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A NOVEL COLLISIONAL RADIATIVE MODEL WITH A NUMERICAL BOTTOM AND AN ANALYTICAL TOP

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Abstract—A cut-off procedure for numerical collisional radiative (CR) models is developed and is based on knowledge of the excitation flow in the collision-dominated part of an atomic system as revealed by analytical models. This new cut-off technique makes it possible to reduce the number of levels in a numerical CR-model drastically in comparison with the older, numerical cut-off technique used by Bates et al, in which the truncation level was demanded to be in Saha equilibrium. The model is applied to an ionizing and recombining argon plasma as an example of a more general technique which can also be applied to other atomic systems. The results are in good agreement with the analytical top model developed previously in our group and also with the experiments and numerical calculations of Vlček and Pelikán.

1. INTRODUCTION

The atomic state distribution function (ASDF), which describes how atoms and ions are distributed over the various excited states, is an important feature of plasmas. The ASDF is related to basic plasma parameters such as the electron density n_e , electron temperature T_e and groundstate density n_1 and contains information on the transport of radiation and particles.

Experimentally determinable by using well-established spectroscopic techniques, modelling of the ASDF is of renewed interest in the fields of spectrochemical analysis, recombination lasers, investigations of impurity compositions of thermonuclear plasmas, astrophysics, etc. This interest is based on the fact that comparisons of experimental data with analytical and numerical calculations may reveal important plasma properties. In the 1930s, astrophysicists such as Baker and Menzel¹ studied analytically the spectra of recombining hydrogen systems in various astrophysical objects. Although the advent of the computer opened the new possibility of a numerical approach initiated by the paper of Bates et al,² there still remained interest in analytical treatments of the problem in various groups, e.g., Fujimoto,³ Biberman et al⁴ and van der Mullen et al.⁵

The advantage of the analytical approach is that it clarifies the influence of various features of plasmas, without the necessity of using tables and graphs. The disadvantage is that it cannot provide a general prediction of population densities of excited states under all possible conditions. In numerical approaches, we are not faced with this problem. However, in numerical models such as that proposed by Bates et al,² the number of excited states has to be very large since the upper state should be in partial local Saha equilibrium (pLSE) to ensure that the truncation does not affect the population of the lower levels.⁶

In this paper, we combine analytical and numerical techniques such that the lower excited states can be described numerically and analytical expressions are then used for a careful truncation at the top levels. The procedure is based on the technique described in Ref. 6. This more rigorous hybrid technique can be applied to ionizing as well as to recombining systems. The aim of this study is to reduce drastically the number of levels that must be taken into account so that the technique can also be used to calculate the particle source terms in plasma-transport models. In this study, the hybrid technique is applied to an argon plasma. Applications to other atomic systems will be essentially the same.

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2. THEORY

2.1. Fundamental equations

The ASDF is mainly determined by elementary collisional and radiative (CR) processes. The manner in which these processes manifest themselves in the ASDF is described by CR-models such as those described in Refs. 2, 4, 7–9. The solution method, which is based on the fact that transport phenomena of atoms in excited levels can be neglected in a large variety of plasmas, is called the quasi-steady-state solution (QSSS). The atom and ion ground-level population densities, for which transport cannot be neglected, are input parameters for the CR-models. We use the following notation: n_1 and n_+ are the densities of the ground level of a general $(Z - 1)$ -fold ionized atomic system and the subsequent ionic (Z) system, respectively; p is used to label the excited levels; if p appears as a variable in a function, it stands for the effective principal quantum number. The temperature and the densities n_1 and n_+ are the main input parameters for the CR-models. The densities n_1 and n_+ are determined by the following zeroth moment of the Boltzmann transport equation:

$$\frac{\partial n_1}{\partial t} + \text{div}[n_1 \mathbf{w}_1] = \left. \frac{\partial n_1}{\partial t} \right|_{\text{CR}}, \quad (1)$$

$$\frac{\partial n_+}{\partial t} + \text{div}[n_+ \mathbf{w}_+] = \left. \frac{\partial n_+}{\partial t} \right|_{\text{CR}}, \quad (2)$$

where $\mathbf{w}_1$ and $\mathbf{w}_+$ are, respectively, the mean velocities of the atom and ion ground levels. The right-hand side (rhs) contains the changes due to CR processes.

Under a wide range of conditions, the relaxation time of the excited levels is much shorter than the relaxation time of the atom and ion ground levels. In addition, the mean thermal energy is assumed to be much less than the first excitation energy⁴ so that, for the excited levels, the relation

$$\sum_{p>1} n(p) \ll n_1, n_+ \quad (3)$$

holds. Under these circumstances, the distribution of the number densities of the excited levels is determined by the QSSS. This statement means that the excited levels follow the relatively slow changes ($10^{-3} \sim 10^{-4}$ sec) of the ground-level densities of the atom and the ion with relatively short time constants ($10^{-7} \sim 10^{-8}$ sec). Therefore, it is justified to neglect temporal and spatial relaxation for excited levels such that the QSSS of the ASDF is given by

$$\left. \frac{\partial n(p)}{\partial t} \right|_{\text{CR}} = 0, \quad p > 1, \quad (4)$$

for all excited levels, while n_1 , n_+ , n_e and T_e are input parameters. We will confine ourselves to plasmas for which Eq. (4) is applicable.

2.2. Basic assumptions

We will now describe an example showing how the analytical and numerical methods for an argon plasma are combined when the following processes are important. Applications to other systems and processes are straightforward. In our example, the following CR processes are taken into account:

- (i) Excitation and deexcitation by electronic collisions given by,

The rate coefficients are, respectively, $K(p, q)$ for the transitions from left to right and $K(q, p)$ for those from right to left.

- (ii) Ionization and three body recombination,

The rate coefficients are, respectively, $S(p)$ and $K_+(p)$.

