Atomic Data and the Modeling of Supernova Light Curves

C J Fontes\textsuperscript{1}, J Colgan\textsuperscript{2}, H L Zhang\textsuperscript{1}, J Abdallah, Jr.\textsuperscript{2}, A L Hungerford\textsuperscript{3}, C L Fryer\textsuperscript{4} and D P Kilcrease\textsuperscript{2}

\textsuperscript{1} Computational Physics Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
\textsuperscript{2} Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
\textsuperscript{3} Theoretical Design Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
\textsuperscript{4} Computer, Computational and Statistical Sciences Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

E-mail: cjf@lanl.gov

Abstract.
We report on preliminary efforts to apply non-local thermodynamic equilibrium (NLTE) effects in the modeling of light curves for Type Ia supernovae. Significant differences are obtained for the opacity of iron at relevant conditions when account is taken of non-thermal electrons resulting from the down-scattering of gamma rays that arise from the radioactive decay of nickel and cobalt. These results provide evidence that a more precise, detailed investigation is warranted.

1. Introduction
The modeling of supernovae (SNe) requires applications from a wide range of numerical and physical disciplines, including hydrodynamics, radiation transport, nuclear physics and atomic physics. Atomic physics can play a particularly important role in determining the integrated light curves and frequency-dependent spectra generated by these objects. More specifically, the atomic opacity is of fundamental importance in determining the frequency and intensity of the radiation that reaches the Earth. The radiation created within a supernova (SN) travels through the surrounding ejecta, undergoing absorption and emission via the standard fundamental atomic processes that ultimately determine the characteristics of the escaping radiation. The opacity at a given point in a SN determines how much of the radiation will be absorbed by the material at that location.

The modeling of SNe has often involved the use of opacities computed under the assumption of local thermodynamic equilibrium (LTE) conditions (see, for example, [1]). The existence of high quality LTE opacity databases \cite{2, 3, 4} provides SN modelers with easy access to LTE opacities for a broad range of elements and mixtures. The generation of such robust LTE databases is possible because LTE conditions, as they pertain to opacities, can be characterized as a function of only temperature and density, allowing for the convenient tabulation of opacities over a wide range of predetermined conditions. On the other hand, non-LTE (NLTE) conditions can occur for a variety of reasons. For example, either the free-electron energy distribution, or...
the photon energy distribution, or both, could be non-thermal in nature, which would require a more specific description than the usual Maxwellian and Planckian distributions prescribed by LTE conditions.

Ultimately, one would like to know how NLTE physics affects the spectrum that is generated by a SN. At the moment, our approach for generating a detailed LTE spectrum involves the post-processing of our radiation-hydrodynamics (rad-hydro) simulations using very detailed (LTE) opacities [1]. This post-processing method assumes that the underlying structure of a SN has been calculated in a reasonably accurate manner, even though the opacity treatment is often rather crude (in order to reduce computational time) during the rad-hydro simulation. In order to ascertain whether the underlying structure is sensitive to NLTE effects, a method for accurately evaluating NLTE physics within a rad-hydro simulation is required. We are currently developing such an in-line NLTE physics approach. Any sensitivity in the opacity to NLTE effects could then be investigated in a more accurate, self-consistent manner to determine how the resulting spectra and light curves are impacted. We note that similar issues have been recently studied by Jack et al [5]. In this work, we focus specifically on the effect of non-thermal electrons on the opacity of iron at conditions found in Type Ia SNe. These SNe are of particular interest as their light curves led to the discovery of dark energy [6]. The non-thermal electrons result from Compton scattering with gamma rays generated from the decay of nickel and cobalt synthesized in the supernova explosion. These electrons provide a high-energy tail to the bulk Maxwellian distribution, which describes the majority of the free electrons characterized by a much lower temperature.

A discussion of the computational approach and atomic physics model used in the present study is provided in the next section, followed by a presentation of the iron opacity example mentioned above. We end with a brief summary.

2. Computational approach and atomic physics model
Our computational approach for calculating the NLTE opacity of iron employed the Los Alamos plasma kinetics code ATOMIC and the associated suite of atomic physics codes [7, 8, 9, 10]. These codes have been used to model plasmas for a variety of applications, ranging from fusion energy to astrophysically relevant cases, e.g. [11, 12, 13]. The Los Alamos suite of atomic physics codes can be used to generate fundamental atomic data for any ion stage of elements of interest. The ATOMIC code receives these data and solves the necessary system of equations to obtain level populations under LTE or NLTE conditions. These populations are then used to generate spectral quantities of interest, such as opacities. The reader is referred to the above references for specific details concerning the theory and computational methods implemented in these codes.

In carrying out this preliminary study, we generated a moderately detailed atomic physics model for the relevant ion stages of iron. The model included excited configurations that can be obtained from the ground configuration of a given ion stage via up to four-electron jumps, and the maximum principal quantum number was chosen to be \( n = 10 \). However, it was decided to calculate all of the atomic data in the configuration-average approximation, rather than in fine-structure detail, in order to keep the computational time at a reasonable level. See table 1 for the number of configurations chosen for the relevant ion stages in this work. Ion stages 2–7 were used in the LTE calculations described in the next section, while stages 3–11 were used in the NLTE calculations, in order to obtain a converged charge state distribution in each case.

