Parametrization of radiative properties of mono- and multi-component plasmas for astrophysics and nuclear fusion applications

Guadalupe Espinosa[1], †*Rafael Rodríguez[1,2], and Juan Miguel Gil[1,2]

[1]IUNAT, Departamento de Física, Universidad de Las Palmas de Gran Canaria, Spain.
[2]Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, Spain.

*Presenting and †corresponding author: rafael.rodriguezperez@ulpgc.es

Abstract

Plasma radiative properties are fundamental in many topics in plasma physics, such as nuclear fusion energy, astrophysics and extreme-ultraviolet lithography. Therefore, they are needed in radiation hydrodynamic simulations of those plasmas. However, the calculation of those properties involve the generation of huge databases of atomic data such as atomic cross sections of several processes that occur in the plasma and the resolution of very large no-linear coupled rate equations to determine the atomic level populations in the plasma. Since these ones depend on the plasma conditions which are determined by the radiation-hydrodynamic simulations at each instant and position, the whole set of equations must be solved self-consistently which makes in-line radiation-hydrodynamics simulations unfeasible. One of the solutions is to perform parametrizations of the plasma radiative properties as a function of the plasma conditions which leads to considerable reductions in computational costs. However, most of the parametrizations available are carried out for particular thermodynamic regimes (Coronal or local thermodynamic equilibria) of the plasmas and are not accurate out of those regimes. In this work, we present parametrizations of average radiative properties as a function of plasma density and temperature useful for astrophysics and nuclear fusion applications. The databases of the properties were generated using a recent code we have developed where a collisional-radiative model is implemented which ensures that the radiative properties obtained are accurate for any thermodynamic regime of the plasma.

Keywords: **Non-local thermodynamic equilibrium plasmas, Plasma radiative properties, Generation of databases and parametrization of radiative properties, Mono- and multicomponent plasmas.**

Introduction

Plasma radiative properties, i.e. the opacity and the emissivity, play a pivotal role in nuclear fusion and astrophysics. In astrophysics, the opacities of the stellar mixtures control the energy transfer in the stars, affecting their structure and evolution [1] and also govern the levitation of metals in stellar interiors [2]. Furthermore, the plasma emissivity is a key quantity in the structure, behavior and stability of radiative shock waves which are present in many astrophysical scenarios. Hence, for example, the onset of thermal instabilities, that can be the responsible of the origin of some astrophysical objects, is related to temperature dependence of the radiative power loss (i.e. the frequency integrated emissivity) in the post-shock medium. In the field of inertial fusion confinement, opacities are relevant in the design of hohlraum walls in the indirect drive scheme and also for the dopants embedded in the ablator of the target since they control the absorption of the thermal radiation coming from the hohlraum [3]. On the other hand, in magnetic confinement fusion, the radiative power loss plays an important role in the current decays after disruptions caused by strongly radiating impurities [4] and also in the radiation losses from impurities that can help in the development of thermal instabilities at the plasma edge of the fusion devices [5].

The numerical simulations of the plasma phenomena above commented require of the resolution of the radiation-hydrodynamic equations (RHE). For a single fluid, that does not involve interior mass sources, the continuity equation is given by [6]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \boldsymbol{u} = 0 \tag{1}$$

where ρ and $\boldsymbol{u}$ are the fluid density and velocity, respectively. The general transport equations for momentum and energy, in the non-relativistic limit, are given by

$$\rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) = -\nabla (p + p_R) + \nabla \cdot \underline{\boldsymbol{\sigma}_{\boldsymbol{\nu}}} + \boldsymbol{F}_{EM} + \boldsymbol{F}' \tag{2}$$

and

$$\frac{\partial}{\partial t} \left(\rho \epsilon + \frac{\rho u^2}{2} + E_R \right) + \nabla \left[\rho \boldsymbol{u} \left(\epsilon + \frac{u^2}{2} \right) + p \boldsymbol{u} \right] = -\nabla \boldsymbol{H} - \boldsymbol{J} \cdot \boldsymbol{E} + \boldsymbol{F}' \cdot \boldsymbol{u} \tag{3}$$

where p and p_R are the fluid and radiation pressures, respectively, $\underline{\boldsymbol{\sigma}_{\boldsymbol{\nu}}}$ is the viscous stress tensor, $\boldsymbol{F}_{EM}$ denotes the force density due to the interaction of the electromagnetic fields and charges and $\boldsymbol{F}'$ the density of other possible forces. In Eq. (3), ϵ and E_R denote the energy density of the fluid and the radiation field, respectively, and $\boldsymbol{J} \cdot \boldsymbol{E}$ represents the volumetric heating by the current induced in the plasma by the electromagnetic waves. The divergence of the energy flux is given by

$$\nabla \boldsymbol{H} = \nabla \left[\boldsymbol{\mathcal{F}}_R + (p_R + E_R) \boldsymbol{u} + \boldsymbol{Q} - \underline{\boldsymbol{\sigma}_{\boldsymbol{\nu}}} \cdot \boldsymbol{u} \right] \tag{4}$$

where $\boldsymbol{\mathcal{F}}_R$is the spectral radiation energy flux which is given by

$$\boldsymbol{\mathcal{F}}_R(\boldsymbol{r}, t) = \frac{1}{4\pi} \int_0^\infty \int I_\nu(\boldsymbol{r}, t, \nu) \mathrm{d}\nu\, \boldsymbol{n} \mathrm{d}\Omega \tag{5}$$