- (iii) Bound-bound absorption and spontaneous emission,

The rates are, respectively, $(1 - A_{qp})A(q, p)n(q)$ and $A(q, p)n(q)$, where $A(q, p)$ is the Einstein coefficient for spontaneous emission and A_{qp} the optical escape factor. This notation convention has the effect that the net result of emission and absorption transitions between q and p may be written as a modified decay rate $n(q)A_{qp}A(q, p)$.

(iv) Photo-ionization and radiative recombination,

$$A(p) + h\nu \leftrightarrow A^+ + e. \quad (8)$$

The rate coefficients are, respectively, $A(p, +)$ and $A(+, p)$. In this study, we will take into account only radiative recombination.

The density of a level will be denoted by $n(p)$. In general, a level $n(p)$ consists of $g(p)$ states. The state density is denoted by $\eta(p) = n(p)/g(p)$. We assume that all states in the same level are equally distributed.² Stimulated emission and transitions induced by ion-ion, ion-atom and atom-atom collisions will be neglected. We assume that this procedure is justified when the ionization degree $\alpha \geq 10^{-3}$.⁴ In this example of using the cut-off procedure, we will use a Maxwellian electron energy distribution function (EEDF). However, this constraint is not really needed as long as the bulk of the EEDF is Maxwellian. The calculation of rate coefficients for transitions between excited levels is straightforward and the principle of detailed balance is valid for the forward and corresponding backward processes. Vlček and Pelikán¹⁰ showed that for a broad class of plasmas, only the high-energy tail of the EEDF is affected so that our cut-off procedure has a wide range of applicability.

2.3. Solution of the problem

The population density $n(p)$ of an excited level p is given by Eq. (4). Explicitly,

$$\begin{aligned} n_e \sum_{q \neq p} n(q)K(q, p) - n_e n(p) \sum_{q \neq p} K(p, q) + \sum_{q > p} n(q)A(q, p)A_{qp} \\ - n(p) \sum_{q < p} A(p, q)A_{pq} + n_e n_+ [n_e K + (p) + A(+, p)] - n_e n(p)S(p) = 0. \end{aligned} \quad (9)$$

In principle, Eq. (9) constitutes an infinite set of linear equations, whereas the summation runs over an infinite number of levels. In order to obtain the solution of Eq. (9) including the bottom levels, we write each component of Eq. (9) in the following form:

$$\sum_{q > 1} C_{qp} n(q) = n_+ C_{+p} + n_1 C_{1p}, \quad (10)$$

where the coefficients C_{qp} are functions of $K(p, q)$, $A(p, q)$, A_{pq} , T_e and n_e . It should be noted that $q = p$ is included in Eq. (10) and that n_1 and n_+ are considered to be independent variables. Therefore, the population density of a level p is determined only by atom and ion ground-level contributions, i.e.,

$$n(p) = n^+(p) + n^1(p), \quad (11)$$

where $n^+(p)$ is the solution of Eq. (10) if there are no ground-level atoms ($n_1 = 0$) and $n^1(p)$ is the solution of Eq. (10) when there are no ions ($n_+ = 0$). The values of the ground levels n_+ and n_1 , which are not predicted by the CR-model, can be calculated by using Eqs. (1) and (2) or they may be determined experimentally. It is convenient to relate $n(p)$ to equilibrium quantities by relating $n^+(p)$ to the Saha population density and $n^1(p)$ to the Boltzmann population density given by

$$\eta^+(p) = r^+(p)\eta^s(p), \quad \eta^1(p) = r^1(p)\eta^b(p), \quad (12)$$

where

$$\eta^s(p) = \eta_e \eta_+ \left(\frac{h^2}{2\pi m_e k T_e} \right)^{3/2} \exp(E_{p1}/kT_e), \quad (13)$$

and

$$\eta^b(p) = \eta_1 \exp(-E_p/kT_e). \quad (14)$$

For the electrons, we have $\eta_e = n_e/2$. The quantity E_{pi} is the ionization energy of level p . The majority of the excited levels is oriented with respect to the ground level of the ion rather than with respect to the ground level of the atom because of the large energy gap between the ground level of the atom and the first excited level. An instructive notation can be found by dividing Eq. (11) by $n^s(p)$, viz.

$$b(p) = n(p)/n^s(p) = \eta(p)/\eta^s(p), \quad (15)$$

$$b(p) = r^+(p) + r^1(p)b(1), \quad (16)$$

where $b(p)$ is the Saha overpopulation [$b(p) > 1$] or underpopulation [$b(p) < 1$] factor. The population coefficients $r^+(p)$ and $r^1(p)$ reflect a purely recombining and a purely ionizing plasma, respectively. In this framework, knowledge of the $r^1(p)$ and $r^+(p)$ population coefficients and of the CR rate coefficients enables us to determine the CR recombination (α_{CR}) and ionization (S_{CR}) coefficients. These two-body rate coefficients are obtained by substituting Eq. (16) and the left-hand side (lhs) of Eq. (9) applied to $p = 1$ into Eq. (1). The result can be written as

$$\frac{\partial n_1}{\partial t} + \text{div}[n_1 \mathbf{w}_1] = n_e n_+ \alpha_{CR} - n_e n_1 S_{CR}, \quad (17)$$

in which

$$\alpha_{CR} = n_e K_+(1) + A(+, 1) + \sum_{q>1} \frac{n^s(q)r^+(q)}{n_e n_+} \{n_e K(q, 1) + A(q, 1)A_{q1}\}. \quad (18)$$

$$S_{CR} = \sum_{q>1} K(1, q) + S(1) - \sum_{q>1} \frac{n^s(q)r^1(q)}{n_e n^s(1)} \{n_e K(q, 1) + A(q, 1)A_{q1}\}. \quad (19)$$