3. Results and discussion
Our study of NLTE effects in Type Ia SNe focused on the effect of gamma rays on the free-electron energy distribution. These gamma rays are produced from the radioactive decay of nickel and cobalt, which also produces iron. While some of these gamma rays directly escape the SN, others undergo Compton scattering with the surrounding ions to produce high-energy
Table 1. Number of configurations for the ion stages of iron used in the present calculations.

| Ionicity | Number of configurations |
|----------|--------------------------|
| 2        | 6798                     |
| 3        | 8208                     |
| 4        | 9213                     |
| 5        | 9752                     |
| 6        | 9848                     |
| 7        | 9867                     |
| 8        | 9465                     |
| 9        | 8606                     |
| 10       | 7280                     |
| 11       | 5889                     |

Non-thermal free electrons. These non-thermal electrons introduce a high-energy tail into the free-electron energy distribution, altering the NLTE rate equations that must be solved to obtain the configuration populations, and ultimately the opacity of the surrounding iron.

In figure 1, we present a color contour plot of the energy distribution of these high-energy electrons at 60 days after explosion. This distribution was obtained from Monte Carlo transport of the gamma rays by explicitly tracking the energy they deposited during Compton scattering. The energy distribution is plotted as a function of distance from the center of the SN. The colors represent the values of the distribution function (in arbitrary units). Taking a vertical line-out provides the energy distribution for a given radius. For example, the energy distribution at a radius of $3 \times 10^{15}$ cm is presented in figure 2.

In order to determine if NLTE effects are important, we specifically considered SN conditions...
where such effects were expected to be most significant. We eventually chose the conditions represented in figure 2, i.e. 60 days after explosion and a radius of $3 \times 10^{15}$ cm. The mass density at this radius was sufficiently low ($2.7 \times 10^{-15}$ g/cm$^3$) that electron equilibration occurs very slowly, ensuring that the high-energy distribution persists for a reasonable amount of time. The bulk (LTE) temperature of the majority of the free electrons is 0.8 eV. Rather than choosing to combine the high-energy distribution in figure 2 with a bulk distribution at 0.8 eV, we simplified the calculation by modeling the high-energy tail as another Maxwellian at a higher temperature. The average energy per electron resulting from the distribution in figure 2 was calculated to be 325 keV. Setting that average energy equal to the usual thermal average, $3/2(kT_{\text{eff}})$, yields the effective temperature of the corresponding Maxwellian distribution, i.e. $kT_{\text{eff}} = 217$ keV. Similarly, the fraction of high-energy electrons, relative to the bulk distribution was obtained by extracting the number density of electrons contained in the distribution in figure 2 and dividing that value by the number density of electrons contained in a Maxwellian at the LTE conditions of 0.8 eV and $2.7 \times 10^{-15}$ g/cm$^3$. The resulting fraction of high-energy electrons was determined to be 2.5\%. Thus, the complete free-electron energy distribution is described by the bi-Maxwellian function displayed in figure 3.

This bi-Maxwellian distribution was then used in the rate equations to calculate the NLTE populations and corresponding opacity for iron at the conditions mentioned above. LTE results were also computed with a single Maxwellian distribution at 0.8 eV. First, we note that the use of the bi-Maxwellian distribution produced a significant shift of 3.66 charge states in the average ionization state, $\langle Z \rangle$, from an LTE value of 2.00 to a NLTE value of 5.66. The LTE and NLTE charge state distributions are presented in figure 4 for further comparison. The deviations in the LTE versus NLTE charge state distributions indicate that the corresponding opacities should also display meaningful differences. This expectation is clearly demonstrated in figure 5, which displays the LTE and NLTE opacities. The presence of high-energy free electrons in the NLTE calculation results in a significant (factor of $\sim 6.6$) enhancement to the free-free contribution to the opacity, which is dominant up to an energy of $\sim 0.02$ eV. This enhancement is reasonably consistent with Kramers’ formula for the free-free opacity, which scales approximately like $\langle Z \rangle^2$. (Note that $\langle Z \rangle_{\text{NLTE}} / \langle Z \rangle_{\text{LTE}} = 2.8$ in the present calculation.) At an energy of $\sim 0.1$ eV, the dominant contribution to the NLTE opacity switches over to scattering.
Figure 3. Plot of the bi-Maxwellian energy distribution used in this work to represent the NLTE case with thermal and non-thermal electrons.

