

Collisional-Radiative modeling of the transient excitation of a carbon atoms beam crossing a tokamak plasma edge

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Abstract. A time-dependent collisional-radiative (CR) model is elaborated in the purpose of modeling the penetration of an atomic carbon beam in the edge plasma of a fusion machine in order to probe it. The excited states population densities of the beam are assumed to be modified by electron-induced processes only. All momentum transfer is neglected: the penetration velocity is assumed constant. In typical conditions for the electron density and temperature gradients ($\partial n_e/\partial x \approx 10^{20} \text{ m}^{-4}$ and $\partial T_e/\partial x \approx 10^7 \text{ K m}^{-1}$), the results illustrate the electrons efficiency to ionize the beam. With a velocity equal to 1 km s^{-1} , the beam is ionized in $20 \mu\text{s}$ in these conditions, which corresponds to a penetration depth of 2 cm. During the conversion in ions, the atomic beam is sufficiently excited to emits spectra whose measurement in coupling with the present CR model can provide information on $\partial n_e/\partial x$ and $\partial T_e/\partial x$.

1. Introduction

The high values of the edge electron density and temperature gradients ($\partial n_e/\partial x \approx 10^{20} \text{ m}^{-4}$ and $\partial T_e/\partial x \approx 10^7 \text{ K m}^{-1}$ in order of magnitude [1]) play a key role in the case of fusion devices [2]. Therefore, these gradients have to be measured. These measurements can be performed using Thomson scattering [3] or Beam Emission Spectroscopy [4]. The latter technique consists in injecting an atomic beam with a sufficiently high center of mass velocity. The resulting penetration through the edge plasma leads to a progressive atomic excitation and to the emission of spectra in part characterized by the values of the gradients [5]. Coupled with a Collisional-Radiative (CR) model, these spectra provide the n_e and T_e profiles. The beam can be produced for instance by ablating plasma facing components made with carbon using a nanosecond laser pulse. In the present paper, we focus our attention on the CR model elaborated to calculate the progressive excitation of such an atomic beam penetrating a typical fusion plasma edge.

2. C excited states considered and assumptions

All excited states belonging to the NIST database have been considered [6]. This set is composed by 268 states. Due to the high gradients values mentioned in Introduction, C atoms in these



excited states can undergo ionization: we have therefore taken into account the ground ionic state. Table 1 lists a part of the set used.

Table 1. Some of the states considered in the present CR model on carbon among the 268 considered from the NIST database [6]. Usual notations are used.

No	Configuration	Term	Energy (eV)	J	No	Configuration	Term	Energy (eV)	J
1	[He] 2s ² 2p ²	³ P	0.000000	0	70	[He] 2s ² 2p 4f	² [7/2]	10.41299	4
2	[He] 2s ² 2p ²	³ P	0.002033	1	95	[He] 2s ² 2p 5d	³ D	10.70759	1
3	[He] 2s ² 2p ²	³ P	0.005381	2	120	[He] 2s ² 2p 6p	¹ S	10.82891	0
4	[He] 2s ² 2p ²	¹ D	1.263725	2	145	[He] 2s ² 2p 7p	³ D	10.92251	2
5	[He] 2s ² 2p ²	¹ S	2.684011	0	170	[He] 2s ² 2p 7f	² [3/2]	10.99062	2
6	[He] 2s 2p ³	⁵ S	4.182631	2	195	[He] 2s ² 2p 8d	¹ P*	11.05502	1
7	[He] 2s ² 2p 3s	³ P	7.480391	0	220	[He] 2s ² 2p 10d	¹ F*	11.13123	3
14	[He] 2s ² 2p 3p	¹ P	8.537096	1	245	[He] 2s ² 2p 15d	¹ P*	11.20760	1
22	[He] 2s ² 2p 3p	¹ D	9.002581	2	268	[He] 2s ² 2p 29d	¹ F*	11.25200	3
44	[He] 2s ² 2p 4p	³ D	10.01575	1	C ⁺	[He] 2s ² 2p	² P*	11.26030	¹ / ₂ - ³ / ₂

