High Energy Density Physics 17 (2015) 219–230

Contents lists available at ScienceDirect

High Energy Density Physics

journal homepage: www.elsevier.com/locate/hedp

The fast non-LTE code DEDALE

Franck Gilleron *, Robin Piron

CEA, DAM, DIF, F-91297 Arpajon, France

ARTICLE INFO

Article history:
Received 15 July 2015
Accepted 16 July 2015
Available online 22 July 2015

Keywords:
Collisional–radiative model
NLTE
Superconfiguration
Rates
Opacity
Emissivity

ABSTRACT

We present Dédale, a fast code implementing a simplified non-local-thermodynamic-equilibrium (NLTE) plasma model. In this approach, the stationary collisional–radiative rates equations are solved for a set of well-chosen Layzer complexes in order to determine the ion state populations. The electronic structure is approximated using the screened hydrogenic model (SHM) of More with relativistic corrections. The radiative and collisional cross-sections are based on Kramers and Van Regemorter formula, respectively, which are extrapolated to derive analytical expressions for all the rates. The latter are improved thereafter using Gaunt factors or more accurate tabulated data. Special care is taken for dielectronic rates which are compared and rescaled with quantum calculations from the Averroès code. The emissivity and opacity spectra are calculated under the same assumptions as for the radiative rates, either in a detailed manner by summing the transitions between each pair of complexes, or in a coarser statistical way by summing the one-electron transitions averaged over the complexes. Optionally, nℓ-splitting can be accounted for using a WKB approach in an approximate potential reconstructed analytically from the screened charges. It is also possible to improve the spectra by replacing some transition arrays with more accurate data tabulated using the SCO-RCG or FAC codes. This latter option is particularly useful for K-shell emission spectroscopy. The Dédale code was used to submit neon and tungsten cases in the last NLTE-8 workshop (Santa Fe, November 4–8, 2013). Some of these results are presented, as well as comparisons with Averroès calculations.

1. Introduction

The modeling of non-local-thermodynamic-equilibrium (NLTE) plasmas is central for many applications involving high-energy density physics. This concerns, for instance, integrated simulations of hohlraums in the context of inertial confinement fusion, the diagnosis of plasma X-ray sources, the estimation of radiative power losses in the ITER reactor or photoionized plasmas in astrophysical environments.

Out of equilibrium, the modeling of atomic physics in plasmas depends closely on the radiation field. In general, radiation transport is coupled to the hydrodynamic motion of matter, so that NLTE physics must be used in integrated radiation–hydrodynamics simulations. This requires fast but accurate methods. At present, the CEA radiation–hydrodynamics codes [1] use different kinds of fast inline NLTE libraries, either based on the NLTE average-atom approach [2,3] or on the notion of ionization temperatures [4,5]. Though largely simplified, these models may be rescaled with more accurate data, for instance from the Averroès code [6,7]. The increase in power of supercomputers nowadays allows one to include more and more complexity in integrated NLTE models. The Dédale code, under development, is an approach similar to models like FLYCHK [8] or DCA-Cretin [9]. The collisional–radiative model determines the NLTE populations of ground and excited states belonging to different ion stages in the plasma. In this framework, it is easier to account for dielectronic processes and electron–electron correlations in NLTE calculations, which are crucial for a realistic ionization balance and for spectra.

The collisional–radiative model on which the Dédale code relies is presented in Section 2. The plasma is viewed as a neutral collection of non-interacting ions and free-electrons. The binding-energy levels of the ions are treated statistically and estimated using the screened hydrogenic model of the atomic structure described in Section 2.1. In more realistic models, interactions among the ions and the free-electrons can lead to pressure ionization of the ions. In order to account for this phenomenon in a crude way, we correct the atomic structure model as described in Section 2.2. The populations of the different species are linked by physical processes and can be obtained either from the thermodynamic equilibrium (under the local thermodynamic equilibrium assumption, i.e. LTE) or from the collisional–radiative equations (CRE) when the plasma is out of equilibrium with the radiation field. In this last case, we solve the master equations given in Section 2.3, and therefore the rates of all relevant processes are obtained using the formula of Section 2.4. Given the populations it is then possible to calculate

PACS: 52.25.Dg 52.20.-j 52.25.Os.