Similarly, if one substitutes Eq. (16) and the lhs of Eq. (9), with p now replaced by the ion level n_+ , into Eq. (2), we obtain

$$\frac{\partial n_+}{\partial t} + \text{div}[n_+ \mathbf{w}_+] = -n_e n_+ \alpha_{CR} + n_e n_1 S_{CR}, \quad (20)$$

where

$$\alpha_{CR} = \sum_{q \geq 1} \{n_e K_+(q) + A(+, q)\} - \sum_{q>1} \frac{n^s(q)r^+(q)}{n_+} S(q), \quad (21)$$

$$S_{CR} = \sum_{q>1} \left\{ \frac{n^s(q)r^1(q)}{n^s(1)} S(q) \right\} + S(1). \quad (22)$$

It is not difficult to show that Eqs. (18) and (19) are equivalent to Eqs. (21) and (22) respectively. Equation (18) expresses the total recombination coefficient as a sum of direct recombination to the atom ground level and deexcitation of that part of the population of excited levels which originates from the ion ground level. Equation (21) states that not every recombination to an excited level leads to effective recombination to the ground level. A part of the population of an excited level originating from the ion ground level is ionized again. In Eq. (19), not every excitation of the atomic ground level leads to effective ionization. A part of the population of the excited levels originating from the ground levels is deexcited back to the ground level, i.e., $\{n^s(q)r^1(q)/[n_e n^s(1)] \times [n_e K(q, 1) + A(q, 1)A_{q1}]\}$. The second expression for the ionization coefficient in Eq. (22) expresses this same result but in a complementary manner. In plasma-transport models, α_{CR} and S_{CR} are important parameters.

2.4. The boundary conditions

2.4.1. Condition for Saha-equilibrium. In view of the main goal of this paper, i.e., a drastic reduction of the work required for calculation of the ASDF, it is important to know under what conditions the ASDF will approach its equilibrium value and how this approach is affected by the various processes. In other words, the question is how the various departures from equilibrium affect the ASDF.

Two primary disturbing phenomena may be distinguished which cause equilibrium departures of the ASDF, namely, transport of radiation and transport of particles. The Saha density is the best candidate for the norm of the ASDF under equilibrium conditions. It can be proved that if the balance

$$A(p) + e \leftrightarrow A^+ + e + e \quad (23)$$

is in equilibrium, then the population density of the excited level p obeys the Saha relation of Eq. (13). To state it differently, the density approaches the Saha value in the limit in which the ratio of the rates of the equilibrium-disturbing to the equilibrium-restoring processes tends to zero. Since the ionization and recombination rate coefficients increase for increasing p values, the Saha balances will approach the equilibrium state more and more closely for increasing p . The upper levels for which Eq. (23) holds at equilibrium are said to be in pLSE (in the usual nomenclature the abbreviation pLTE is used). If a disturbing process has a radiative character, the demand for the presence of Saha equilibrium and thus the validity of the Saha formula (13) may be implemented by writing

$$\tilde{N}_e(p) \equiv n_e K(p) / A(p) \gg 1, \quad (24)$$

where $K(p)$ and $A(p)$ refer, respectively, to the total collisional and radiative depopulation processes of level p . The dimensionless quantity $\tilde{N}_e$ represents the number of electron-induced transitions per radiative lifetime.⁶ This well known criterion sets an n_e -dependent boundary p_{CR} in the atomic system for which $\tilde{N}_e(p_{CR}) = 1$. It should be noted that the $K(p)$ in the criterion of Eq. (24) includes the rate coefficients of all (de)excitation processes, of which ionization is only a minor part. This result means that p_{CR} is *not* a boundary between radiative levels and pLSE but rather between radiatively- and collisionally-determined levels. It is the boundary between the corona balance (CB) and the excitation-saturation balance (ESB) in ionizing plasmas and between the capture radiative-cascade (CRC) balance and the deexcitation saturation-balance (DSB) in recombining plasmas.^{3,5,9}

The (de)excitation balances ESB and DSB differ only in the direction of the (de)excitation flow. This flow, which is important in the cut-off procedure, will be discussed presently. When we refer to the common properties of the de(excitation) flow, we use the abbreviation D/ESB.

The condition $p > p_{CR}$, i.e., that levels are collisionally instead of radiatively dominated, is in most cases *needed* but not at all *sufficient* for the presence of pLSE.⁶ A second demand for the presence of Saha equilibrium deals with the transport of particles. In an ionizing system in which the ground level n_1 is overpopulated with respect to the Saha-equilibrium value, i.e., $b(1) \gg 1$, there will be a net excitation flow $J(p)$ over the excited levels in the atomic system to support the outward transport $\nabla \cdot n_+ w_+$ of charged particles. This flow can be described analytically for levels p for which stepwise excitation and deexcitation processes are dominant, i.e., if

$$p > p_{hc} = Z \sqrt{Ry / kT_e \delta_c}, \quad (25)$$

where Ry designates the Rydberg energy and δ_c represents a parameter depending on the atomic system.⁶ For hydrogenic systems, the value of δ is model-dependent ($\delta_c = 1.5$ in Biberman et al.⁴ and $\delta_c = 3.83$ in Mansbach and Keck¹¹). For non-hydrogenic systems, the level spacing may be smaller and δ_c may be somewhat greater. In fact, p_{hc} defines a hot-cold boundary level for which the excitation and deexcitation processes are in balance.¹² This dependence of the (de)excitation kinetics on the temperature was discussed by Byron et al.¹²