where ν is the photon frequency, $\boldsymbol{n}$ is a unit vector in the direction of propagation for any value of Ω and I_ν is the spectral radiation intensity. The radiation energy density and the radiation pressure also depend on the spectral radiation intensity

$$E_R(\boldsymbol{r}, t) = \frac{1}{c} \int_0^\infty \int I_\nu(\boldsymbol{r}, t, \nu) \mathrm{d}\nu\, \mathrm{d}\Omega \tag{6}$$

$$p_R(\boldsymbol{r}, t) = \frac{1}{c} \int_0^\infty \int I_\nu(\boldsymbol{r}, t, \nu) \cos^2\theta \mathrm{d}\nu\, \mathrm{d}\Omega \tag{7}$$

with c the speed of light. Therefore, the spectral radiation intensity is the basic macroscopic quantity to describe the radiative transfer and is obtained solving the radiative transfer equation (RTE) given by

$$\frac{1}{c}\frac{\partial I_\nu(\mathbf{r},t,\nu,\boldsymbol{n})}{\partial t} + \boldsymbol{n}\cdot\boldsymbol{\nabla} I_\nu(\mathbf{r},t,\nu,\boldsymbol{n}) = -\kappa(\mathbf{r},t,\nu)I_\nu(\boldsymbol{r},t,\nu,\boldsymbol{n}) + j(\mathbf{r},t,\nu) \tag{8}$$

where $j(\boldsymbol{r},t,\nu)$ and $\kappa(\boldsymbol{r},t,\nu)$ are the monochromatic emissivity and absorption coefficients, respectively. Both coefficients include electron transitions in the plasma between atom bound levels (line transitions or bound-bound contributions), between bound and free levels (photoionization and radiative recombination which are bound-free contributions) and between electron free levels (direct and inverse bremsstrahlung or free-free contributions). The expressions used to calculate them can be found elsewhere [7]. Two ingredients are needed to compute them. First, the cross sections of the radiative processes, which are obtained through atomic simulations. Secondly, the populations of the atomic levels in the plasma. In general, plasmas are in non-local thermodynamic equilibrium (NLTE) regime and the atomic-level populations (for a given plasma condition, i.e. for a plasma density and temperature) are obtained from the solution of a system of rate equations of a so-called collisional-radiative model (CRM) [8][9]. This set of kinetic equations is given by

$$\frac{dN_{\zeta i}(\mathbf{r},t)}{dt} = \sum_{\zeta' j} N_{\zeta' j}(\mathbf{r},t)\mathbb{R}^{+}_{\zeta' j\to\zeta i} - \sum_{\zeta' j} N_{\zeta i}(\mathbf{r},t)\mathbb{R}^{-}_{\zeta i\to\zeta' j} \tag{9}$$

where $N_{\zeta i}$ is the population density of the atomic level i of the ion with charge state ζ. The terms $\mathbb{R}^{+}_{\zeta' j\to\zeta i}$ and $\mathbb{R}^{-}_{\zeta i\to\zeta' j}$ take into account all the collisional and radiative processes which contribute to populate and depopulate the level ζi, respectively. Since the rate equations included the radiative processes in the plasma, i.e. the absorption and emissivity coefficients, these equations are coupled to the RTE. Furthermore, since the CRM depends on the plasma density and temperature, which are obtained from the single fluid RHE of the plasma (and an equation of state), the rate equations are also coupled to them.

Radiation-hydrodynamic simulations (RHS) of nuclear fusion and astrophysical plasmas require the calculation of plasma radiative properties for density and temperature profiles that could include between $10^2 - 10^3$ different plasma conditions. For each plasma condition, the set of rate equations of the CRM must be solved, which could involve around 10^4 non-linear equations including 10^6 radiative and collisional processes. Furthermore, the RTE for each photon frequency, the RHE and the rate equations must be solved self-consistently. Therefore, in-line RHS are unfeasible and approximations are usually made. In the RTE is common to assume that the radiation does not depend explicitly on time. Moreover, the RTE is solved under the grey approach, in which appropriate mean opacities are used (Planck or Rosseland mean opacities) instead of monochromatic radiative properties, thus preventing the solution of the RTE for each photon frequency. Even so, huge radiative properties databases should be generated solving the CRM coupled to the RHE, which is still a complex problem that involves large computational times. An appropriate solution to this problem is to perform parametrizations of the plasma mean radiative properties in terms of plasma density and temperature. Thus, these properties can be obtained for given plasma conditions from polynomial fittings obtained from reduced databases, greatly decreasing the computational cost.

There are several available analytical expressions for the mean radiative properties, but more of them are accurate only for Coronal equilibrium [10]-[15], i.e. for plasmas at very low density in which they are density independent, or for the range of high photon energies assuming the plasma in LTE [16][17], i.e. for high density plasmas, but not for NLTE situations. In this work, we present a parametrization of the average radiative properties which are essential for RHS of plasmas in nuclear fusion and astrophysics scenarios, such as the average ionization, Rosseland and Planck mean opacities (which are weighted averages in frequency of the monochromatic opacities) and the radiative power loss, for mono- and multi-component plasmas. The parametrization was performed using the PARPRA code [18] and is based on polynomial functions where the coefficients of the fitting were determined by means of a least square regression. A quad-tree algorithm was used to optimize the division of the space of plasma conditions to parametrize. The databases of the radiative properties to parametrize are generated for a representative set of plasma conditions using the RAPCAL code [19][20] using the the plasma atomic level populations obtained from the resolution of the rate equations of the CRM implemented in the POLAR code (a recent extension of the MIXKIP code [21]) and for this reason the parametrizations obtained are valid for Coronal equilibrium, LTE and NLTE regimes. The paper is structures as follows. Next section is devoted to a presentation of the theoretical and computational models used to perform the parametrizations. Thereafter, some examples of parametrizations for both mono- and multicomponent plasmas are shown. Finally, conclusions and future extensions are commented.

