission coefficients for the Boltzmann plot method, a spectrum was first simulated using a code based on the radiation transport equations in LTE plasmas, as previously shown in [6]. A copper plasma was assumed for further calculations, since it has atomic lines with different energy levels in a small wavelength range that are very suitable for temperature calculation.

Furthermore, as a first approximation, it was assumed that the plasma is spatially homogeneous in temperature and density or pressure. This assumption is supported on the fact that the use of line intensity instead of emission coefficient determination is usually coupled with fiber-based spectroscopic measurements, which do not provide spatially solved information.

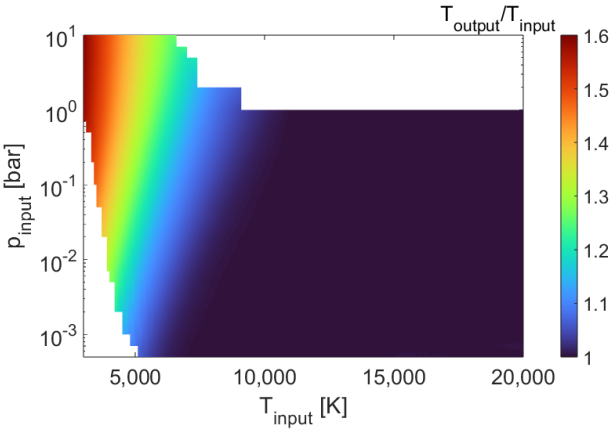

Figure 3. Ratio between the calculated electron temperature T_{out} using the Boltzmann plot method and the input electron temperature T_{input} as indication for the accuracy of the method. The line integrated intensities L_i of simulated spectra were used as an approximation to the emission coefficients ϵ_i. The simulation has the following boundary conditions: pure copper plasma, line width is $10^{-5}\,nm < \Delta\lambda < 1\,nm$ and LTE is required. Parameters: plasma diameter of $d = 0.2\,mm$, atomic lines at 510.6 nm and 521.8 nm, atomic data from [1, 7–9].

3.1. Calculating the output temperature using line intensities

Further, the reliability of using the line intensity instead of the emission coefficient was investigated. For this purpose, simulated spectra with different known electron temperatures and plasma pressures were evaluated using the Boltzmann plot method, or more precisely the two-line method, and shown in figure 3.

It can be observed that the calculated value of electron temperature deviates increasingly from the actual electron temperature at high pressures and low temperatures, giving always an overestimated temperature value. This indicates that the line intensities in these range are no longer linearly related to the emission coefficients. The most likely reason is that the absorption coefficient κ_i that is no longer negligibly small. This changes the ratio of the line intensity of different lines because their absorption coefficients differ. Therefore, the dependence of the accuracy of the Boltzmann plot method on various parameters related to the absorption coefficient is investigated in the following section.

3.2. Parameter dependence of the accuracy of the temperature calculation

When the emission coefficient reaches the order of magnitude of the spectral radiation density by Planck's law, absorption becomes significant (see formula 6). However, the actual emission is distributed over a spectral line profile, where a broader profile results in lower emission at its peak, while a narrower profile leads to higher peak emission, given that the total emission remains constant in both cases, as sketched in

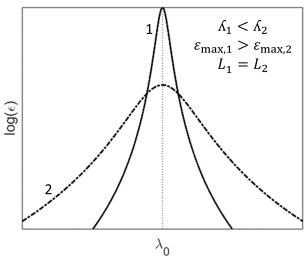

Figure 4. Sketch of dependence between maximum in line center and line width.

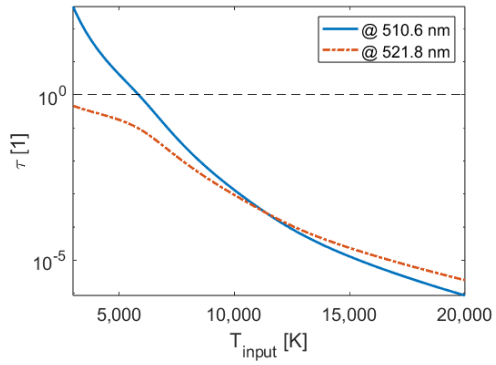

Figure 5. Optical depth τ, i.e. absorption coefficient (see formula 6) integrated over the line of sight, in the line center of two atomic lines of a 1 mbar copper plasma, which are used for the electron temperature calculation using the Boltzmann plot method. Parameters: plasma diameter of $d = 0.2$ mm, atomic lines at 510.6 nm and 521.8 nm, atomic data from [1, 7–9].

figure 4. Unfortunately, information about the actual line broadening of a spectral line is often not available, since the apparatus profile often dominates. Even if the line broadening due to the apparatus profile makes it seem that the measured spectral radiation density is significantly smaller than the value given by Planck' law, this may not actually be the case with the actual plasma-related line broadening (e.g. Stark width), which can be many orders of magnitude smaller (as indicated in figure 4).