Concerning $J(p) \simeq \nabla \cdot n_+ w_+ \simeq n_+ w_+ / \lambda_+$ as a disturbance of the Saha balance, the second criterion for the presence of pLSE is

$$\frac{n_e S(p) \lambda_+}{n_+ w_+} \gg 1, \quad (26)$$

in which λ_+ is a characteristic geometrical length. It is noteworthy that this criterion is p -dependent. If the criterion in Eq. (26) is fulfilled, then the collision processes responsible for restoring Saha equilibrium for the level p dominate over stepflow⁵ at level p , which is generated by the particle transport. In contrast to the first or Griem criterion¹³ in Eq. (24), the second criterion in Eq. (26) is seldom considered. It should be stressed that especially for laboratory plasmas for which λ_+ may

Fig. 1. Upward (a) and downward (b) excitation flows in the excitation-saturation balance.

be rather small, Eq. (26) may be the most stringent criterion; the disturbing influence of particle transport on the ASDF is important.^{5,9,14} This result means that the level p_{es} for which $n_e S(p_{es}) = n_+ w_+ / \lambda_+$ may be very high. The cut-off technique of Bates et al.² is based on the presence of pLSE and is such that many more levels have to be taken into account than the maximum of p_{CR} and p_{es} . In our cut-off technique, we take advantage of the fact that collision-dominated levels can be treated analytically if $p > \max(p_{hc}, p_{CR})$ by using the analytical top model (ATM)⁵ so that we can lower the cut-off level to the first collisional hot level.

2.4.2. The analytical top model (ATM). The fact that the cut-off procedure can be used for ionizing as well as for recombining plasmas is based on what is called the complementary principle,⁶ as will be illustrated presently. In Eq. (16), we introduced the population coefficients $r^l(p)$ and $r^+(p)$. We first consider the situation of large n_e -values, for which the $r^l(p)$ and $r^+(p)$ coefficients are determined by electron collisions only. The $r^l(p)$ value is obtained by setting $n_+ = 0$. As a result, there can be no Saha equilibrium since the recombination process in Eq. (23) is missing. The population density of an excited level p will be mainly determined by a so-called improper balance between excitation from level $p-1$ to p and excitation from level p to $p+1$ [Fig. 1(a)]. By analogy, the $r^+(p)$ coefficient describes the ASDF for a purely recombining plasma. For sufficiently large n_e -values, all levels are collisionally dominated and a downward recombination flow is created. This flow is characterized by the reverse improper balance [Fig. 1(b)] such that the two flows cancel each other for the case that $b(1) = 1$ so that the relation $b(p) = r^l(p) + r^+(p) = 1$ should hold (see also Fig. 2).⁷ This complementary principle allows us to treat $r^l(p)$ and $r^+(p)$ in a complementary manner provided that n_e is sufficiently large so that, if $r^l(p)$ is known we immediately have $r^+(p) = 1 - r^l(p)$.

In the case of a purely ionizing, collisionally-dominated, hot system, it can be shown by using the ATM⁵ that

$$r^l(p) = f(p) = b_0 p^{-x}. \quad (27)$$

Fig. 2. For the levels below p_{CR} , radiative decay is important. The densities of these levels must be calculated numerically. This procedure defines the boundary for the top levels. Above the boundary level p_{CR} , the excitation flow (a) or the deexcitation flow (b) are analytically determined. For increasing electron densities, p_{CR} will decrease.

The function $f(p)$ is the solution of a differential equation derived from the continuity equation for the excitation flow $J(p)$ in the excitation space, i.e.

$$\text{div } J(p) = R - I, \quad (28)$$

where R and I represent, respectively, the recombination and ionization sinks. The excitation flow $J(p)$ is described by stepwise collision processes and their rate coefficients. The exponent x is determined by the competition between ionization and excitation. Its minimum value is 5 when there is no ionization and, in general, it takes a value of about 6 for ionizing⁷ as well as for recombining plasmas.⁵ It is interesting to note that a differential equation, comparable to Eq. (28), has been set up by Seaton in the treatment of planetary nebulae.¹⁵ The overpopulation expressed in Eq. (27) decreases rapidly for increasing p values. For a purely recombining, collision-dominated plasma, the ASDF is given by

$$r^+(p) = 1 - f(p) = 1 - b_0 p^{-x} \quad (29)$$

in view of the complementary principle. It can be shown that this solution satisfies Eq. (28) as well.⁶

For decreasing n_e -values, the influence of radiative transitions at the bottom of the system will become increasingly important. However, Eqs. (27) and (28) can be retained for the top levels. The $b_0(n_e)$ value is then n_e -dependent. The boundary value b_0 in ionizing systems is determined by the boundary with CB and by the boundary with CRC for recombining systems. This power law for the collisional part of the ASDF has indeed been observed in various experiments (Fig. 3).^{7,16}

Summarizing, we may state that collisionally-dominated levels in both ionizing and recombining systems are described by the same differential equation (28). Only the boundary conditions are different. This information and especially knowledge of the stepflow will be used to construct the cut-off procedure.

2.5. A hybrid cut-off technique

For the collisionally-dominated part of the atomic system, an analytical solution may be derived for the ASDF for levels $p > \max(p_{\text{hc}}, p_{\text{CR}})$ in the ESB and pLSE. However, peculiarities in the lower

Fig. 3. Relative overpopulation $\delta b(p)$ as a function of the effective principal quantum number for argon (van der Mullen et al.¹⁶): (Δ) $n_e = 1.5 \times 10^{19} \text{ m}^{-3}$; ($\circ$) $n_e = 6.7 \times 10^{19} \text{ m}^{-3}$; ($\bullet$) $n_e = 1.5 \times 10^{20} \text{ m}^{-3}$; $T_e = 3\text{--}5 \text{ eV}$.

part of the atomic system such as the presence of metastable and resonant states cannot be accounted for analytically.