The atomic beam injected into the fusion machine interacts with the plasma already formed. The following assumptions have been made:

- (i) *the C atoms enter the plasma under weak density and low temperature conditions.* According to its production mode, the atomic beam produced by laser ablation of solid materials can reach a temperature higher than their melting point after few microseconds [7]. However, the beam is produced from a plasma facing component carbon tile whose typical temperature is of $T_0 = 2000$ K. The initial beam temperature has been therefore chosen equal to T_0 .
- (ii) *the properties of the plasma are not significantly modified by the carbon beam.* The mean density order of magnitude in the edge plasma is $10^{21} - 10^{22} \text{ m}^{-3}$. Even if the smallest initial density of the beam obtained by laser ablation is classically of some 10^{22} m^{-3} under weak fluence [8], we can assume that the plasma is very weakly modified by the penetration of the beam owing to the high electron temperature.
- (iii) *the beam velocity is uniform.* The density of the plasma is weak. In addition, the plasma is mainly composed by light particles as protons, hydrogen, deuterium, tritium and helium atoms. Their momentum transfer cross section with carbon is therefore weak and the resulting retardation can be neglected. In addition, the atoms velocity distribution function is assumed narrow with respect to the center of mass velocity: the beam is assumed monokinetic and there is no spreading during the propagation.
- (iv) *the free electron density and temperature gradients are uniform.* As we will see in the following, the penetration depth is of the order of some centimeters. The characteristic length over which the electron parameters gradients are uniform is higher [9]: these gradients have been therefore considered as uniform.
- (v) *the contribution of the protons to the C excitation is negligible.* At same energy, protons are much less efficient than electrons to excite or ionize another particle owing to the mass ratio: proton-induced elementary processes have been therefore disregarded. This assumption leads to neglect the collisions between C atoms as well.

- (vi) *the C^+ ions are only produced on the $[He]2s^2 2p$ ground state.* The first excited electronic state of C^+ is the $[He] 2s 2p^2 \ ^4P$ state whose energy is 16.59203 eV from the C ground state. We have assumed in the present preliminary study that the number of electrons with this energy or higher is negligible.
- (vii) *the C emission lines are optically thin.* The divergence of the beam is assumed small [10]: the escape factor is therefore close to unity [11].

3. CR model and balance equation

The previous hypotheses lead to a simple form for the balance equation of a carbon atom on the excited state subscripted j :

$$\frac{D[C_j]}{Dt} = \left(\frac{\partial[X_j]}{\partial t} \right)_{Rad.} + \left(\frac{\partial[X_j]}{\partial t} \right)_{Coll.} \quad (1)$$

where a Lagrangian approach is used. The two terms in the right-hand side are the radiative and collisional terms respectively. The elaboration of the CR model consists in calculating realistically the elementary processes involved in these terms. Using the NIST database for the spontaneous emission probabilities $A_{k \rightarrow j}$ and $A_{j \rightarrow i}$, the radiative term is:

$$\left(\frac{\partial[X_j]}{\partial t} \right)_{Rad.} = \sum_{k>j} A_{k \rightarrow j} [C_k] - \sum_{i<j} A_{j \rightarrow i} [C_j] \quad (2)$$

The radiative recombination has been neglected.

The collisional term involves the elementary processes changing the excitation and ionization degrees of the beam and can be written as:

$$\left(\frac{\partial[X_j]}{\partial t} \right)_{Coll.} = \sum_{i<j} k_{i \rightarrow j} [C_i] n_e - \sum_{k>j} k_{j \rightarrow k} [C_j] n_e - k_{j \rightarrow ion} [C_j] n_e - \quad (3)$$

$$\sum_{i<j} k_{j \rightarrow i}^* [C_j] n_e + \sum_{k>j} k_{k \rightarrow j}^* [C_k] n_e + k_{ion \rightarrow j}^* [C^+] n_e^2 \quad (4)$$

