White Paper for *Frontiers of Plasma Science Panel*

Date of Submission:	20 June 2015

Indicate the primary area this white paper addresses by placing "P" in right column.
Indicate secondary area or areas by placing "S" in right column

	"P", "S"
• Plasma Atomic physics and the interface with chemistry and biology	P
• Turbulence and transport	
• Interactions of plasmas and waves	
• Plasma self-organization	
• Statistical mechanics of plasmas	

Indicate type of presentation desired at Town Hall Meeting.

	"X"
Oral	
Poster	X
Either Oral or Poster	
Will not attend	

Title:	Validation and Verification of Collisional-Radiative Models
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- ***Describe the research frontier* and importance of the scientific challenge.**

Advanced collisional-radiative (CR) models are extensively used in plasma spectroscopy to analyze plasma kinetics and spectra produced far from local thermodynamic equilibrium (LTE). Non-LTE atomic models also play a critical role in radiation-hydrodynamic simulations used to help design plasma experiments. Verification and validation (V&V) of these widely used and complex CR models are thus topics of significant interest. Experimental benchmarks for validation are challenging, requiring carefully designed and extensively diagnosed experiments where the general plasma parameters such as temperature and density are determined independently from the kinetic parameters, e.g., mean ion charge and detailed spectra. Temporal and spatial uniformity are also desirable and difficult to obtain. Thus, computational experiments and comparisons are one of the primary tools for V&V of CR codes.

Since the first meeting in 1996, the non-LTE (NLTE) Code Comparison Workshops [1-6] have become a venue for such efforts. These meetings not only allow the developers of CR models to test their codes under various plasma conditions but also provide an opportunity for the participants to have extensive discussions on outstanding problems, physical effects, numerical issues, and new experiments. It would not be an exaggeration to say that the noticeable progress in collisional-radiative modeling seen over the last two decades is no small degree related to the NLTE workshops.

- ***Describe the approach to advancing the frontier and indicate if new research tools or capabilities are required.***

The most important part of the NLTE workshops is the comparisons of different CR code calculations for test cases. The call for submissions that is prepared well in advance contains a number of cases characterized by an element and a set of temperatures and densities with possible addition of non-Maxwellian effects, opacities, external radiation field, and other non-equilibrium features. The calculated results are then submitted to be uploaded into a relational databases with a dedicated user-friendly interface allowing online comparisons. Examples of databases for NLTE-3 and NLTE-4 workshops can be found at http://nlte.nist.gov/SAHA and http://nlte.nist.gov/NLTE4.

The list of plasma kinetics parameters available for code comparisons is very extensive. The main group of parameters include quantities related to general characteristics (e.g., mean ion charge and central momenta, total statistical weights, radiative power losses), ion characteristics (e.g., ion populations, effective total and fractional ionization and recombination rates, net rates), level characteristics (e.g., level populations, ratios of populations to equilibrium populations, shell populations, occupation numbers, total and fractional population influxes and outfluxes) and synthetic spectra. The database interface allows one to perform detailed comparisons of any set of codes for any submitted case.

The comparisons and code differences are then discussed in detail during the meeting. The participants are then given three months to resubmit their improved calculations. Sometimes benchmark experimental measurements are brought in for comparisons and discussions on related spectroscopic diagnostics. An example comparing the measured radiative power losses of Kr at magnetic fusion conditions of (electron density $n_e = 10^{14}$ cm^{-3}) with the calculations from the NLTE-7 workshop is presented in figure 1.

- ***Describe the impact of this research on plasma science and related disciplines and any potential for societal benefit.***

Validation and verification of collisional radiative models has immediate and extensive impact on quality of plasma diagnostics and understanding of physical processes in various plasmas. From laser-produced plasmas to magnetic fusion to EUV lithography, NLTE modeling provides crucial input for reliable analysis of plasmas and their spectra.

References

1. R.W. Lee, J.K. Nash, Yu. Ralchenko. J. Quant. Spectrosc. Radiat. Transfer **58**, 737 (1997).
2. C. Bowen, A. Decoster, C.J. Fontes, et al., J. Quant. Spectrosc. Radiat. Transfer **81**, 71 (2003).
3. C. Bowen, R.W. Lee, Yu. Ralchenko. J. Quant. Spectrosc. Radiat. Transfer **99**, 102 (2006).
4. J.G. Rubiano, R. Florido, C. Bowen, et al. High Energy Density Phys. **3**, 225 (2007).
5. C.J. Fontes, J. Abdallah Jr., C. Bowen, et al. High Energy Density Phys. **5**, 15 (2009).
6. H.-K. Chung, C. Bowen, C.J. Fontes, et al. High Energy Density Phys. **9**, 645 (2013).

