Atomic Physics Modeling and Applications for ICF Plasmas*)

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The Atomic Physics Group at the Institute of Nuclear Fusion (DENIM) in Spain has accumulated experience over the years in developing a collection of computational models and tools for determining some relevant microscopic properties of, mainly, ICF and laser-produced plasmas in a variety of conditions. In this work several applications of those models in determining some relevant microscopic properties are presented.

Keywords: ICF plasma, computational model to calculate plasma property, average ionization, thermodynamic regime, mean opacity, radiative power loss

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1. Introduction

Fundamental research and modelling in plasma atomic physics continues to be essential for both providing basic understanding and advancing on many different topics relevant to high-energy-density systems community. For that reason, the Atomic Physics Group at the Institute of Nuclear Fusion (DENIM) in Spain has accumulated experience over the years in developing a collection of computational models and tools for determining some relevant microscopic properties of inertial confinement fusion (ICF) plasmas. Thus, for instance, the computational package ABAKO/RAPCAL [1] was developed and used for detailed calculations of population kinetics and spectroscopic diagnosis of direct-drive ICF targets, or ATMED code [2], based on a new average-atom screened-hydrogenic model [3] and which was developed with the purpose of providing fast computation of mean and frequency-dependent emissivities and opacities for hot and dense LTE single- and multi-component plasmas. This code allows an easy coupling to a potential hydrodynamic code and it has been also used to compute the plasma equation of state (EOS) and shock Hugoniot curves.

These two models are also useful for determining the optical data for simulating the radiation hydrodynamic in the laser reactor chambers where residual gas interacts with the plasma, being the temperatures and densities spread over 1 eV to 1 keV and 10^{-8} to 1 g/cc respectively. The procedure is to create a data table of opacities in these ranges. Radiation hydrodynamic codes will read this table and interpolate for the real temperature and density.

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2. Computational Models

2.1 ABAKO/RAPCAL package

The computational package ABAKO/RAPCAL [1] consists of two codes, ABAKO [4] and RAPCAL [5, 6]. The first one is devoted to the calculation of the plasma level populations for arbitrary optical depths in both local thermodynamic equilibrium (LTE) and non-LTE (NLTE) conditions, using a collisional-radiative steady state (CRSS) model. This model solves level by level (or configuration by configuration, depending on the atomic description) and it is applied to low to high Z ions under a wide range of plasma conditions. RAPCAL is used to determine several relevant plasma radiative properties such as the spectrally resolved opacities and emissivities, mean and multigroup opacities, source functions, radiative power losses, specific intensities and plasma transmission.

2.2 ATMED code

ATMED code [2] has been designed to compute the spectral radiative opacity as well as the Rosseland and Planck means for single element and mixture plasmas under LTE conditions. Furthermore, it has been also used to compute the plasma EOS and the shock Hugoniot case in the adiabatic situation. The model developed is fast, stable and reasonably accurate into its range of application (LTE) and it can be a useful tool to simulate ICF experiments in plasma laboratory. The code has been developed in the context of the average atom (AA) model approximation. The atomic data needed are computed using a Relativistic Screened Hydrogenic Model based on a new set of universal screening constants including j-splitting that were obtained from the fit to a wide database of atomic energies, ionization potentials and transition energies of high quality [3].

3. Results

3.1 ABAKO/RAPCAL simulations

As said before, ABAKO/RAPCAL has been widely and succesfully used in the determination of relevant plasma microscopic properties such as the average ionization, the charge state distributions or the radiative properties. In this work, we consider C and Xe which are relevant elements for reactor chambers, being the first one a debris coming from the target and Xe the gas in the reactor. The average ionization maps of C and Xe are obtained (Figs. 1 and 2, respectively), in a wide range of plasma conditions, covering both NLTE and LTE situations. This kind of maps permits a subsequent optimization in the computation of level populations and radiative properties since it reduces the number of ions to include in the calculations.