where the part (3) of the right-hand side is related to the forward (inelastic) processes and the part (4) is related to the backward (superelastic) processes. The rate coefficients $k_{i \rightarrow j}$, $k_{j \rightarrow k}$ and $k_{j \rightarrow ion}$ are calculated assuming valid the cross sections of Drawin [12] whose main interest is to distinguish correctly the forbidden from the allowed transitions, even if they have been identified in the case of hydrogen-like species as rare gas atoms. These cross sections are integrated over Maxwellian distribution for the electron energy according to the electron temperature T_e and finally written as:

$$\text{Optically allowed transition: } k_{m \rightarrow n} = \frac{3.45 \times 10^{-6} \alpha_A}{[(E_n - E_m) k_B]^{1.6454}} T_e^{0.1454} e^{-\frac{E_n - E_m}{k_B T_e}} \quad [m^3 s^{-1}] \quad (5)$$

$$\text{Optically forbidden transition: } k_{m \rightarrow n} = \frac{5.24 \times 10^{-17} \alpha_F}{[(E_n - E_m) k_B]^{0.5067}} T_e^{-0.0067} e^{-\frac{E_n - E_m}{k_B T_e}} \quad [m^3 s^{-1}] \quad (6)$$

$$\text{Ionization: } k_{m \rightarrow n} = \frac{3.45 \times 10^{-6} \alpha_I}{[(E_n - E_m) k_B]^{1.6454}} T_e^{0.1454} e^{-\frac{E_n - E_m}{k_B T_e}} \quad [m^3 s^{-1}] \quad (7)$$

with $E_n > E_m$. The backward rate coefficients are calculated using the detailed balance principle.

By writing the balance equation (1) for the 269 species here considered, an ordinary differential equations system is obtained and finally solved using the DVODE library [13]. The time evolution of the different $[C_j]$ population densities is derived, which can be easily converted in spatial profiles owing to the constant velocity of the beam.

4. Results

The test-case studied corresponds to usual conditions observed in fusion machine plasma. The gradients values adopted are $\partial n_e / \partial x = 2.75 \times 10^{20} \text{ m}^{-4}$ and $\partial T_e / \partial x = 3 \times 10^7 \text{ K m}^{-1}$ with $n_e(x = 0) = 0$ and $T_e(x = 0) = T_0 = 2000 \text{ K}$. The velocity of the beam depends on the laser pulse characteristics. However, the order of magnitude is typically of some km s^{-1} in low fluence conditions [14]: we have therefore adopted $v = 1 \text{ km s}^{-1}$.

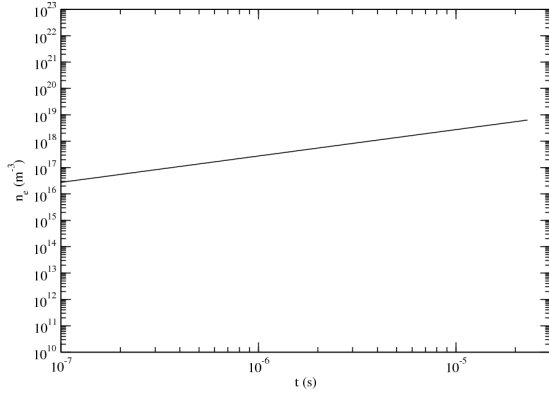


Figure 1. Time-evolution obtained for the electron density n_e in the test-case studied.

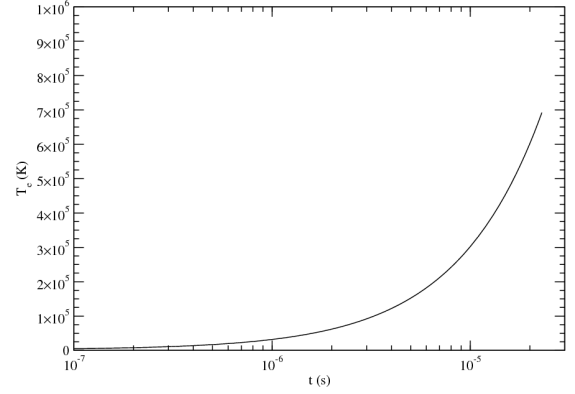


Figure 2. Time-evolution obtained for the electron temperature T_e .