In the numerical approach, we are not faced with these problems but with a complementary problem. In the ATM, a boundary condition for the ASDF is needed in the lower part of the atomic system, whereas for numerical models we need a boundary condition in the upper part to reduce the number of excited levels. The truncation of the atomic system at a certain cut-off level N stops the (de)excitation flow and leads to erroneous pLSE-like results because, for the level N , there is only the Saha balance (van der Sijde et al¹⁷). To overcome this problem, we combine the ATM with the numerical model. Knowledge of the (de)excitation flow $J(p)$ revealed by the ATM gives us a prescription for the upper boundary condition for the cut-off in numerical CR-models while, at the same time, the numerical model will give a lower boundary condition for the ATM. This cut-off procedure, in which we use the boundary value of an *excitation flow* rather than that of a *level density*, can be implemented in the well known procedure given in the publication of Bates et al.² The authors in Ref. 2 use as the boundary condition the requirement that there exists a cut-off level N such that collisional ionization and recombination processes are dominant and in equilibrium. Stated in another way: in their cut-off procedure, it is assumed that the pLSE balance is valid for the cut-off level N . This level and all higher levels obey the Saha relation of Eq. (13), which is equivalent to the condition $b(u \geq N) = 1$ or $r^1(p) = 0$. In view of this, we group the terms involving the upper levels with the terms involving the continuum (see Ref. 6). Then Eq. (9) becomes

$$\begin{aligned}
 & n_e n(p) \sum_{q \neq p}^N K(p, q) + n_e n(p) \left[\sum_{u > N} K(p, q) + S(p) \right] + n(p) \sum_{q < p} A(p, q) A_{pq} \\
 & - \sum_{1 < q \neq p}^N n_e n(q) K(q, p) - \sum_{q > p}^N n(q) A(q, p) A_{qp} \\
 & = n_e n_+ [n_e K_+(p) + A(+, p)] + \sum_{u > N} n^s(q) A(q, p) A_{qp} + \sum_{u > N} n_e n^s(q) K(q, p) \\
 & + n_e n_1 K(1, p).
 \end{aligned} \tag{30}$$

With the principle of detailed balance, we can write this last equation in the form of an equation for $b(p)$, viz.

$$\begin{aligned}
 & n_e b(p) \sum_{q \neq p}^N K(p, q) + n_e b(p) \left\{ \sum_{u > N} K(p, q) + S(p) \right\} + b(p) \sum_{q < p} A(p, q) A_{pq} \\
 & - \sum_{q \neq p, 1}^N n_e b(q) K(p, q) - \sum_{q > p}^N \frac{b(q) n^s(q)}{n^s(p)} A(q, p) A_{qp} \\
 & = \sum_{u > N} n_e K(p, q) + n_e [S(p) + n_+ A(+, p)/n^s(p)] + \sum_{u > N} \frac{n^s(q)}{n^s(p)} A(q, p) A_{qp} \\
 & + b(1) n_e K(p, q).
 \end{aligned} \tag{31}$$

A curve drawn through the solution $b(p)$ as a function of p must be tangential to $b(p) = 1$. If this is not the case, the excitation flow over the excited levels is mutilated by the cut-off. To avoid this problem, N should be increased. Depending on the conditions of the plasma, N can be very large. Many authors^{8,18} use this cut-off procedure. In this paper, we employ a different approach for the cut-off procedure. In our approach, the flow predicted by the ATM is used as the upper boundary condition.

The excitation flow across the cut-off level is mainly determined by step processes and may be written as

$$J(N, N+1) = n_e n(N) K(N, N+1) - n_e n(N+1) K(N+1, N). \tag{32}$$

Using the principle of detailed balance and the factor $b(N)$, we find

$$J(N, N+1) = n_e n^s(N) K(N, N+1) [b(N) - b(N+1)]. \tag{33}$$

The step flow across the cut-off level for the case when $b(N+1)$ is set equal to unity would be given by

$$J^{\text{cut}}(N, N+1) = n_e n^s(N) K(N, N+1) [b(N) - 1] \quad (34)$$

so that we may write

$$J(N, N+1) = J^{\text{cut}}(N, N+1) \left[\frac{b(N) - b(N+1)}{b(N) - 1} \right]. \quad (35)$$

From analytical and experimental results, it is known that⁶

$$\frac{b(N) - b(N+1)}{b(N) - 1} = 1 - \frac{N^6}{(N+1)^6} \equiv \gamma(N). \quad (36)$$

We note that the correction factor $\gamma(N)$ tends to zero if $N \rightarrow \infty$. If we rewrite the boundary flow as

$$J(N, N+1) = n_e n(N) K(N, N+1) \gamma(N) - n_e n^s(N) K(N, N+1) \gamma(N), \quad (37)$$

it is clear that the factor $\gamma(N)$ can be used to correct the rate coefficients involved at the cut-off level. When the first term on the rhs of Eq. (37) is added to the lhs of Eq. (31) and the second term to the rhs of Eq. (31), we find for the cut-off level N the following relation:

$$\begin{aligned} & n_e b(N) \sum_q^{N-1} K(N, q) + n_e b(N) \left[\sum_{u>N} K(N, q) + S(N) + \gamma(N) K(N, N+1) \right] \\ & + b(N) \sum_{q<N} A(N, q) A_{Nq} - \sum_{q>1}^N n_e b(q) K(N, q) \\ & = [n_e K(N, N+1) \gamma(N) + n_e S(N)] + \frac{n_e n_+}{n^s(N)} A(+, N) \\ & + \frac{1}{n^s(N)} \sum_{u>N} n^s(u) A(u, N) + n_e b(1) K(N, 1). \end{aligned} \quad (38)$$

In this cut-off procedure, a simple correction of the rate coefficient $K(N, N+1)$ for the cut-off level enables us to lower the upper boundary level to almost the first collisionally-dominated level. This procedure drastically reduces the number of levels that must be considered.