Furthermore, we also present the thermodynamic regimes maps for both C and Xe plasmas (Figs. 3 and 4, respectively). In these maps the plasma conditions in which LTE or NLTE regimes can be assumed are swown. In the literature, some qualitative criteria to estimate when an ion or ion level can be considered under LTE conditions are available. However, in this work a criterion that can state the regime of the whole plasma is employed, which is based on the weigthed relative differences between the ion populations calculated from Saha-Boltzmann (SB) equations and those obtained from the CRSS model [5, 7]. When theat criterion is fulfilled we can assume that LTE regime has been achieved. Otherwise, the plasma is under NLTE conditions. This kind of map is very useful since allows us to know where SB equations are accurate enough to obtain plasma level populations, which represents and advantage since they are easier and faster than CRSS models.

As it is known, radiation-hydrodynamics simulations of radiative shocks need the calculation of several plasma parameters such as the average ionization, radiative power losses or mean opacities for many plasma conditions. Due

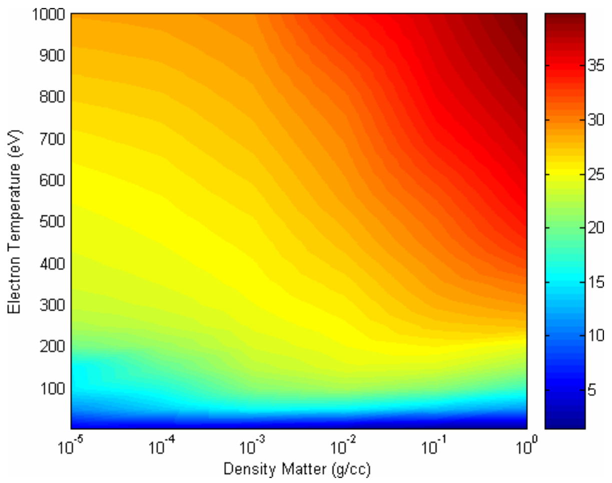

Fig. 1 Map of the average ionization for C plasmas.

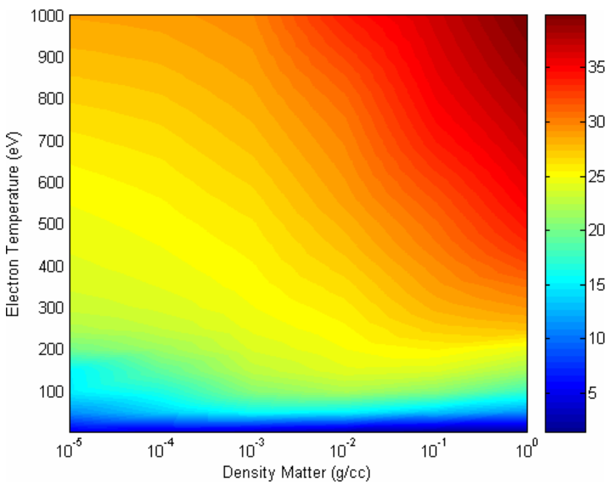

Fig. 2 Map of the average ionization for Xe plasmas.

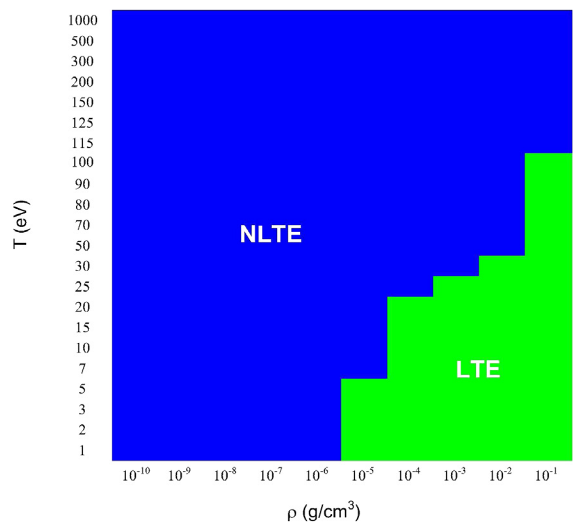

Fig. 3 Carbon thermodynamic regimes as a function of the temperature and density.