* Corresponding author. CEA, DAM, DIF, F-91297 Arpajon, France.
E-mail address: franck.gilleron@cea.fr (F. Gilleron).

http://dx.doi.org/10.1016/j.hedp.2015.07.001
1574-1818/

the radiative properties of the plasma using the approach of Section 2.5.

In Section 3, results of the present model are compared with Averroès calculations on some low-, medium- and high-Z plasma cases. We then draw some preliminary conclusions.

2. Presentation of the Dédale model

2.1. Atomic structure modeling

We use a statistical approach based on Layzer complexes, i.e. superconfigurations with supershells gathering all orbitals with the same principal quantum number (up to n = 10):

$$\mathcal{C} = (1s)^{P_1}(2s2p)^{P_2}(3s3p3d)^{P_3}\ldots(10s10p\ldots10m)^{P_{10}} \tag{1}$$

The occupation number P_n of shell n can vary from 0 to the shell degeneracy $2n^2$. The calculation uses a list ranging from a few hundreds up to several tens of thousands of complexes, depending on the user's need as regards the computation time. Ground complexes are first set up for each ion charge state. They are then used to generate automatically the excited complexes by moving one or more electrons to higher shells according to several parameters and criteria.

All levels or configurations within the same complex are considered to be in LTE at a temperature much higher than the energy spread of the complex (statistical weigth approximation). Only transitions involving different shells participate in the kinetic equations (see Section 2.3). The total energy of complex $\mathcal{C}$ is approximated using the screened hydrogenic model (SHM) as

$$E_{\mathcal{C}} = \sum_{n=1}^{10}\frac{P_n[\mathcal{C}]}{2n^2}\sum_{\kappa=1}^{n}4\kappa\left(1-\frac{1}{2}\delta_{\kappa,n}\right)\varepsilon_{n\kappa}[\mathcal{C}] \tag{2}$$

where the expression for the energies $\varepsilon_{n\kappa}$ (<0) follows the exact solution of the Dirac equation for hydrogenic atoms,

$$\varepsilon_{n\kappa}[\mathcal{C}] = \frac{2\mathcal{R}}{\alpha^2}\left(\left(1+\left(\frac{\alpha Q_n[\mathcal{C}]}{n-|\kappa|+\sqrt{\kappa^2-\alpha^2Q_n^2[\mathcal{C}]}}\right)^2\right)^{-1/2}-1\right) \tag{3}$$

in which the nuclear charge Z has been replaced by the effective charge $Q_n[\mathcal{C}]$ seen by the electrons in shell n of complex $\mathcal{C}$. $\mathcal{R}$ is the Rydberg energy and α is the fine-structure constant. The effective charges are evaluated using the screening factors $\sigma_{n,n'}$ of More [10] as

$$Q_n[\mathcal{C}] = Z-\frac{1}{2}\sigma_{n,n}\max(0,P_n[\mathcal{C}]-1)-\sum_{n'<n}\sigma_{n,n'}P_{n'}[\mathcal{C}]. \tag{4}$$

This expression accounts for the screening by inner electrons only ($n'<n$) and includes a correction to avoid electron self screening, as mentioned in Ref. 11 to obtain a better accuracy for hydrogenic atoms.