Theoretical and computational models

The POLAR code was developed in order to obtain the atomic level populations at typical plasma conditions obtained in nuclear fusion and astrophysics. For that purpose, a CRM was implemented including, in the rate equations (Eq. (9)), the following atomic processes that populate and de-populate the atomic levels: collisional ionization and three-body recombination, spontaneous decay, collisional excitation and deexcitation, radiative recombination, autoionization and electron capture, photoexcitation, photodeexcitation and photoionization, which are the most common processes in this kind of plasmas. In this work, we have considered that the atomic level populations do not depend on time. Under this assumption, the rate equations of the collisional-radiative steady-state (CRSS) model are given by

$$\sum_{\zeta' j} N_{\zeta' j}(\mathbf{r},t)\mathbb{R}^{+}_{\zeta' j\to\zeta i} - \sum_{\zeta' j} N_{\zeta i}(\mathbf{r},t)\mathbb{R}^{-}_{\zeta i\to\zeta' j} = 0 \tag{10}$$

Steady-state approach implies that the characteristic times of the atomic processes are significantly lower than the characteristic time of the plasma evolution. This approach becomes invalid, for example, if the plasma is under the interaction with ultra-short pulsed laser (~fs). However, for the plasmas of interest in this work that assumption is accurate. Two complementary equations have to be satisfied together with Eq. (10). First, the requirement that the sum of fractional level populations equals to the total ion particle density, n_{ion}

$$\sum_{\zeta=0}^{Z}\sum_{i=1}^{M_\zeta} N_{\zeta i} = n_{ion} \tag{11}$$

where Z is the atomic number and M_ζ is the total number of levels for the charge state. Second, the charge neutrality condition in the plasma

$$\sum_{\zeta=0}^{Z} \sum_{i=1}^{M_\zeta} \zeta N_{\zeta i} = n_e \tag{12}$$

with n_e the electron particle density. The average ionization of the plasma, $\bar{Z}$, is then defined as the ratio between the electron and the ion particle densities.

The effect of radiative processes in the low density plasmas obtained in magnetic fusion devices and stellar atmospheres can be neglected since they can be assumed as optically thin (plasma radiation self-absorption is not significant). Furthermore, we have not considered external radiation fields in this work. On the other hand, for the high density plasmas obtained in stellar interiors and inertial confinement targets the relevance of radiative processes is significantly lower than collisional processes and can also be neglected. Therefore, the atomic processes considered in the CRSS model were collisional ionization and three-body recombination, spontaneous decay, collisional excitation and deexcitation, radiative recombination, autoionization and electron capture and the rate equations and the RTE will be uncoupled.

The calculation of the rate coefficients of those processes requires of atomic data such as atomic energy levels, oscillator strengths and cross sections. Before then, the first problem to address is the selection of a suitable set of atomic configurations for the CRM since, in principle, the number of atomic levels for a given ion is infinite. There is not a priori criterion to determine which configurations should be considered in the model and, in general, the kind of configurations to include depends on the plasma conditions, the presence of external radiation fields (such as thermal radiation or ultra-intense lasers) or the interaction with particle beams. However, since we are interested in the generation of databases of radiative plasma properties and their parametrization in wide range of plasma conditions, the criterion employed was based on a rule of thumb in which the configurations included for each ion in the model are those with energies up to twice the ionization energy of the ground configuration of the ion. With this criterion we cannot guarantee that all the configurations that have some influence in the radiative properties for a given plasma condition are included but the ones that have a large contribution are considered. The second question to address is related with the degree of detail of the atomic description. The most detailed description is the so-called detailed level accounting (DLA) approach. However, this description entails very large computational times and, therefore, it is only useful for chemical elements of low atomic number. In this work, the atomic data were generated in the detailed configuration accounting (DCA) approach. This is a statistical average of the atomic properties obtained in the DLA approach and is more accurate for elements of high atomic number. Nevertheless, since we are interested in average radiative properties, DCA approach is accurate enough for that purpose. Once the set of atomic configurations and the atomic description were selected, the atomic data used in the POLAR code were generated with the FAC code [22]. For a given ion with N electrons the energy levels are obtained in FAC by means of the diagonalization of the relativistic Hamiltonian. The wave functions are then obtained as antisymmetric sums of products of N monoelectronic Dirac spinors. Configuration interactions effects are also considered. The cross sections of the forward-going processes (collisional ionization, collisional excitation and autoionization) are calculated quantum-mechanically in the relativistic distorted wave approach [22]. The cross sections for the corresponding inverse processes were determined from the appropriate micro-reversibility relations [23].