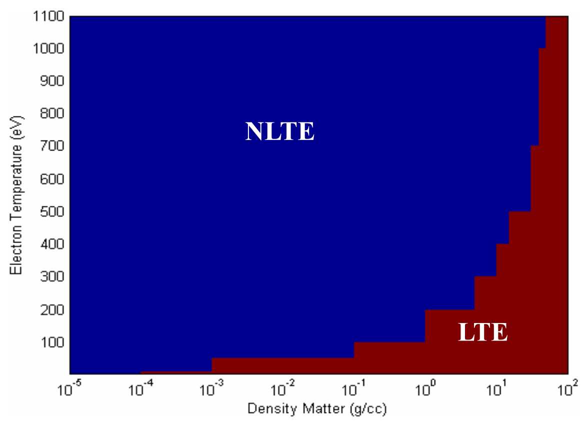

Fig. 4 Xenon thermodynamic regimes as a function of the temperature and density.

to the large computational cost of these calculations it is usual to make use of fittings to analytical expressions of those parameters. However, most of these fittings are only valid for low density plasmas since they were made assuming coronal equilibrium, and, therefore, the fittings are density independent. Furthermore, the atomic models that underlie those calculations are, in general, quite simple, based on hydrogenic models and average atoms. We have developed analytical expressions in powers of densities and temperatures for the calculation of the average ionization, the radiative power loss and the Planck mean opacity which are valid for low-to-high densities and temperatures. The data employed for the fittings are those provided by ABAKO/RAPCAL computational package. If A denotes the magnitude to fit, the analytical expression employed for the fitting is the following

$$\log A(\rho, T) = \sum_{i=0}^{n} \sum_{j=0}^{m} C_{ij} (\log \rho)^i (\log T)^j. \quad (1)$$

The maximum degrees of the polynomial fitting both for the matter density and electron temperature were fixed to 7 in order to avoid oscillating behavior. For the fitting relative errors lower than 1% for the average ionization and lower than 5% for the radiative power loss and the Planck mean opacity were required. Obviously, as the error imposed becomes more restrictive the number of polynomial functions needed to make the fit of the whole range of plasma conditions increases. In order to optimize the searching method of the polynomial functions a quad-tree algorithm was implemented. Fittings for the average ionization, mean opacities and radiative power losses for Xe and Kr plasmas in a range of plasma conditions of interest for laboratory astrophysics have been presented in a previous work [8].

3.2 ATMED simulations

In Table 1, for an iron plasma with density 1 $\mathrm{g cm^{-3}}$ and several temperatures (0.5 to 1.25 keV), we compare or results with experimental data provided by Avrorin *et al.* [9], and data provided by a Thomas-Fermi calculation and those given by THERMOS [10], LEDCOP [11] and OPAL [12] codes. Looking at the results we can see that our model agrees into the experimental margins with experimental results and shows a very good behaviour in relation to more sophisticated codes used for several laboratories as LLNL and LANL.

In Fig. 5 we present a comparison of a monochromatic opacity for iron plasma between ATMED and LEDCOP. From the figure we observe that ATMED reproduces quite well the absorption spectra although the number of lines is lower than in LEDCOP, which is expected since the former is based on an average atom model and the latter is a DCA one.

ATMED has been also used in the calculation of radiative opacities of mixtures of ICF plasmas. For example, in Figs. 6 and 7 we show the monochromatic opacities calculated for a beryllium-copper mixture (Be(99.1%)-Cu(0.9%)), essential to describe the fusion ignition target compression [13]. They have been compared with those calculated using LEDCOP code. As we can see there are good agreements between ATMED and LEDCOP in both cases.

In Tables 2 and 3 we have have compared Rosseland mean opacities with those calculated by SPECTR code [13] for the same mixture and for temperatures from 40 eV to 360 eV and densities in the range from 10^{-3} to

Table 1 Rosseland mean opacities in $\mathrm{cm^2/g}$ for iron plasma at several temperatures.

