LANL Contributions to the NLTE-7 Code Comparison Workshop– Argon Test Case

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We report on the LANL contributions to the recent NLTE-7 Code Comparison Workshop that was held in Vienna, Austria in December 2011. The purpose of the workshop is to provide a detailed comparison among kinetics codes that simulate the properties of non-local-thermodynamic-equilibrium (NLTE) plasmas. Comparisons are made for a range of plasma properties such as ion populations and radiative losses. The LANL contributions were made using the LANL suite of atomic physics codes and the ATOMIC kinetics code, and included calculations for all of the test problems. In general, the LANL contributions compared very well to the other submissions, which came from various kinetics codes from institutions worldwide.

The NLTE Code Comparison Workshops [1] were first organized more than 10 years ago in an effort to provide critical comparisons between atomic kinetics codes that model populations of non-local-thermodynamic-equilibrium (NLTE) plasmas and their radiative properties under a range of plasma conditions. Such comparisons are particularly useful since there are few (if any) experiments with which to compare such kinetics calculations in large portions of the range of plasma conditions of interest. The Code Comparison Workshops are held every few years, and typically attract from 10 to 15 different code contributions from institutions worldwide. Usually a small number of test cases are chosen, with the intention of making a very detailed comparison among the different calculations at the workshop within a highly focused interactive forum. A dedicated website (hosted by Yu. Ralchenko at the National Institute of Standards and Technology [NIST]) was constructed to facilitate detailed code comparisons. These workshops are very useful to the atomic physics effort at LANL, since they provide important verification and validation of our atomic physics and kinetics modeling codes, which is the principal set of codes used to generate local-thermodynamic-equilibrium (LTE) and NLTE emissivities and opacities.

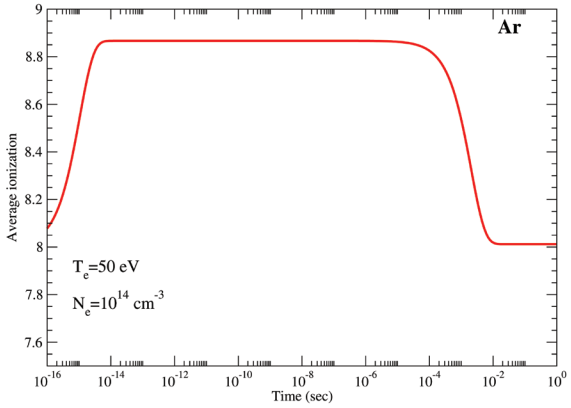

Fig. 1. ATOMIC calculations of the average ionization of Ar plasma as a function of time, at an electron temperature of 50 eV and an electron density of 10^{14} cm^{-3}. The initial condition of the plasma is that all population is in the $1s^1\ 2s^2\ 2p^6\ 3p^1$ levels of Ne-like Ar (corresponding to an average ionization of 8.0 at time=0).

The seventh workshop, which was held in Vienna, Austria in December 2011, compared four test cases, each of which offered some insight into plasma properties at various conditions. The LANL contributions to the workshop were made using the LANL suite of atomic physics codes and the ATOMIC kinetics code [2]. The calculations were made in a close collaboration of T-1 personnel (Gregory Armstrong, James Colgan, David Kilcrease, and Joe Abdallah) and XCP-5 staff members (Chris Fontes and Honglin Zhang). Much of the work performed for this workshop is expected to result in journal publications. In this report, we summarize the argon test case, with particular emphasis on the LANL calculations that were made. We also briefly describe the conclusions reached at the workshop.

The argon (Ar) test case for the NLTE-7 workshop was divided into two parts. Steady-state calculations were made for a range of electron temperatures (10 to 100 eV) and at two electron densities (10^{10} and 10^{20} cm^{-3}) to perform a detailed analysis of the role of dielectronic recombination and excitation-autoionization in the population kinetics. This case used a well-defined list of electronic configurations to facilitate the best comparison possible among the different submissions. The ATOMIC calculations for this test case, made using the configuration-average approximation, found that for a low electron density (10^{10} cm^{-3}) it was necessary to include configurations with principal quantum number up to n=18 to obtain fully converged autoionization and recombination rates. For the higher electron density case, comparisons were complicated by the need to include continuum lowering in the kinetics calculations–that is, lowering of the ionization thresholds of the atomic species due to plasma density effects.