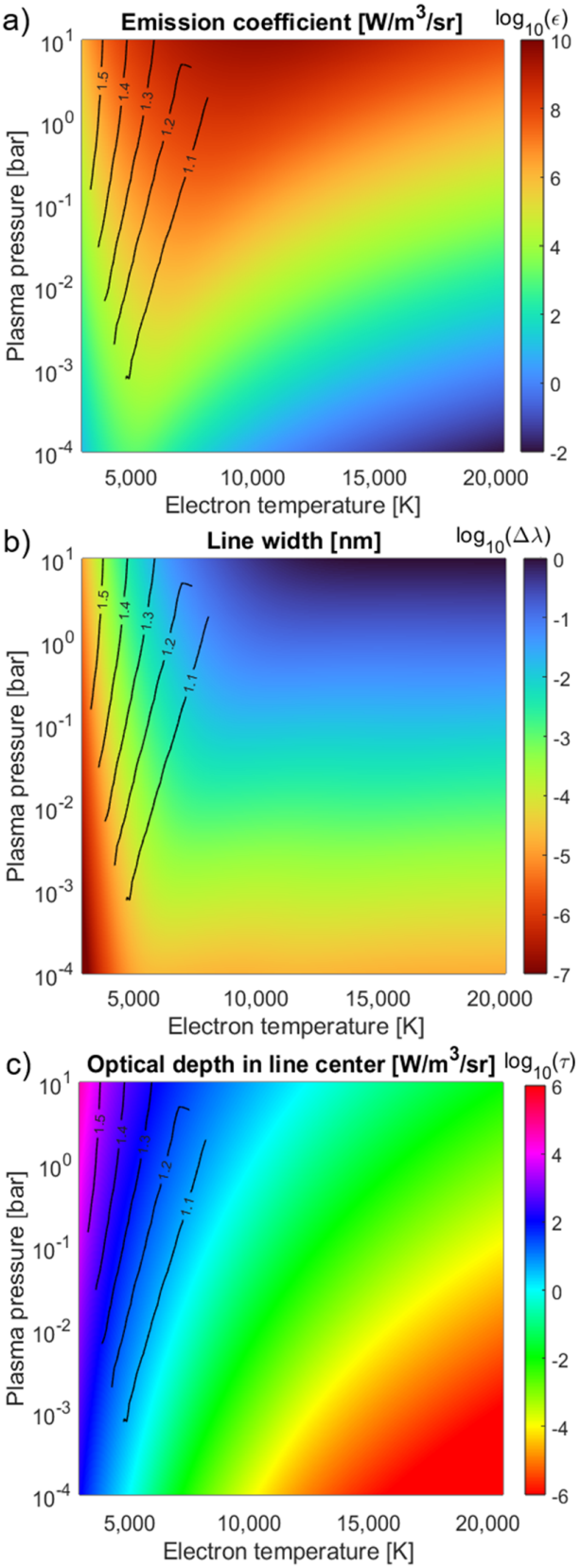

Figure 6. a) emission coefficient, b) line width (full-width-half-maximum) and c) optical depth in the line center. All for the atomic line at 521.8 nm from a copper plasma. Simulated assuming an homogeneous plasma with electron temperature T_e and plasma pressure p as input parameters. Parameters: plasma diameter of 0.2 mm, atomic lines at 510.6 nm and 521.8 nm, atomic data from [1, 7–9].

As can be seen in figure 5, the optical depth in the line center at 510.8 nm is significantly above 1, especially for low temperatures, which means that there is a non-negligible absorption. This is also indicated by the fact that an underestimation of the corresponding emission coefficient in combination with the low energy level leads to an increase in the calculated electron temperature, as can be seen in figure 3. Therefore, this line is used in the following to investigate the dependencies.

