LANL Contributions to the NLTE-7 Code Comparison Workshop–Three Test Cases

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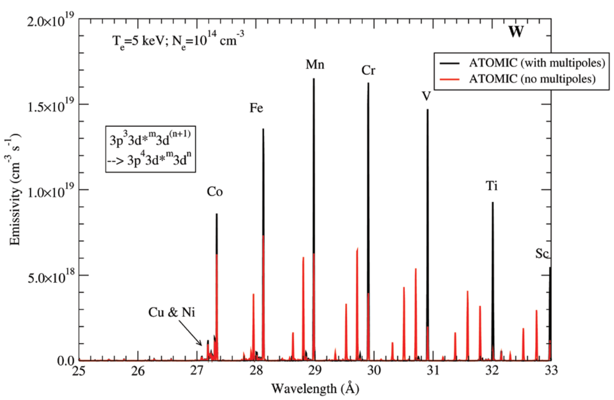
We report here on three of the LANL contributions to the recent NLTE-7 Code Comparison Workshop that was held in Vienna, Austria, in December 2011. The purpose of the workshop is to provide a detailed comparison among kinetics codes that simulate the properties of nonlocal-thermodynamic-equilibrium (NLTE) 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 nonlocal-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. Calculated emission spectra for W at an electron temperature of 5 keV and an electron density of 10^{14} cm^{-3}. We compare ATOMIC calculations that include multipole radiative transitions with ATOMIC calculations that omit multipole transitions. The labels on the emission features indicate the ion stage of W from which the transitions arose.



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 three workshop test cases, with particular emphasis on the LANL calculations made for each case. We also briefly describe the conclusions reached at the workshop.

The first test case considered the properties of neon (Ne) plasma. This case was designed to explore the convergence of kinetics modeling with respect to the highest principal quantum number included within a model. Relatively cold electron temperatures (10 and 30 eV), and a range of electron densities (10^{14}, 10^{18}, and 10^{20} cm^{-3}) were chosen, so that the plasma properties arose from open-shell ions, which are often more difficult to model. (In previous workshops, it was found that when the plasma conditions resulted in plasmas dominated by a closed-shell ion stage, most kinetics codes were in good agreement and so the comparisons were of limited value.) Calculations were then made for six different cases per temperature/density combination, where each of the six calculations used a different maximum principal quantum number in the list of configurations employed. Two further types of LANL calculations were made, one using a configuration-average approximation, and one using a fine-structure approximation. The latter set of calculations included full configuration-interaction between the configurations used, resulting in a set of fine-structure (LSJ) levels. When considering emission spectra, fine-structure calculations are

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generally more accurate than configuration-average calculations, but fine-structure calculations usually are much more time-consuming and computationally demanding to perform. The emission spectra from the ATOMIC calculations made at the various temperature/density cases resulted in a very large number of bound-bound transitions in almost all cases. Convergence of the emission spectra was obtained for almost all temperature/density cases using a model with a maximum principal quantum number of 12.

The next workshop case considered here was a study of krypton (Kr) plasma. This case was unique due to the availability of an experimental spectrum [3], measured several years ago in France, with which to compare the contributed calculations. These previously published experimental results were initially compared to kinetics calculations with only moderate agreement found between experiment and theory. Two sets of ATOMIC calculations were made for this case. Full fine-structure calculations were performed using a model containing a relatively small number of configurations for the ion stages of interest (centered around Ne-like Kr). A mixed unresolved transition array (UTA) calculation was also performed, in which the population kinetics were calculated within a configuration-average approximation, but where detailed lines were used to accurately model the emission spectrum. The ATOMIC calculations were in reasonable agreement with the measured spectrum. It became apparent that opacity effects modified the measured spectra and had to be taken into account in the calculations. Work is ongoing to improve how ATOMIC treats such opacity effects in the spectral generation.

The final workshop case chosen was an examination of tungsten (W) plasma. Tungsten is an important element in magnetic fusion plasma devices, and will be used extensively in the planned ITER (International Thermonuclear Experimental Reactor) device [4]. It is therefore important to understand the radiative properties of W at conditions expected in magnetic fusion plasmas. This is the third time W has been chosen as an NLTE workshop case. The large number of electrons in W, and the need for relativistic treatments of the atomic structure and collision processes in the W ions of interest complicate comparisons. Calculations were made for a range of electron temperatures from 2.5 keV to 12 keV, at an electron density of 10^{14} cm^{-3}. In Fig. 1 we present an example of the emission spectrum for the 5-keV case. Two sets of ATOMIC calculations are shown–one that includes higher-order multipole radiative transitions (i.e., those beyond the E1 transition, such as electric quadrupole [E2] and magnetic dipole [M1] radiative transitions) in the calculation, and one in which only E1 transitions are considered. We found that the inclusion of higher-order multipole transitions makes a significant difference to the spectrum, and in particular transfers population to the lowest (relativistic) configuration in each of the ion stages present at these conditions, so that fewer strong lines are observed when the multipole transitions are included. This was unexpected for two reasons. Usually, higher-order multipole transitions are expected to be important only at low ($\leq 10^{10}$ cm^{-3}) electron densities, and their inclusion typically results in more emission lines, not fewer. This study shows that the emission from W plasma at magnetic fusion conditions explores some very interesting atomic physics. The workshop comparisons showed that several bulk plasma properties (such as the average ionization of the plasma) were in reasonable agreement among the contributors, but that fine-structure calculations were required to fully characterize the emission spectra. More detailed studies of W plasma at these conditions are ongoing with ATOMIC.

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).
[3] Bastiani-Ceccotti, S. et al., *High Energ Density Phys* **3,** 20 (2007).
[4] Ralchenko, Yu. et al., *Proc 16th Int Conf Atom Process Plasma* **1161,** 242 (2009).

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