The atomic data provided by the FAC code are obtained for isolated atoms. However, the plasma surrounding (ions, free electrons and photons) modify the atomic data since they change the potential experimented by the bound electrons. This effect is commonly modelled in plasma physics through the so-called continuum lowering, that represents the depression of the potential with respect to the isolated situation due to the electric fields generated by the plasma charged particles. In this work, the model used for the continuum lowering is based on the widely used proposal developed by Stewart and Pyatt [24] where the correction to the ionization potential I_ζ is given by

$$\Delta I_\zeta = \frac{3a_0 I_H}{2R_\zeta}(\zeta+1)\left\{\left[1+\left(\frac{D}{R_\zeta}\right)^3\right]^{2/3} - \left(\frac{D}{R_\zeta}\right)^2\right\} \tag{13}$$

where a_0 is the Bohr radius, I_H is the Rydberg constant, $R_\zeta = [3(\zeta+1)/4\pi n_e]^{1/3}$ is the sphere-ion radius assuming the plasma composed of ions with charge ζ only and the Debye radius is $D = \left[4\pi\left(\bar{Z}+\overline{Z^2}\right)n_{ion}/T_e\right]^{-1/2}$, with T_e the electron temperature and $\overline{Z^2}$ the second order moment of the population distribution. The inclusion of the continuum lowering the kinetics rate equations of the CRSS model imply to solve them iteratively since the atomic data are now modified by the shifts caused by plasma effect.

The set of rate equations constitutes a system of M equations for the level populations, where M denotes the total number of levels included in the CRM. Therefore, the size of the collisional-radiative matrix scales like M^2. Even in the DCA approach, the number of levels involved in collisional-radiative simulations can easily reach 10^4 which entails matrix with 10^8 elements. However, in CRM the atomic processes usually connect only levels belonging to ions with either the same charge state or to adjacent ones which means that the matrix is sparse and for this reason POLAR use sparse techniques to store and operate on only the non-zero elements, decreasing the memory requirements.

Once the plasma level populations are calculated with the POLAR code, these ones along with the oscillator strengths and the photoionization cross sections obtained using the FAC code are the input to the RAPCAL code to calculate the plasma radiative properties. Since in this work we show some examples of the parametrization of the radiative power loss, in the following we present a brief explanation about its calculation. The method to calculate the other plasma radiative properties in RAPCAL can be found in [19][20]. The radiative power loss is the frequency integrated plasma emissivity, if the plasma may be considered as optically thin. The emissivity, $j(\mathbf{r},t,\nu)$, has three contributions. The bound-bound contribution, $j_{bb}(\mathbf{r},t,\nu)$, is given by

$$j_{bb}(\nu) = \sum_\zeta \sum_{i,j} j_{\zeta j\to\zeta i}(\nu), \quad j_{\zeta j\to\zeta i}(\nu) = \frac{h\nu}{4\pi} N_{\zeta j} A_{\zeta j\to\zeta i} N \phi_{ij}(\nu) \tag{14}$$

where we have omitted the dependence on the position and time in the formula for simplicity. $A_{\zeta j\to\zeta i}$ is the Einstein coefficient for spontaneous deexcitation between the bound states j, i of the ion ζ and h is the Planck's constant. $\phi_{ij}(\nu)$ is the line profile and in its evaluation of the line profile, natural, Doppler, and electron-impact [25] broadenings were included and also the Unresolved Transition Array width [26], which is a statistical method to take into account the atomic fine structure of the spectra in the DCA atomic approach used in this work. The line-shape function is applied with the Voigt profile that incorporates all these broadenings. The bound-free contribution to the emissivity, $j_{bf}(\mathbf{r},t,\nu)$, is determined by means of

$$j_{bf}(\nu) = \sum_{\zeta+1,j} \sum_{\zeta,i} j_{\zeta+1,j\to\zeta,i}(\nu)$$

$$j_{\zeta+1,j\to\zeta,i}(\nu) = \frac{h^4\nu^3 n_e}{2\pi c^2 \varepsilon^{\frac{1}{2}}}\left(\frac{1}{2m_e}\right)^{\frac{3}{2}} N_{\zeta+1,j} f(\varepsilon)\, \frac{g_{\zeta,i}}{g_{\zeta+1,j}} \sigma^{\text{pho}}{}_{\zeta+1,j\to\zeta,i}(\nu) \tag{15}$$

where ε is the free electron energy and m_e the electron mass. In this work, a Maxwell-Boltzmann distribution $f(\varepsilon)$ at the electron temperature is assumed. Photoionization cross section, $\sigma^{\text{pho}}{}_{\zeta+1,j\to\zeta,i}(\nu)$, were calculated quantum-mechanically using the FAC code in the relativistic distorted wave approach. $g_{\zeta,i}$ denotes the statistical weight of level i. Finally, for the free-free contribution to the emissivity a semi-classical expression, based on the Kramer's inverse bremsstrahlung cross section [27], was used

$$j_{ff}(\nu) = \frac{32\pi^2 e^4 a_0^2 \alpha^3}{\sqrt{3}(2\pi m_e)^{3/2} h}\left(\frac{m_e}{2\pi k_B T_e}\right)^{1/2} \overline{Z^2} n_{\text{ion}} n_e e^{-h\nu/k_B T_e} \tag{16}$$

where $k_B$is the Boltzmann's constant and α is the fine structure constant. Therefore, the total emissivity is the sum of these three contributions and the radiative power loss is the emissivity integrated in frequency, as said above.