T (keV)	0.5	0.75	1	1.25
Thomas-Fermi	62.5	7.81	2.7	1.59
THERMOS	79.6	8.37	3.14	2.29
LEDCOP	74.8		2.79	2.14
OPAL	84.2		3.48	
Experiment	82 ± 12	7.8 ± 1	2.3 ± 0.4	1.3 ± 0.2
ATMED	**79.93**	**8.31**	**2.70**	**1.75**

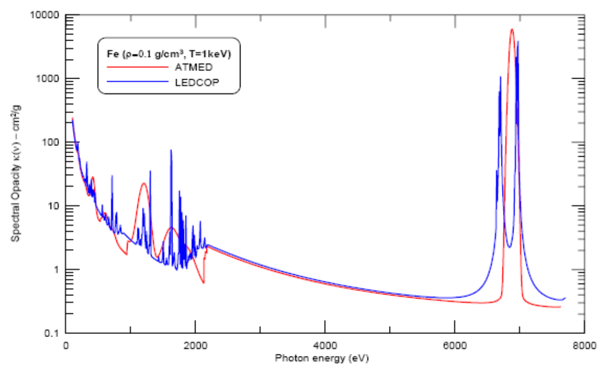

Fig. 5 Spectral opacity for Fe at $T = 1$ keV and $\rho = 0.1$ g/cm^3.

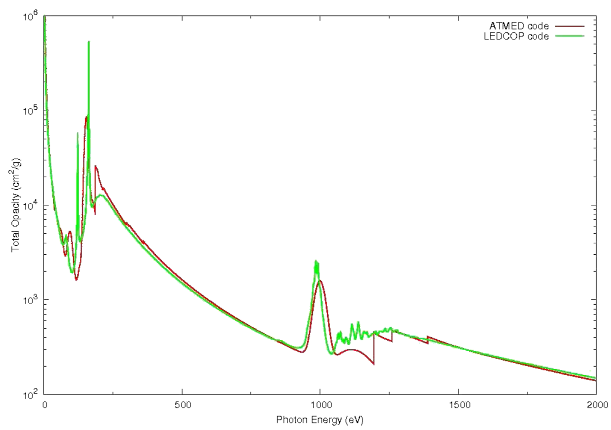

Fig. 6 Spectral opacity for Be-Cu mixture at $T = 50$ eV and $\rho = 0.1$ g/cm^3.

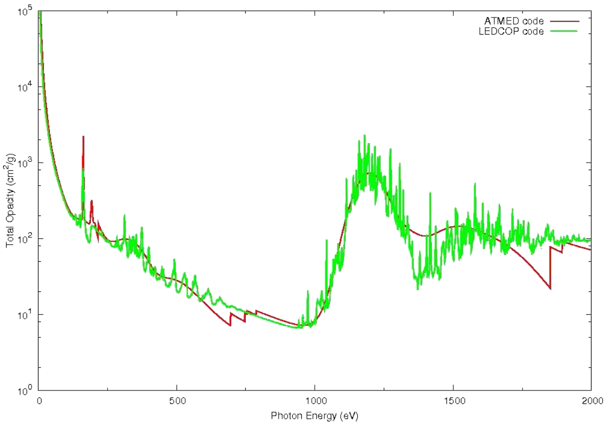

Fig. 7 Spectral opacity for Be-Cu mixture at $T = 250\,\mathrm{eV}$ and $\rho = 0.1\,\mathrm{g/cm^3}$.

Table 2 Comparison of the Rosseland mean opacities in cm^2/g for Be-Cu mixture.

ρ (g/cm^3)	40 eV		100 eV	
	SPECTR	ATMED	SPECTR	ATMED
10^{-3}	516.900	776.800	8.177	8.760
10^{-2}	2916.000	2905.000	66.700	61.240
10^{-1}	11430.000	8792.000	257.600	272.900
10^{0}	26810.000	17640.000	929.600	892.200

Table 3 Comparison of the Rosseland mean opacities in cm^2/g for Be-Cu mixture.

ρ (g/cm^3)	250 eV		360 eV	
	SPECTR	ATMED	SPECTR	ATMED
10^{-3}	0.693	0.747	0.270	0.318
10^{-2}	4.286	3.653	1.066	1.044
10^{-1}	22.130	22.200	9.516	9.673
10^{0}	116.600	90.560	46.950	44.430

10^{-1} g/cm^3. According as the temperature increases the opacity values obtained from ATMED are closer to the SPECTR ones, since the atoms are more ionized and the screened hydrogenic model has a better behaviour.

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