3. THE ARGON-SYSTEM AND RATE COEFFICIENTS

The numerical CR-model will be applied to an argon plasma composed of atomic Ar and singly-ionized Ar^+ in the ground level. In the CR-models of Katsonis¹⁹ and of Vlček and Pelikán,¹⁰ the Ar atom is divided into two subsystems according to the two core quantum states $^2P_{1/2}$ (primed system) and $^2P_{3/2}$ (unprimed system). In our Ar model, we also separate the two resonant and the two metastable levels of the $4s$ and $4s'$ groups in accord with the model of Vlček.¹⁸ However, in view of our main goal to observe the effect of the cut-off procedure, it is not necessary to take into account the separate subsystems and an extensive electron-coupling scheme between the various groups in the neutral argon system. For levels higher than $4s$, the two subsystems corresponding to nl and nl' are lumped together into one effective level as follows:

$$\sum_n g_n E_n / \sum_n g_n. \quad (39)$$

The energy difference between nl and nl' in the two subsystems is almost constant and amounts to 0.18 eV. For plasmas with temperatures of 3 eV, this difference will be negligible. The energy of the lumped effective levels, which are confined to the s , p , d , and f groups, is $1/3 \times 0.18$ eV above the subsystem $nl(^2P_{3/2})$, which agrees with the statistical weights of both subsystems. It is not difficult to extend our Ar model and to incorporate the special features of the two subsystems. In our computations, the Ar atom has at most 64 effective levels (see Table 1) which, because of the cut-off procedure, can be reduced to 14 effective levels.

Table 1. Data for the Ar-I system used in the model.

Level number n	Effective pqn (eV)	Excitation energy ϵ_n	Statistical weights	Group
1	1.797	11.548	5	4s [3/2] ₂
2	1.813	11.623	3	4s [3/2] ₁
3	1.836	11.723	1	4s'[1/2] ₀
4	1.860	11.828	3	4s'[1/2] ₁
3	2.260	13.096	36	4p
6	2.786	14.007	60	3d
7	2.843	14.077	12	5s
8	3.297	14.508	36	5p
9	3.727	14.780	60	4d
10	3.851	14.842	12	6s
11	3.991	14.905	84	4f
12	4.310	15.027	36	6p
13	4.710	15.146	60	5d
14	4.855	15.182	12	7s
15	4.991	15.213	84	5f
16	5.317	15.278	36	7p
17	5.718	15.343	60	6d
18	5.860	15.363	12	8s
19	5.990	15.380	84	6f
20	6.315	15.418	36	8p
21	6.678	15.454	60	7d
22	6.848	15.469	12	9s
23	6.994	15.481	84	7f
24	7.317	15.505	36	9p
25	7.706	15.530	60	8d
26	7.845	15.538	12	10s
27	7.991	15.546	84	8f
28	8.330	15.563	36	10p
29	8.668	15.578	60	9d
30	8.841	15.585	12	10s
31	8.997	15.591	84	9f
32	9.337	15.603	36	10p
33	9.652	15.613	60	10d
34	9.856	15.619	12	12s
35	10.000	15.623	84	10f
36	10.348	15.632	36	12p
37	10.690	15.640	60	11d
38	10.875	15.644	12	13s
39	11.069	15.648	84	11f
40	11.327	15.653	36	13p
41	11.662	15.659	60	12d
42	11.841	15.662	12	14s
43	11.965	15.664	84	12f
44	12.362	15.670	36	14p
45	12.649	15.674	60	13d
46	12.958	15.678	84	13f

3.1. Excitation cross-sections

Since there is a lack of experimental data for electronic transitions between excited levels, semi-empirical (SE) expressions are required for the inelastic electron-atom collisions. Drawin²⁰ proposed SE formulae for the cross-sections based on extensions to the Bethe formulae.²¹ These formulae contain parameters for optically-allowed, spin-allowed and parity-forbidden transitions between the excited levels and have been calculated for Ar by Kimura et al.²² The computations of Ref. 10 are based on these data. In our study, we employ the SE excitation cross-section formulae proposed by Vriens and Smeets²³ for neutral hydrogen and alkali atoms. However, for electronic transitions between the ground level and the first 7 excited levels {4s[3/2]₂, 4s[3/2]₁, 4s'[1/2]₀, 4s'[1/2]₁, 4p, 3d, and 5s}, experimental data sets of Chutjian and Cartwright,²⁴ Tachibana,²⁵ and Peterson and Allen²⁶ are employed. These were also incorporated in the CR-model of Vlček.¹⁸

The radiative transition probabilities are taken from Wiese et al.²⁷ For the ionization cross-sections, the SE formulae of Ref. 23 are employed as well. The SE formulae of Ref. 19 were used for radiative recombinations. The plasma will be transparent except for the resonance lines and free-bound radiation. For these levels, the escape factor in a plasma with cylindrical configuration with radius R is given by (Holstein,²⁸ Klein²⁹)

$$A_{ln} = g_0 T(R), \quad (40)$$

where g_0 is of the order unity and the transmission factor is^{18,29}

$$T(R) = T_D \exp\left(-\frac{\pi T_{LD}^2}{4T_L}\right) + T_L \operatorname{erf}(\sqrt{\pi} T_{LD}/2T_L); \quad (41)$$

here, T_D and T_L are, respectively, by the transmission coefficients for Doppler-broadened and Lorentz-broadened spectral lines. The quantity T_{LD} is the transmission coefficient for a Voigt profile, i.e.

$$T_D = \frac{1}{k_0 R \sqrt{\pi \ln(k_0 R)}}, \quad T_L = \sqrt{\frac{a}{\pi k_0 R}}, \quad T_{LD} = \frac{2a}{\pi \sqrt{\ln(k_0 R)}}; \quad (42)$$

here, a is the ratio of Lorentz to Doppler broadening and $k_0 R$ is the optical depth.