The ranges of plasma conditions of interest in RHS are, in general, very wide, covering several orders of magnitude in temperature and density. For this reason, we have obtained that an optimum grid in which generating the databases of the radiative properties using POLAR is based on logarithmic meshes with steps of 0.1 and 0.5 for the temperature and density grids, respectively, since the radiative properties are more sensitive to the plasma temperature than to the density. Once the databases have been generated we can proceed to their parametrization. Due to the nature of the radiative properties, we have obtained that the parametrization of the decimal logarithm of the radiative property than the property itself [28] shows numerical advantages. The polynomial employed for the fitting is given by

$$P(d,T_e) = \sum_{i=0}^{n} \sum_{j=0}^{m} C_{ij} (\log d)^i (\log T_e)^j \tag{17}$$

where d denotes either the electron particle density, the ion particle density or the density of matter of the plasma. The coefficients of the parametrization, C_{ij}, are obtained by the minimization of the following function through least square regression

$$F(C_{ij}) = \sum_{k=1}^{n_d} \sum_{l=1}^{n_T} \left[P(d_k, T_{e,l}) - \log A(d_k, T_{e,l})\right]^2 \tag{18}$$

where $A(d_k, T_{e,l})$ is the radiative property evaluated at a given plasma condition. Then, from the equation of the minimization

$$\frac{\partial F(C_{ij})}{\partial C_{ij}} = 0 \tag{19}$$

the following set of $(n+1) \cdot (m+1)$ coupled algebraic equations is obtained

$$\sum_{k=1}^{n_d} \sum_{l=1}^{n_T} \sum_{i=0}^{n} \sum_{j=0}^{m} C_{ij} (\log d_k)^{i+q} \left(\log T_{e,l}\right)^{j+r} = \sum_{k=1}^{n_d} \sum_{l=1}^{n_T} \log A\left(d_k, T_{e,l}\right) (\log d_k)^q \left(\log T_{e,l}\right)^r \tag{20}$$

with $q = 0, \ldots, n$ and $r = 0, \ldots, m$. Polynomial of high degree for the fittings can be highly oscillatory and may provide very inaccurate values for the radiative properties for plasma conditions not belonging to the databases. This fact is avoided fixing the maximum degree of the polynomial both for the temperature, m, and density, n, to 7, which are enough for the properties in which we are interested. To obtain the coefficients of the fitting we start from the lowest degree and we increase it until the relative difference between the fitting and the database value is lower than an imposed criterion. If the maximum degree is reached and the criterion has not been fulfilled, then the range of density and temperature considered must be sub-divided in short ranges and then the procedure starts again. In order to optimize this division, we have employed a quad-tree algorithm. Obviously, the number of polynomials obtained (and of sub-divisions of the space of plasma conditions) depends on the criterion imposed. As the criterion becomes more restrictive, the number of polynomial needed increases. This procedure is integrated in a computational code named PARPRA [18] which, in addition, was developed with a graphic interface to ease its use by the user. A detailed explanation of the code can be found in [29].

The databases of the radiative properties are generated for monocomponent plasmas. However, both in nuclear fusion and astrophysics, multicomponent plasmas (i.e. plasma mixtures) are commonly found. In this case, the fittings of the individual elements of the mixture can be used for determining its radiative properties. The procedure followed to obtain the mixture radiative properties depend on the type of density given as an input. If the input is the electron density, then the procedure is very simple since we only have to add the fitted radiative property of each single element, weighted by the abundance of each element in the mixture, in order to obtain the total one. On the other hand, if the input is the ion number density or the mass density we have to make an iterative procedure. Hence, we start assuming an electron density for the mixture equal to the ion density or to the mass density divided by the Avogadro's number and multiplied by the mixture atomic mass. With this electron density we obtain the average ionizations of the different elements in the mixture form the fitting of the average ionization of the single elements for that electron density. With this set of average ionizations and weighted by their fractional abundances in the mixture we obtain a new electron density and we repeat this procedure until the relative difference between the average ionizations of the mixture in two consecutive steps of the iterative procedure will be lower than an imposed criterion. We would like to point out the relevance of this procedure since it avoids the resolution of the CRM for a mixture which involves to solve as many set of rates equations as elements of the mixture, that, for example, in astrophysics can easily reach 26 elements.

Results

In this section we present some examples of the fittings of some of relevant microscopic radiative properties in order to show the utility and the accuracy of the fitting proposed. In Figure 1 we show an example of characteristic databases, generated using POLAR, to parametrize. In this case the property is the average ionization for Xe and Kr in a range of plasma conditions typically obtained in experiments of laboratory astrophysics in which scaled astrophysical phenomena are reproduced in laboratory with ultra-intense laser and noble gases.

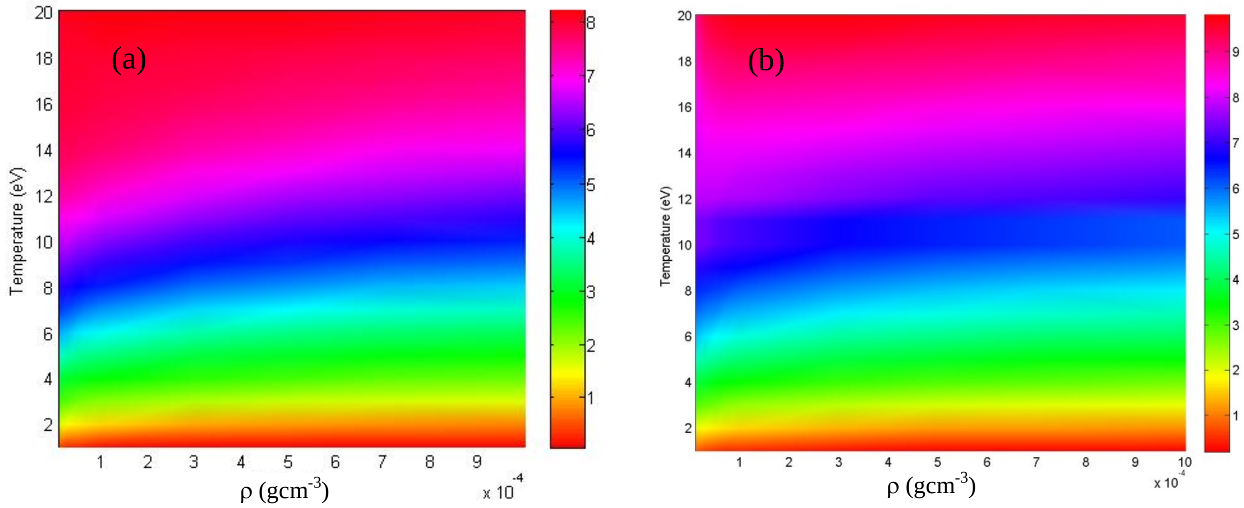

Figure 1. Representation of the databases of the average ionization generated by POLAR as a function of the electron temperature and density for plasmas of (a) Kr and (b) Xe.