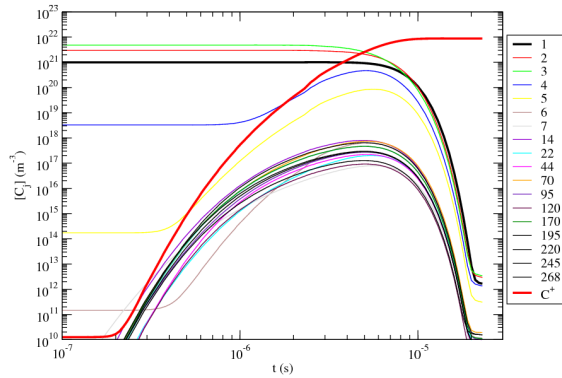


Figure 3. Evolution of the population density of some C excited states listed in table 1. The evolution of $[C^+]$ is also displayed.

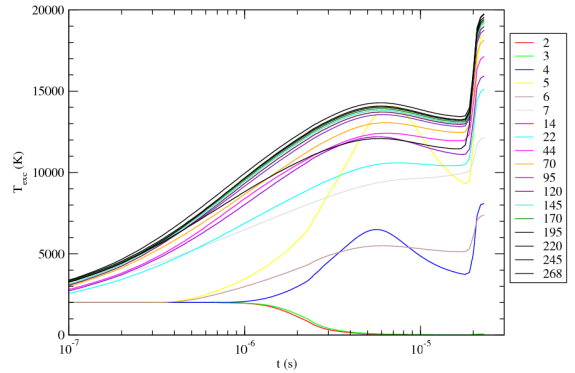


Figure 4. Evolution of the excitation temperature of some C states calculated with respect to the ground state density (see equation 8).

Figures 1 and 2 display the time-evolutions of n_e and T_e obtained in our Lagrangian approach. These values of the electron density and temperature correspond to the fluid particle location at time t . The electron density values are rather weak, but we can expect an important modification of the distribution of the beam particles among the excited states owing to the high electron temperature levels.

Figure 3 illustrates the time-evolution derived for the states of carbon atoms accounted for in table 1 in the test-case conditions. We can notice first that the population densities vary strongly. These excited states can be separated in two groups. The first group corresponds to

states weakly excited forming the fine structure of the ground state (levels i such that $1 \leq i \leq 3$) and the two metastable states ^1D and ^1S at 1.26 and 2.68 eV from the ground respectively. These states have population densities well coupled to each other for $t > 8 - 9 \times 10^{-6}$ s. The second group is formed by all other states whose population densities are coupled as early as $t = 10^{-6}$ s. This behavior can be easily explained by the energy distribution of these excited states. The C energy diagram exhibits indeed a cut due to the existence of the two metastable states reinforced by a large empty interval of 3.3 eV between the ^5S and ^3P states preventing a complete coupling. We have already noted such a characteristics with rare gas atoms whose cut of energy diagram is deeper [15]. Despite this bad coupling, the behavior of both groups is similar: they undergo a brutal depopulation owing to the beam ionization.