4. RESULTS

4.1. An ionizing plasma

The first computations have been carried out for an ionizing Ar plasma under the following conditions:

$$n_e = 6.7 \times 10^{19} \text{ m}^{-3}, n_1 = 10^{19} \text{ m}^{-3}, T_e = 3 \text{ eV},$$

for which the collisional-radiative and the hot-cold boundary are, respectively, given by

$$p_{CR} \simeq 3.5, p_{hc} \simeq 1.$$

This approach means that the principal quantum number of the cut-off level must be at least 3.5.

For a correct cut-off procedure, the ASDF must not depend on the number of excited levels. We will demonstrate the consequences of an inadequate cut-off and compare this procedure with the novel hybrid cut-off procedure. Figure 4 shows four calculations of the ground level contribution $r^1(p)$ of the ASDF as a function of the effective pqn with 14, 26, 34, and 46 effective levels, respectively, using an incorrect cut-off. Using the Ar-atom model of Table 1 with normal statistical weights for s , p , d , and f , namely, 12, 36, 60, and 84, means that a double truncation is executed: one truncation at the effective pqn side and one at the orbital quantum number side because g , h , ... effective groups with $l \geq 4$ are not taken into account. As can be seen in Fig. 4, the population of the levels in the neighbourhood of the cut-off level are increased artificially. The reason is that the excitation flow $J(p)$ is truncated totally and thus incorrectly; it becomes zero at the truncation level since for the cut-off level in this calculation, there is only the Saha balance left. The slope of the $r^1(p)$ coefficient varies from -4.0 ± 0.1 ($N = 46$) to -2.5 ± 0.2 ($N = 14$), whereas a constant slope of -6 is to be expected according to analytical and experimental results. The level 14 shows r^1 -values of 2.0×10^{-5} ($N = 14$) and 3.7×10^{-6} ($N = 46$), which differ by a factor of 6. These calculations show that if $J(N)$ is suppressed, the overpopulation of the ASDF in ionizing systems decreases too slowly. As a consequence, the ASDF depends also on the number of levels N .

To avoid the truncation at the orbital quantum number side, we include the g , h , ... by increasing the statistical weight of the f -group artificially, i.e., we use $12p^2 - 108$ as statistical weight of the f -group. The $12p^2$ stands for the statistical weight of the whole Ar energy shell with effective pqn p , while $108 = 12 + 36 + 60$ represents the sum of the statistical weights of the s , p , and d groups, as previously retained in the model. When the truncation of the orbital quantum number is removed, the slope of the $r^1(p)$ coefficient varies from -4.7 ± 0.1 ($N = 46$) to -2.8 ± 0.2 ($N = 14$) and is still too low.

Fig. 4. The $r^1(p)$ coefficient as a function of the effective principal quantum number obtained with a double truncation. The plasma conditions are $n_e = n_i = 6.7 \times 10^{19} \text{ m}^{-3}$; $T_e = 3 \text{ eV}$, $n_1 = 10^{19} \text{ m}^{-3}$, $T_a = 1 \text{ eV}$: (Δ) 46 effective levels; (+) 34 effective levels; (∇) 26 effective levels; ($\diamond$) 14 effective levels.

In Fig. 5, the $r^1(p)$ and $\delta b(p) = b(p) - 1$ coefficients are shown as functions of the effective pqn when the hybrid cut-off technique is applied. The slope shown in Fig. 5 is calculated with all 46 levels included. However, the first excited levels are not collisionally dominated but are influenced by radiative processes. The slope of the $r^1(p)$ for $p > p_{\text{CR}}$ varies from -6.1 ± 0.2 ($N = 46$), -6.2 ± 0.3 ($N = 34$) to -5.7 ± 0.5 ($N = 26$). For $N = 14$, it makes no sense to carry out a linear regression analysis for the collision-dominated part. But the ASDF as a whole, calculated with $N = 14$, coincides within 2% with the ASDF calculated with $N \geq 26$. Furthermore, the slope of $r^1(p)$ agrees well with the results predicted by the ATM and the experimental data.¹⁶ It is clear that the slope of the $\delta b(p)$ coefficient is the same as the slope of the $r^1(p)$ as predicted by the theory⁶ and found in experiments¹⁶ and is independent of the number of levels. As can be seen, the level densities of the d and f groups are systematically a little too high. The result is probably due to the fact that we were using the Vriens and Smeets²³ cross-section formulae. These give large cross-sections for electron excitation between the p - d and d - f groups. Also shown are some experimental values measured in a hollow cathode-arc discharge¹⁶ for the following plasma parameters: $n_e = 6.7 \times 10^{19} \text{ m}^{-3}$, $n_1 = 10^{19} \text{ m}^{-3}$, $T_e = 3$ – 5 eV , and a radius of 1 cm. Our numerical calculations agree very well with the calculations of Ref. 10 (broken curve). In our calculations, it may be sufficient to take only 14 effective levels to calculate the constant b_0 in the analytical formula (27).

The two-body rate coefficients α_{CR} and S_{CR} [see Eqs. (18) and (19)] are the same for all calculations with $N = 14, 26, 34$, and 46, namely,

$$S_{\text{CR}} = 2.11 \times 10^{-16} \text{ m}^3 \text{ sec}^{-1}, \quad \alpha_{\text{CR}} = 1.05 \times 10^{-19} \text{ m}^3 \text{ sec}^{-1}.$$

4.2. Recombining plasma

We have applied the hybrid cut-off procedure for a recombining plasma under conditions

Fig. 5. The $r^1(p)$ and $\delta b(p)$ coefficients as functions of the effective pqn obtained with the hybrid cut-off technique and the same conditions as in Fig. 4. The $r^1(p)$ calculated with 46, 34, 26, and 14 effective levels are represented as follows: (Δ) 46 effective levels; (+) 34 effective levels; ($\diamond$) 26 effective levels; ($\blacklozenge$) 14 effective levels. The δb are represented as follows: (+) 46 effective levels; ($\circ$) 34 effective levels; (∇) 26 effective levels; ($\square$) 14 effective levels; ($\blacksquare$) experimental values (van der Mullen et al¹⁶). (---) Calculations of Vlček and Pelikán.¹⁰

corresponding to an inductively-coupled plasma (see Nowak et al³⁰), viz.