Under the assumption that free electrons form a non-interacting partially-degenerate gas in local thermodynamic equilibrium, their density is given by the formula

$$n_e = \frac{4\pi}{h^3}(2mkT_e)^{3/2}F_{1/2}\left[\frac{\mu}{kT_e}\right] \tag{5}$$

where k is the Boltzmann constant, h is the Planck constant, m is the electron mass, μ is the chemical potential and $F_{1/2}[x]$ is the Fermi-integral of order 1/2. The chemical potential μ is determined by assuming charge neutrality for the overall plasma, $n_e = \bar{Z}n_{\text{ion}}$, where n_{ion} is the number of ions per unit volume. The plasma mean ionization is defined as:

$$\bar{Z} = \frac{1}{n_{\text{ion}}}\sum_{\mathcal{C}}Z_{\mathcal{C}}N_{\mathcal{C}}, \tag{6}$$

where $Z_{\mathcal{C}} = Z-\sum_n P_n[\mathcal{C}]$ is the charge state of the Layzer complex $\mathcal{C}$ and $N_{\mathcal{C}}$ its population. The populations of the complexes are computed either from the thermodynamic equilibrium condition or using a collisional–radiative approach detailed in Section 2.3.

2.2. Density effects

To mimic the pressure–ionization effects on bound states and their progressive delocalization, the degeneracy of shell n is gradually reduced as the ion density increases [12]:

$$g_n = 2n^2\Lambda_n[\rho] \tag{7}$$

The total degeneracy of complex $\mathcal{C}$ is evaluated as

$$g_{\mathcal{C}} = \prod_n \Theta[g_n,P_n] \tag{8}$$

using a modified binomial function which reads:

$$\Theta[g_n,P_n] = \begin{cases}\dfrac{\Gamma(1+g_n)}{\Gamma(1+P_n)\Gamma(1+g_n-P_n)} & \text{if} \quad 0\le P_n\le g_n\le 2n^2\\ e^{-a_n\left(\frac{P_n}{g_n}-1\right)} & \text{if} \quad 0\le g_n<P_n\le 2n^2\end{cases} \tag{9}$$

where $\Gamma[x]$ is the Euler gamma function. The parameter a_n is a real positive number which controls the progressive disappearance of shell n. Simultaneously, ionization-potential lowering is taken into account by adding a positive density-dependent contribution to the total energy of complex $\mathcal{C}$:

$$E_{\mathcal{C}} \to E_{\mathcal{C}} + \sum_n P_n[\mathcal{C}]\delta E_n[\rho] \tag{10}$$

To speed-up the calculations, complexes may be removed from the collisional–radiative modeling if its degeneracy is considered to be sufficiently small.

The simplest approach is to express $\Lambda_n[\rho]$ and $\delta E_n[\rho]$ as a function of the parameter R_n/R_0, where R_n is the mean radius of shell n, $R_0 = \left(\frac{3}{4\pi n_{\text{ion}}}\right)^{1/3}$ is the Wigner–Seitz radius, $n_{\text{ion}} = \rho N_a/A$ is the ion density (with the Avogadro number N_a and the ion mass A). Indeed, it is expected that $\Lambda_n \to 1$ and $\delta E_n \to 0$ when $R_n \ll R_0$ (no density effects), and that $\Lambda_n \to 0$ when $R_n \gg R_0$ (delocalization of shell n). Many options are available in the code, based on various formulas found in the literature (see for instance Refs. 13–15).

We compare in Fig. 1 the Al 20 eV-isotherm mean ionization obtained using Dédale to that stemming from the well-known Inferno Ion-in-Cell Average-Atom model [17]. The latter calculation uses the following definition of the mean ionization: $\bar{Z} = Z-\sum_{n,\ell}P_{n,\ell}$, where $P_{n,\ell}$ are the LTE fractional subshell occupation numbers. This last definition is similar to Eq. (6) and leads to the characteristic step features corresponding to closed shell ions (Ne-like, He-like).[1]

As can be seen, with the Dédale model, LTE is reached along this isotherm around 10^{-3} g.cm^{-3} matter density. The pressure ionization also occurs starting from a few 10^{-3} g.cm^{-3} and the Dédale calculations with degeneracy reduction yield in this region the qualitative behavior of increasing mean ionization.

[1] Using Inferno with the definition of the mean ionization based on the chemical potential, i.e. that used in the Thomas–Fermi model lead to a much smoother curve, close to that from the Thomas–Fermi model.