In Figure 2, we present the parametrizations carried out with PARPRA of the average ionization and the radiative power loss of a krypton plasma as a function of the temperature and for several mass densities. For the fitting, the criterion imposed was a relative error lower than 1%. We also show in the figure the relative errors obtained between values obtained with POLAR and the parametrization either for plasma conditions used in the parametrization or not. We can observe that for the latter the relative error is sometimes larger than the criterion used in the fitting although they are still small and near to the criterion (lower than 1.5%). The errors obtained are slightly greater for the radiative power loss than for the average ionization since the former is a less average property than the latter and, therefore, is more sensitive to the plasma conditions. The number of polynomial functions required for the parametrization of the whole set of plasma conditions was 4 both for the average ionization and the radiative power loss.

The examples presented in the images correspond to parametrizations of radiative properties of monocomponent plasmas (krypton in particular). As commented above, a great advantage of this kind of parametrization is that it can be used to obtain the radiative properties of multicomponent plasmas without making any new parametrization or the calculation of the databases for the mixture. In Table 1 we present the comparison of the average ionization and the radiative power loss for a plasma mixture of four elements (neon, argon, aluminium, which are of interest in astrophysics, and xenon, which is commonly used as temperature moderator in nuclear fusion chambers) from the database and the ones obtained from the parametrization of the individual elements. We have assumed the same relative abundance of the four elements in the mixture. The databases of the single elements were parametrized with a relative error of 1% for the plasma conditions of the mesh of the database. From the table, we can observe that although the radiative properties of the multicomponent plasma in PARPRA are generated from the ones fitted for each single element of the mixture, the agreement with the values obtained from the collisional-radiative simulations using POLAR is really good. This is a remarkable result since this means a considerable reduction both in the complexity of the problem of dealing with plasma mixtures and also in the computing time.