$$n_e = 4 \times 10^{20} \text{ m}^{-3}, \quad n_i = 5 \times 10^{23} \text{ m}^{-3}, \quad T_e = 0.6 \text{ eV}.$$

For these conditions, the highest boundary value for p is $\max(p_{hc}, p_{CR}) = p_{hc} \simeq 3$. In Fig. 6, the $r^1(p)$ and $1 - r^+(p)$ coefficients are plotted as functions of the effective pqn . The slope of the $r^1(p)$ coefficient is -5.9 ± 0.2 and is in good agreement with the expected value -6 . The $1 - r^+(p)$ has a slope of -4.8 ± 0.1 and seems to be too small in absolute value since the $r^+(p)$ and $r^1(p)$ should have the same slope. In this numerical calculation, we did not take photo-ionization into account so that radiative recombination is not a balanced process. The slope of the $r^+(p)$ calculated without radiative recombination and photo-ionization amounts to -5.4 ± 0.2 and this is in better agreement with the expected value of $x = -6$. In this case, 14 effective levels are found to be sufficient to calculate b_0 and the remaining top part of the ASDF can be expressed analytically. The two-body rate coefficients S_{CR} and α_{CR} are found to be

$$S_{CR} = 9.34 \times 10^{-24} \text{ m}^3/\text{sec}, \quad \alpha_{CR} = 2.04 \times 10^{-19} \text{ m}^3/\text{sec}.$$

4.3. Comparison with another numerical model and with experimental data

In Fig. 7, the population coefficient $r^1(4p)$ calculated with $N = 26$ is shown as a function of n_e for $T_e = 3 \text{ eV}$ with different ground-level densities ($n_i = 10^{17} - 10^{21} \text{ m}^{-3}$). The indicated range corresponds to an opacity range from optically-thin to optically-thick plasmas for resonant radiation. The plasma column has a radius of 0.01 m. For low and intermediate n_e -values, the $r_1(4p)$ is proportional to n_e in the CB, as can be proved by analytical calculations.^{6,7} For high n_e -values, the $r^1(4p)$ saturates, i.e., it is completely dominated by electronic collisions in the ESB since both production from lower and destruction to a higher level are proportional to n_e . The numerical

Fig. 6. The $r^1(p)$ and $1-r^+(p)$ coefficients as functions of the effective principal quantum number obtained with the hybrid cut-off technique. The conditions are $n_e = n_i = 4 \times 10^{20} \text{ m}^{-3}$, $T_e = T_a = 0.6 \text{ eV}$ and $n_1 = 5 \times 10^{23} \text{ m}^{-3}$. The $1-r^+$ are represented as follows: (Δ) 46 effective levels; (+) 34 effective levels; ($\diamond$) 26 effective levels; ($\blacktriangle$) 14 effective levels. The r^1 are represented as follows: (+) 46 effective levels; ($\circ$) 34 effective levels; (∇) 26 effective levels; ($\square$) 14 effective levels.

Fig. 7. The $r^1(4p)$ as functions of the electron density ($T_e = 3 \text{ eV}$ and $T_a = 1 \text{ eV}$). Results: (—) $n_1 = 10^{17} \text{ m}^{-3}$; (---) 10^{18} m^{-3} ; (-·-) 10^{19} m^{-3} ; (---) 10^{20} m^{-3} ; (···) 10^{21} m^{-3} ; curve A shows the calculations of Vlček and Pelikán;¹⁰ (●) experimental results from van der Sijde et al.³¹

results of the extensive 65-level model of Ref. 18 for the single $4p'[1/2]_1$ are also shown. It should also be noted that our calculations have been carried out with $4p$ representing a whole group. If we take into account the energy shift of the effective $4p$ and $4p'[1/2]_1$ levels, our result lies systematically 35% above the result of Ref. 10. This difference may at least partly be due to different cross-section data (see Ref. 20 for the work of Ref. 10 and Ref. 23 for ours). Also shown are the experimental values of $r^1(4p'[1/2]_1)$ of the $4p$ group in Ar I obtained in a plasma column generated by a hollow cathode-arc discharge measured by van der Sijde et al.³¹ Our computations agree well with these experimental data. For a comparison with other numerical CR-models,^{17,19} we refer to Ref. 10.

5. CONCLUSIONS

The use of an inadequate cut-off in numerical CR-models results in an incorrect ASDF. In our work, a numerical CR-model with a hybrid cut-off procedure⁶ has been applied to an ionizing plasma (hollow cathode-arc discharge) and a recombining plasma. The main conclusions which can be drawn from our computational results are the following: (i) the hybrid cut-off technique, based on knowledge of the analytical excitation flow,^{5,6} may be used successfully in reducing the number of excited levels below the number of levels needed in the cut-off technique proposed in Ref. 2. With this new technique, the computational effort required to calculate the two-body ionization and recombination rate-coefficients and the ASDF is relatively small. (ii) In calculations of the ASDF, it is sufficient to deal with only 14 effective levels for an ionizing as well as a recombining Ar plasma. (iii) The calculated ASDF agrees well with the experimental values of Ref. 31 for an ionizing plasma. (iv) The $r^1(p)$ for the whole $4p$ group calculated with 26 effective levels is typically a factor of 1.35 greater than the $r^1(4p)$ for the $4p'[1/2]_1$ level calculated with an extensive 65-level Ar-model.¹⁰ This difference may be due to the fact that the calculations of Ref. 10 are based on excitation cross-sections of Refs. 20 and 22 and not on Ref. 23 as are ours.

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