Figures

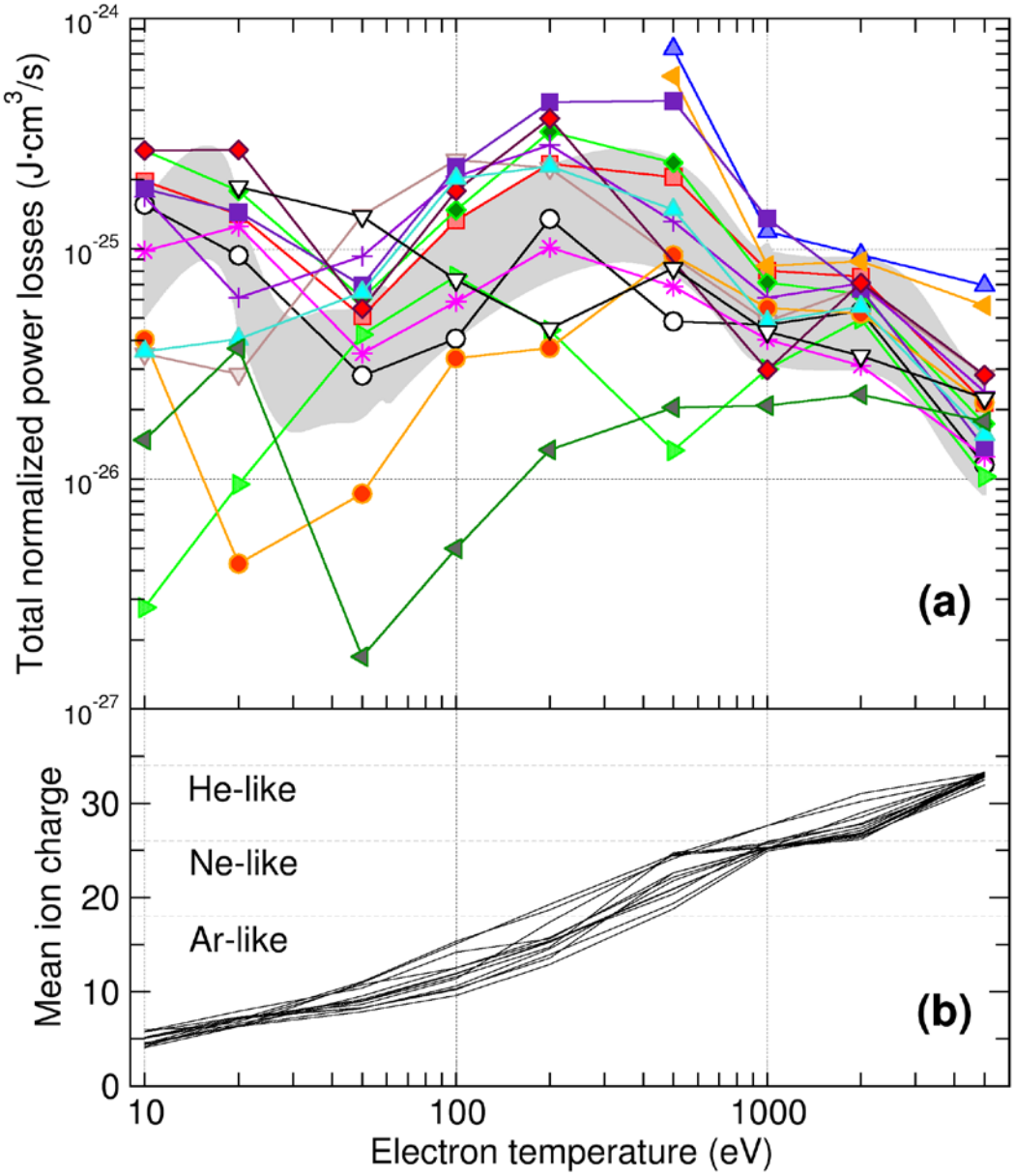

Figure 1 – Comparison of radiative power losses (a) and mean ion charges (b) for Kr at 10^{14} cm^{-3}. (a): shaded area – experimental data, lines with symbols – NLTE7 results; (b) lines – NLTE7 results.