First of all, it must be said that coefficients without profile (such as the emission coefficient) and values with spectral profile (such as optical depth) must be clearly distinguished. As can be seen in figure 6a, there is no directly recognizable dependence between the emission coefficient and the deviation of the electron temperature calculation. There is a recognizable trend for higher pressures, where also higher emission coefficients occurs , lead to a larger deviation in the temperature calculation. However, the temperature dependence does not show a comparable trend. For the line width, which is an indicator of the distribution of the emission over a spectral profile and thus the behavior in the line center, the trend is exactly the opposite as shown in figure 6b. Low temperatures lead to smaller line broadening (here dominant Stark broadening) and thus to a higher radiation density and absorption in the line center. However, no comparable effect is evident for high plasma pressures.

The deviation of the calculated electron temperature from the actual temperature therefore depends neither only on the emission or absorption coefficient, nor only on the line width. However, the behavior of the optical depth in the line center, which is defined by the absorption coefficient, line broadening and plasma size, corresponds very well with the behavior of the deviation of the calculated temperature, as shown in figure 6c.

It is also interesting that an overestimation by the Boltzmann plot method is quickly reached at low temperatures due to a weaker line broadening and thus a higher optical depth value in the line maximum, comparable to figure 4. In contrast, for higher temperatures the considered line broadening is stronger and therefore leads to a decrease of the line maximum value. This effect is much stronger than the increasing due to higher emission coefficients in the investigated ranges of electron temperature and particle density or plasma pressure. That's why, such an effect did not occur for high temperatures and pressures in the studied setting. As a result, the optical depth in the line center does not increase equally and a limit value exceed is only reached for electron temperatures below a certain limit, which is below 10,000 K for copper.

In order to finally be able to make a statement about the parameter range for a reliable temperature calculation using line intensities with the Boltzmann plot method, the optical depths in the respective line center and the ratio of calculated and actual electron temperatures were determined for several elements. As can be seen in figure 7, a limit of about $\tau \approx 1$ can be observed.

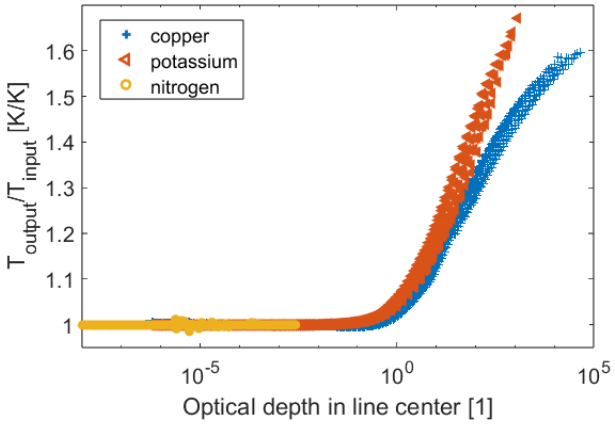

Figure 7. Ratio between calculated electron temperature using the Boltzmann plot method and input electron temperature of the spectra simulation in dependence on the the highest optical depth of the atomic lines involved for different elements. Parameters: plasma diameter of 0.2 mm. Copper: atomic lines at 510.6 nm and 521.8 nm, atomic data from [1, 7–9]. Potassium: atomic lines at 693.9 nm and 766.5 nm, atomic data from [1, 10]. Nitrogen: atomic lines at 493.5 nm and 742.4 nm, atomic data from [1, 10, 11].

The exact parameter ranges for which this is valid are different for each element, since values such as the transition probability of the transitions involved, ionization energies, etc. play a role. However, in general can be stated that temperature calculations using line intensities instead of emission coefficients for the Boltzmann plot method become increasingly inaccurate at low electron temperatures.

4. Conclusions

This study highlights the challenges associated with using line intensities instead of actual emission coefficients for electron temperature determination for via the Boltzmann plot method. Our simulations of a copper plasma demonstrated that significant overestimation of the electron temperatures occur, particularly at low plasma temperatures and high pressures, where the optical depth becomes non-negligible. The results indicate that the assumption $L \sim \epsilon$ fails when the optical depth reaches a magnitude of 1, leading to inaccuracies in temperature calculations.

It is important to note that measured spectra do not always clearly reveal whether the conditions for accurate temperature determination are met. For instance, additional line broadening caused by instrumental effects can lead to an underestimation of the optical depth, resulting in an inaccurate assessment of the temperature calculation's reliability. This emphasizes the need for caution when interpreting spectroscopic data. Nevertheless, a finding of this investigation is that lower temperatures are associated with increasing

deviations in the temperature determination.

These results emphasize the importance of understanding the conditions under which the approximation $L \sim \epsilon$ holds true. Accurate electron temperature diagnostics are critical for various plasma applications, and our research identifies key parameter ranges that researchers should consider to ensure reliable results.

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