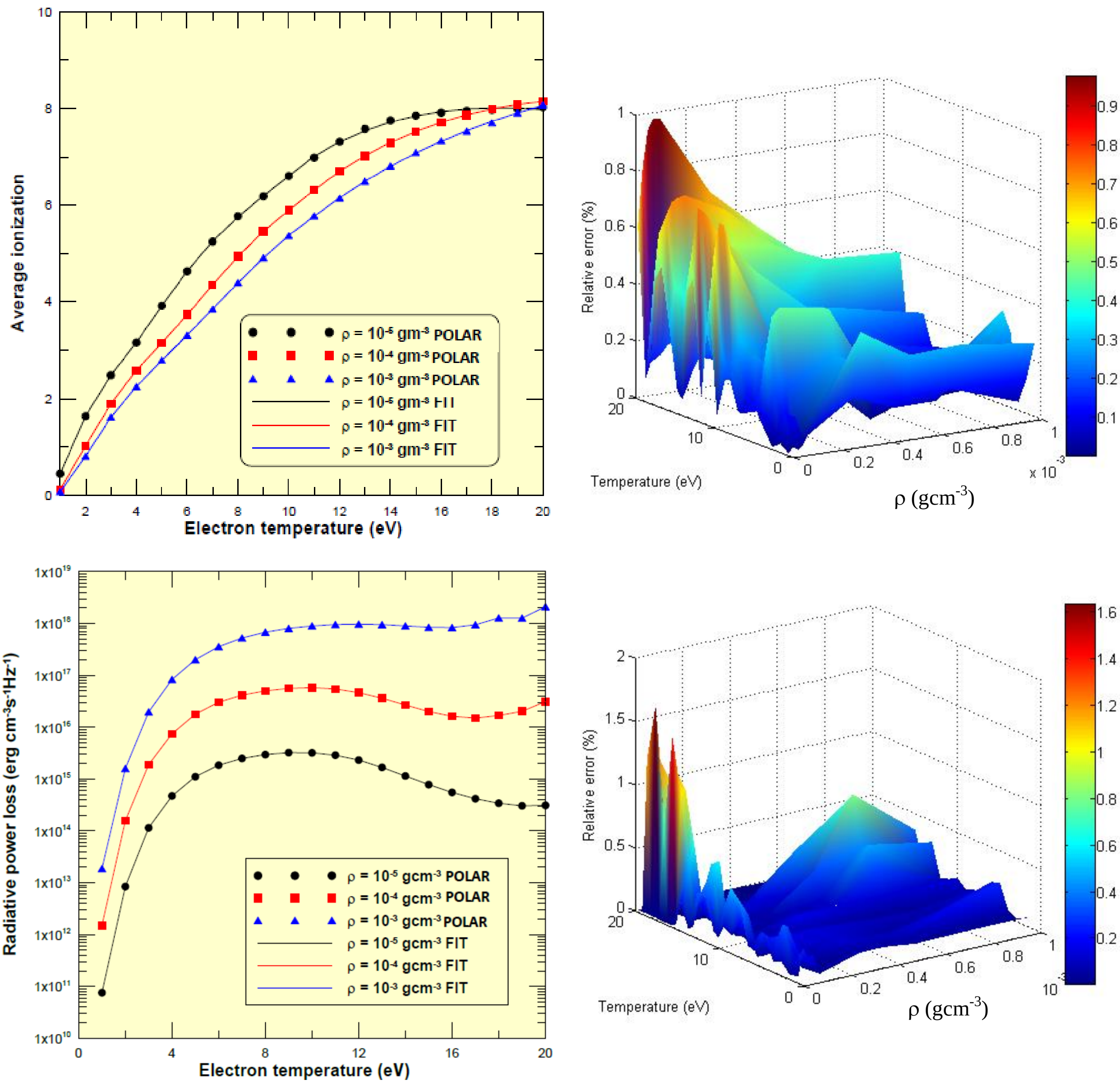

Figure 2. Parametrization of the average ionization and radiative power loss for several mass densities and for the range of temperatures 1-20 eV for a Kr plasma. The figure also shows the relative errors in the fitting for values of the properties belonging or not to the database fitted.

Table 1. Comparison of the average ionization ($\bar{Z}$) and the radiative power loss (RPL), in erg/s/cm3, for a plasma mixture of four elements, provided by the POLAR simulations and their parametrization with PARPRA.

T (eV)	d (gcm^{-3})	$\bar{Z}$ (POLAR)	$\bar{Z}$ (PARPRA)	RPL (POLAR)	RPL (PARPRA)
2	10^{-5}	1.293	1.239	3.564×10^{13}	3.579×10^{13}
10	10^{-5}	4.046	4.046	5.352×10^{15}	5.351×10^{15}
20	10^{-5}	6.060	6.058	1.286×10^{16}	1.287×10^{16}
20	10^{-4}	6.164	6.158	3.963×10^{17}	3.973×10^{17}

Conclusions

In this work we have presented a method to parametrize average plasma radiative properties, implemented in the PARPRA code in terms of the plasma temperature and density by means of polynomial functions, which is very useful in RHS since these parametrizations considerably reduce the computational costs. The databases of the radiative properties to parametrize are generated using a recently developed code named POLAR which has implemented a CRM. Therefore, the radiative properties and, therefore, their parametrizations, are accurate for any plasma thermodynamic regime. The criterion imposed in the parametrization is fixed by the user. Obviously, as the criterion becomes more restrictive the number of polynomial functions required to parametrize the whole set of plasma conditions increases. We have presented, as example, a parametrization of the average ionization and the radiative power loss of a Kr plasma imposing a relative error in the fitting of 1%. The number of polynomials required was 4 for both properties and the errors obtained in the calculation of the properties from the parametrization at plasma conditions not included in the fitting were also very near to the criterion. We have also showed the utility and the accuracy of the parametrization of the radiative properties of the single elements for obtaining those for plasma mixtures. It is worth pointing out the advantage of providing this kind of parametrizations since the radiative properties are needed in radiation-hydrodynamics simulations of plasmas in nuclear fusion and astrophysics in wide range of plasma conditions being their calculation very complex and computing time consuming.

In this work we have limited the parametrization to mean radiative properties since we have assumed the gray approach for the RTE in the RHS. However, this may be a rude approach in several scenarios. More realistic radiative transfer simulations require more detailed descriptions of the radiative properties such as those based on multigroup descriptions (the gray approach can be considered as one group approach). Parametrizations of multigroup radiative properties as a function of the plasma conditions and photon frequency groups would be highly useful and this will be a future goal of this work.

Acknowledgements

This work has been supported by the EUROfusion Consortium TASK AGREEMENT WPENR: Enabling Research IFE, Project No. AWP15-ENR-01/CEA-02, by the Project of the Spanish Government with reference FIS2016-81019-P.

References

[1] Fengtao, J., Jiaolong, Z., Jianmin, Y., Guoxing, H., Zeqing, W., Yun, Y., Wan, M. and Peng, Y. (2005) L to M shell transitions and model comparisons for radiative opacities of sodium fluoride plasmas, *Journal of Quantitative Spectroscopy and Radiative Transfer* **95**, 241-253.

[2] Bailey, J.E., Rochau, G.A., Mancini, R.C., Iglesias, C.A., MacFarlane J.J., Golovkin, I.E., Blancard, C., Cosse, Ph. and Faussurier, G. (2009) Experimental investigations of opacity models for stellar interior, inertial fusion and high energy density plasmas, *Physics of Plasmas* **16**, 058101.

[3] Benredjem, D., Jarrah, W., Gilleron, F., Pain, J.C., Ferri, S. and Calisti, A. (2015) Opacity calculations. Ge and Si dopants in ICF, *High Energy Density Physics* **16**, 23-27.

[4] Smith, H.M. and Verwitche E. (2008) Hot tail runaway electron generation in tokamak disruptions, *Physics of Plasmas* **15**, 072502.

[5] Tokar, M.Z. and Kelly, F.A. (2003) The role of plasma-wall interactions in thermal instabilities in tokamak edges, *Physics of Plasmas* **10**, 4378-4386.

[6] Drake, R. P. (2005) *High energy density physics: fundamentals, inertial fusion and experimental astrophysics*, Springer, The Netherlands.