Figure 4. LTE (black, solid curve) and NLTE (red, dashed curve) charge state distributions of iron for the conditions described in the text.

indicated by the horizontal portion of the curve. The NLTE scattering contribution is enhanced by approximately a factor of 2.9 relative to the LTE result, consistent with the formula for the Thomson-scattering opacity, which scales linearly with \( \langle Z \rangle \). As displayed in figure 4, several of the higher ion stages in the NLTE model contained significantly more population compared to the LTE results. These differences result in significant changes to the bound-bound and bound-free features. For example, the most prominent LTE bound-free feature occurs at \( \sim 32 \) eV (the M-edge from the Cr-like stage, ionicity 3 in figure 4). This feature is significantly reduced in the NLTE case, due to the negligible population in the Cr-like stage in the NLTE calculation. Instead, in the NLTE case, the M-edge features progressively increase in magnitude from the
Figure 5. LTE (black, solid curve) and NLTE (red, dashed curve) opacities of iron for the conditions described in the text.

Cr- to Sc-like stages, mimicking the relative strength of those stages (ionicities 3–6) in the charge state distribution of figure 4. On the other hand, we note that the K- and L-shell bound-bound and bound-free features are virtually identical when comparing the LTE and NLTE spectra. From a practical perspective, the differences in the iron opacity mentioned above could have an important effect on the light emitted by Type Ia SNe. For example, visible photons, which have energies of ~2–3 eV, make up a significant portion of the light curve. As noted above, the iron opacity is dominated by scattering in this energy range, and the NLTE value is enhanced by a factor of 2.9.

4. Summary
We have presented a preliminary study of the importance of NLTE effects on the opacity of iron under conditions found in Type Ia SNe. The NLTE effects investigated here are caused by non-thermal free electrons arising from Compton scattering with gamma rays. The presence of non-thermal electrons in the energy distribution resulted in significant changes to the average ionization and opacity of iron. These results provide justification for a more detailed study. Possible avenues of research include an expansion from configuration-average to fine-structure atomic models, consideration of a more realistic distribution function for the high-energy electrons when solving the rate kinetic rate equations, an investigation of the importance of this NLTE effect over a broader range of conditions that occur in Type Ia SNe, and implementation of an in-line atomic physics package that would make possible a more integrated approach to evaluating the relevance of NLTE effects in rad-hydro simulations.

Acknowledgments
This work was performed under the auspices of the U.S. Department of Energy by Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

References
[1] Fryer C L, Brown P J, Bufano F, Dahl J A, Fontes C J, Frey L H, Holland S T, Hungerford A L, Immler S, Mazzali P, Milne P A, Scannapieco E, Weinberg N and Young P A 2009 Astrophys. J. 707 193
[2] Magee N H, Abdallah J Jr, Clark R E H, Cohen J S, Collins L A, Csanak G, Fontes C J, Gauger A, Keady J J, Kilcrease D P and Merts A L 1995 Astronomical Society of the Pacific Conference Proceedings vol 78 ed S J Adelman and W L Wiese (ASP: New York) pp 51–55 (http://www.t4.lanl.gov/cgi-bin/opacity/tops.pl)

[3] Rogers F J and Iglesias C A 1992 Astrophys. J. Suppl. 79 507 (http://opalopacity.llnl.gov)

[4] Badnell N R, Bautista M A, Butler K, Delahaye F, Mendoza C, Palmeri P, Zeippen C J and Seaton M J 2005 Mon. Not. R. Astron. Soc. 360 458

[5] Jack D, Hauschildt P H and Baron E 2011 Astron. Astrophys. 528 A141

[6] Perlmutter S et al (The Supernova Cosmology Project) 1998 Nature 391 51

[7] Magee N H, Abdallah J Jr, Colgan J, Hakel P, Kilcrease D P, Mazevet S, Sherrill M, Fontes C J and Zhang H L 2004 Atomic Processes in Plasmas, Fourteenth APS Topical Conference, Santa Fe, NM ed J S Cohen, S Mazevet and D P Kilcrease AIP Conf. Proc. No. 730 (AIP: New York) pp 168–179

[8] Abdallah J Jr, Zhang H L, Fontes C J, Kilcrease D P and Archer B J 2001 Journal of Quantitative Spectroscopy & Radiative Transfer 71 107

[9] Hakel P, Sherrill M E, Mazevet S, Abdallah J Jr, Colgan J, Kilcrease D P, Magee N H, Fontes C J and Zhang H L 2006 Journal of Quantitative Spectroscopy & Radiative Transfer 99 265

[10] Fontes C J, Colgan J, Zhang H L and Abdallah J Jr 2006 Journal of Quantitative Spectroscopy & Radiative Transfer 99 175

[11] Colgan J, Abdallah J Jr, Sherrill M E, Foster M, Fontes C J and Feldman U 2008 Astrophys. J. 689 585

[12] Oelgoetz J, Fontes C J, Zhang H L, Nahar S N and Pradhan A K 2009 Mon. Not. R. Astron. Soc. 394 742

[13] Abdallah J Jr, Colgan J, Clark R E H, Fontes C J and Zhang H L 2011 J. Phys. B: At. Mol. Opt. Phys. 44 075701