Journal of Quantitative Spectroscopy & Radiative Transfer 99 (2006) 272–282

Journal of Quantitative Spectroscopy & Radiative Transfer

www.elsevier.com/locate/jqsrt

A comparison of detailed level and superconfiguration models of neon

S.B. Hansen[a,*], K.B. Fournier[a], C. Bauche-Arnoult[b], J. Bauche[b], O. Peyrusse[c]

[a]*Lawrence Livermore National Laboratory, P.O. Box 808, L-473, Livermore, CA 94550, USA*
[b]*Laboratoire Aimé Cotton, Campus d'Orsay, Bâtiment 505, 91405 Orsay, France*
[c]*CELIA, UMR 5107 Université Bordeaux I-CEA-CNRS, 33405 Talence, France*

Accepted 26 April 2005

Abstract

The superconfiguration (SC) approach to collisional-radiative modeling can significantly decrease the computational demands of finding non-LTE level populations in complex systems. However, it has not yet been fully determined whether the statistical averaging of SC models leads to a significant loss of accuracy. The present work compares results from two independent models: a detailed-level accounting (DLA) model based on HULLAC data and the SC model MOST. The relatively simple level structures of the K- and L-shell ions of the neon test system ensure a tractable number of levels for the DLA model but challenge the statistical assumptions of the SC approach. Nonetheless, we find fair agreement between the two models for average ion charges, SC populations, and various effective temperatures.

Keywords: Superconfiguration; Collisional-radiative; Non-LTE; Effective temperature

1. Introduction

The determination of effective temperatures that may govern the population distributions of energy levels in plasma ions has long held promise as a way to ease the significant computational burden of non-LTE modeling [1–3]. Recently, the collisional and radiative atomic processes that

*Corresponding author.
E-mail address: hansen50@llnl.gov (S.B. Hansen).

0022-4073/$ - see front matter
doi:10.1016/j.jqsrt.2005.05.021

couple energy levels have been shown to promote Boltzmann-like population distributions, i.e., populations varying as $e^{-\Delta E/T_{\mathrm{eff}}}$, among levels within electronic configurations and among configurations within larger ensembles called superconfigurations (SCs) [4]. The resultant effective temperature laws have been confirmed both analytically [2] and numerically [5–7], and suggest that some of the spectral character of ions in plasma can be adequately described using statistical methods rather than explicit treatment [8,9]. To exploit this simplification of the general collisional-radiative (CR) problem, various SC models which statistically average detailed level structure into large ensembles have been developed [10–12].

With the significant compression of level structure achieved through the SC approach, the ions can be described with a completeness that is computationally prohibitive for more detailed models [2,13,14]. The advantage of this compression is substantial: for many-electron systems, the number of fine structure levels can easily reach several million, pushing the limits of practical computing capabilities. Averaging these levels into a few hundred SC ensembles makes complex systems tractable. However, in order for the computational advantages of the SC approach to be fully utilized, it must be proven to be reliable. Recently, successful comparisons of the results of SC models with experiments have been made [2,6,11,14,15], and iterative models which split SCs into successively smaller ensembles have been shown to converge [13], suggesting internal consistency between detailed-configuration accounting (DCA) and SC models. But while the effective temperature law foundations of the SC approach have been numerically confirmed by detailed-level accounting (DLA) models (sometimes also called detailed term accounting, or DTA) [5,6], to our knowledge no direct and systematic comparison between the results of SC and DLA models has yet been made.

In this work, we present a direct comparison between two independent models of neon: the SC model MOST [12] and a DLA model. The low-Z test system was chosen so that a DLA model of reasonable size and sufficient completeness could be constructed for comparison with the SC model over a wide range of plasma conditions. While the relatively small modeled system accommodates the practical computational limits of the DLA approach, it challenges the statistical foundations of the SC approach: A few SCs in the present system contain only a single level, and the configurations and SCs of the modeled K- and L-shell ions are generally much smaller than those of the M-shell systems treated by MOST in previous work [6,12]. Nonetheless, MOST gives good agreement with the DLA model for average ion charges and ion populations across a wide range of temperatures and densities and predicts reasonable values for effective temperatures within ions and SCs.

In the following sections, we:

(1) describe the SC and DLA approaches and the modeled neon system;
(2) compare SC and DLA results for average ion charge, SC populations, and various effective temperatures; and
(3) develop an analytical formulation of a general effective temperature as a heuristic tool.

2. Description of models

Two CR models have been constructed to describe the non-LTE populations of neon ions in plasma. Both models are based on the same relatively simple and reasonably complete set of energy levels in neon, but while the DLA model treats each of more than 4500 fine-structure levels