Figure 3 displays also the C^+ density evolution. We can note the complete conversion of the beam: firstly only composed by neutrals, the beam is totally ionized under electron impact over almost 1 μ s. When a C^+ ion is produced, an electron is of course produced as well. The initial density of the neutral beam is 10^{22} m^{-3} : in these conditions, the electron density rapidly increases and becomes higher than the one resulting from the fusion plasma. We assumed that the beam penetration does not modify significantly the plasma properties: is our approach finally inconsistent? Actually not, because electrons formed during the ionization processes have a low kinetic energy: they cannot penetrate the plasma and are moved perpendicularly to the beam direction owing to the confinement strong magnetic field. Equations 3 and 4 involve therefore only the electron properties of the fusion plasma. The C^+ ions are much more heavy: the magnetic field action is limited and is neglected. Anyway, the C^+ ions play a role only through the three-body recombination. The term $k_{ion \rightarrow j}^*[C^+]n_e^2$ of equation 4 takes this process into account. A thorough study of the different contribution to $(\partial[X_j]/\partial t)_{Coll.}$ shows that three-body recombination is negligible at any time owing to the increase of T_e .

At time $\tau_p \approx 2 \times 10^{-5}$ s, the beam is thus totally ionized: this corresponds to a position of $x_p \approx 2$ cm from the surface where the beam is produced by the laser pulse. This distance can be therefore considered as the "penetration depth" of the carbon beam. The observation of a rich emission spectrum can be expected over this distance: the final determination of the n_e and T_e gradients can be only performed over x_p .

The calculation of the excitation temperature of each excited state with respect to the ground state gives further insight into the global ionization process. This excitation temperature is calculated by:

$$T_{exc}(j) = \frac{E(j) - E(1)}{k_B} \left\{ \ln \left(\frac{g_e(i)}{g_e(1)} \frac{[C_1]}{[C_i]} \right) \right\}^{-1} \quad (8)$$

Figure 4 displays the resulting time-evolutions. Starting from 2000 K owing to the initial equilibrium, T_{exc} increases for each state according to a very similar way, except for the less excited ones. The different behaviors can be ascribed again to the energy diagram peculiarities discussed above. However, we can notice the moderate increase of the excitation temperature in comparison with the one observed for T_e . This weak increase results from the good coupling previously observed and from the rapid ionization of the ground state. When the conversion of the beam is complete ($t \approx 2 \times 10^{-5}$ s), one can note the quick increase of the excitation temperature followed by a slower one whose interpretation necessitates further investigations.

In the past, laser blow-off (LBO) diagnostics were performed on different fusion machines. They are based on the production of Li-C atoms beam obtained by lighting with a laser pulse the rear side of layers deposited on a glass or a quartz substrate. The beam is then formed by atoms with a center of mass velocity of 10^4 m s^{-1} approximately [16]. In these conditions, a more important penetration depth is expected. The usual value for x_p is indeed around 10 cm [17] which leads to ability of the method to diagnose the edge plasma assessed to $n_e \times x_p = 10^{18} - 10^{19} \text{ m}^{-2}$ [18, 19]. In our case, this product is five times lower owing to the value of x_p . However the

production mode of the plasma is easier: the present method offers an interesting economical alternative to the LBO method to perform edge plasmas n_e and T_e measurements.

5. Conclusion

A Collisional-Radiative model is elaborated in order to provide information on the penetration of a carbon atomic beam in the edge plasma of a fusion machine. Numerous excited states of C are accounted for and their chemistry is assumed governed by the main electron-induced elementary processes (excitation/deexcitation and ionization/recombination). The plasma is assumed unchanged by the beam interaction. The calculations are based on the solution of the ordinary differential equations system obtained by writing the balance equation of each state population density under a Lagrangian approach. The results put forward the rapid conversion of the atomic beam into an ionic beam which lasts approximately 20 μ s in the typical conditions adopted. This characteristic delay corresponds to a penetration depth of the beam equal to 2 cm for a beam velocity of 1 km s⁻¹. The conversion occurs through a high correlation between excited states illustrated by the population densities and excitation temperature time-evolutions.

These results are certainly highly depending on the set of cross sections used. Further investigations will be performed with at least one different set. In addition, the interaction with the plasma is assumed reduced to electron-induced processes only. The density and energy of protons are important and the role of momentum transfer can be studied: in future calculations, these processes will be accounted for. Helium atoms exhibit an energy diagram more favorable to the present diagnostic method and can be implemented more easily experimentally: other calculations based on He will also be performed.

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