[7] Rodriguez, R., Espinosa, G., Gil, J.M., Stehle, C., Suzuki-Vidal, F., Rubiano, J.G., Martel, P. and Minguez, E. (2015) Microscopic properties of xenon plasmas for density and temperature regimes of laboratory astrophysics experiments on radiative shocks, *Physical Review E* **91**, 053106.

[8] Bates, D.R., Kingston, A.E. and McWirther, R.W. P. (1962) Recombination between electrons and atomic ions. I. Optically thin plasmas, *Proceedings of the Royal Society of London Series A: Mathematical and physical sciences* **267**, 297-312.

[9] McWirther, R.W. P. (1978) Data needs, priorities and accuracies for plasma spectroscopy, *Physics Reports* **37**, 165-209.

[10] Post, D.E., Jensen, R.V. and Tarter, C.B. and Grasberger, W.H. and Lokke, W.A. (1977) Steady-state radiative cooling rates for low density, high-temperature plasmas, *Atomic Data and Nuclear Data Tables* **20**, 397-439.

[11] Summers, H.P. and McWhirter, R.W.P. (1979) Radiative power loss from laboratory and astrophysical plasmas. I. Power loss from plasmas in steady-state ionisation balance, *Journal of Physics B: Atomic and Molecular Physics* **12**, 387-411.

[12] Fournier, K.B., Pacella, D., May, M.J., Finkenthal, M. and Goldstein, W.H. (1997) Calculation of the radiative cooling coefficient formolybdenum in a low density plasma, *Nuclear Fusion* **37**, 825-834.

[13] Fournier, K.B., Cohen, M., May, M.J. and Goldstein, W.H. (1988) Ionization state distribution and radiative cooling rate for argon in a low density plasma, *Atomic Data and Nuclear Data Tables* **70**, 231-254.

[14] Fournier, K.B., May, M.J., Pacella, D., Finkenthal, M., Gregory, B.C. and Goldstein, W.H. (2000) Calculation of the radiative cooling coefficient for krypton in a low density plasma, *Nuclear Fusion* **40**, 847-863.

[15] Schure, K.M., Kosenko, D., Kaastra, J.S., Keppens, R. and Vink, J. (2009) A new radiative cooling curve based on an up-to-date plasma emission code, *Astronomy &. Astrophysics* **508**, 751-U240.

[16] Minguez, E., Ruiz, R., Martel, P., Gil, J.M., Rubiano, J.G. and Rodriguez, R. (2001) Scaling law of radiative opacities for ICF elements, *Nuclear Instruments and Methods in Physics Research A* **464**, 218-224.

[17] Minguez, E, Martel, P., Gil, J.M., Rubiano, J.G. and Rodriguez, R. (2002) Analytical opacity formulas for ICF elements, *Fusion Engineering. Design* **60**, 17-25.

[18] Rodriguez, R., Espinosa, G., Gil, J.M., Rubiano, J.G., Mendoza, M.A., Martel, P. and Minguez, E. (2014) Parametrization of Mean Radiative Properties of Optically Thin Steady-State Plasmas and Applications, *Communications in Computational Physics* **16**, 612-631.

[19] Rodríguez, R., Florido, R., Gil, J.M., Rubiano, J.G., Martel, P. and Mínguez, E. (2008) RAPCAL: a computational package to compute radiative properties of optically thin and thick low and high-Z plasmas in a wide range of density and temperature, *Laser and Particle Beams* **26**, 433-448.

[20] Rodriguez, R., Florido, R., Gil, J.M., Rubiano, J.G., Suarez, D., Martel, P., Minguez, E. and Mancini, R.C. (2010) Collisional-Radiative calculations of optically thin and thick plasmas using the computational package ABAKO/RAPCAL, *Communications in Computational Physics* **8**, 185-210.

[21] Espinosa, G., Rodríguez, R., Gil, J.M., Suzuki-Vidal, F., Lebedev, S.V., Ciardi, A., Rubiano, J.G. and Martel, P. (2017) Influence of atomic kinetics in the simulation of plasma microscopic properties and thermal instabilities for radiative bow shock experiments, *Physical Review E* **95**, 033201.

[22] Gu, M.F. (2008) The flexible atomic code, *Canadian Journal of Physics* **86**, 675-689.

[23] Blatt, J.M. and Weisskopf, V.F. (1991) *Theoretical Nuclear Physics*, Dover Publications, New York.

[24] Stewart, J.C. and Pyatt, K.D. (1966) Lowering of ionization potentials in plasmas (1966), *The Astrophysical Journal* **144**, 1203-1211.

[25] Dimitrijevic, M.S. and Konjevic, N. (1987) Simple estimates for Stark-broadening of ion lines in stellar plasmas, *Astronomy & Astrophysics* **172**, 345-349.

[26] Bauche, J., Bauche-Arnoult, C. and Klapisch, M. (1987) Transition arrays in the spectra of ionized atoms, *Advance Atomic Molecular Physics* **23**, 131-195.

[27] Rose, S.J. (1992) Calculation of the radiative opacity of laser-produced plasmas, *Journal of Physics B: Atomic and Molecular Physics* **25**, 1667-1681.
[28] Espinosa, G., Rodríguez, R., Gil, J.M., Suzuki-Vidal, F., Lebedev, S.V., Ciardi, A., Rubiano, J.G. Martel, P. (2017) *Physical Review E* **95**, 033201.
[29] Espinosa, G. (2015) *Determinación y parametrización de propiedades radiativas de plasmas para la simulación y análisis de experimentos de astrofísica de laboratorio*. Ph. D Thesis, Las Palmas de Gran Canaria.