The second Ar test case was a model time-dependent calculation inspired by the selective K-shell photoexcitation that can be accomplished using existing X-ray Free Electron Lasers (FEL). The

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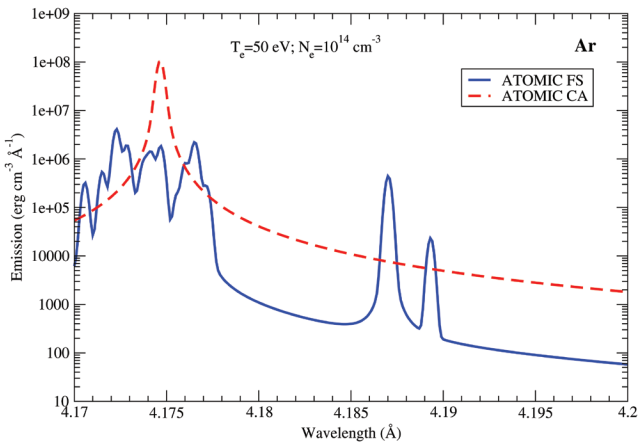

Fig. 2. ATOMIC calculations of the time-integrated emission spectrum of Ar plasma in an X-ray wavelength range, for an electron temperature of 50 eV and an electron density of 10^{14} cm^{-3}. The time-dependent kinetics calculations were made for the same initial conditions as in Fig. 1. We present configuration-average (red line) and fine-structure (blue line) calculations of the emission spectrum.

test case called for three calculations, at an electron temperature of 50 eV, and at three different electron densities (10^{14}, 10^{18}, and 10^{20} cm^{-3}). All cases were propagated in time with the initial condition that all population is assumed to be in the levels of the $1s^1\ 2s^2\ 2p^6\ 3p^1$ ($\equiv 1s^{-1}\ 3p^1$) configuration of Ne-like Ar. The ATOMIC contribution for this case again consisted of configuration-average and fine-structure calculations. Figure 1 shows the ATOMIC fine-structure calculations of the average ionization of the Ar plasma, as a function of time, for the 10^{14} cm^{-3} electron density case. This case exhibits some unusual features–in particular it was found that the plasma takes a relatively long time (0.01 s) to reach a steady state.

We found that the plasma, starting with all populations in the Ne-like stage, rapidly ionizes so that by a time of 10^{-14} s the average ionization rises to around 8.8. This behavior is due to the rapid autoionization of the $1s^{-1}\ 3p^1$ levels. However, about 25% of the destruction of these levels is also due to radiative decay from the 2p to 1s sub-shells, which gives rise to the X-ray spectra in the 4.17 to 4.2 Å wavelength range (see the time-integrated spectrum in Fig. 2). By a time of around 10^{-14} s, the $1s^{-1}\ 3p^1$ levels have completely depopulated. At this point the majority of the population is in the $1s^2\ 2s^2\ 2p^4\ 3p^1$ levels of fluorine (F)-like Ar. These levels decay via a two-step process (involving two E1 transitions) to the ground level of F-like Ar, and there is also some recombination into the Ne-like ion stage. The soft X-ray spectral region of 40-50 Å contains many spectral lines due to the 3l-2l' transitions in F-like Ar. At a time of 10^{-9} s (for the 10^{14} density case), most of the population is in the two ground levels of F-like Ar ($2p^5\ 2P_{3/2,1/2}$) and in the ground level of Ne-like Ar ($2p^6\ ^1S_0$). These levels retain population for a sizeable time, until recombination eventually forces all population back to the ground level of Ne-like Ar, at which time the plasma is in a steady state with an average ionization of 8.02. This latter value was confirmed by an explicit steady-state calculation.

Figure 2 shows the time-integrated emission spectrum of the Ar plasma, again for the 10^{14} cm^{-3} case. The ATOMIC fine-structure calculation is compared to the ATOMIC configuration-average calculation. This comparison shows clearly that the more detailed fine-structure calculation results in many more features in the emission spectrum in this X-ray wavelength range. As mentioned previously, the features in this region are due to transitions from the 2p to 1s sub-shells in Ne-like Ar, that is, transitions between levels arising from the $1s^1\ 2s^2\ 2p^6\ 3p^1$ configuration to levels arising from the $1s^2\ 2s^2\ 2p^5\ 3p^1$ configuration. The ATOMIC calculations were found to be among the most detailed of those presented at the workshop, and also underscored the importance of accurate atomic structure in constructing large-scale atomic kinetics calculations.

In conclusion, we have reported on detailed atomic kinetics calculations that were contributed to the NLTE-7 Code Comparison Workshop. Such calculations are instructive as a verification and validation of our kinetics-modeling capabilities, and also allow us to form collaborations within this community. We aim to contribute to NLTE workshops that are planned in the future.

[1] Fontes, C.J. et al., *High Energ Density Phys* **5,** 15 (2009).
[2] Magee, N.H. et al., *Proc 14th Topical Conf Atom Process Plasma,* 168 (2004).

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