NON-LTE LINE-BLANKETED MODEL ATMOSPHERES OF HOT STARS. II.
HOT, METAL-RICH WHITE DWARFS

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ABSTRACT

We present several model atmospheres for a typical hot metal-rich DA white dwarf, $T_{\text{eff}} = 60,000$ K, log $g = 7.5$. We consider pure hydrogen models, as well as models with various abundances of two typical "trace" elements—carbon and iron. We calculate a number of LTE and non-LTE models, taking into account the effect of numerous lines of these elements on the atmospheric structure. We demonstrate that while the non-LTE effects are not very significant for pure hydrogen models, except for describing correctly the central emission in Hz, they are essential for predicting correctly the ionization balance of metals, such as carbon and iron. Previously reported discrepancies in LTE abundance determinations using C\textsc{iii} and C\textsc{iv} lines are easily explained by non-LTE effects. We show that if the iron abundance is larger than $10^{-4}$, the iron line opacity has to be considered not only for the spectrum synthesis, but also in the model construction itself. For such metal abundances, non-LTE metal line-blanketed models are needed for detailed abundance studies of hot, metal-rich white dwarfs. We also discuss the predicted EUV spectrum and show that it is very sensitive to metal abundances, as well as to non-LTE effects.

Subject headings: line: formation — stars: abundances — stars: atmospheres — ultraviolet: stars —
white dwarfs

1. INTRODUCTION

In recent years, it has been amply demonstrated that the atmospheres of many hot DA white dwarfs, originally thought to be of pure hydrogen composition, or to have a stratified hydrogen-helium structure, are appreciably contaminated by heavier elements. Weak lines of C\textsc{iv}, Si\textsc{iv}, and N\textsc{v} were first detected in the IUE high-resolution spectra by Dupree & Raymond (1981) and Bruhweiler & Kondo (1983) in two stars, Feige 24 and G191-B28, which later became the prototypes of hot, metal-rich DA white-dwarfs. The above authors have presented evidence for their photospheric origin and suggested that these elements are supported against the downward diffusion by radiative levitation. More evidence came from X-ray observations. Kahn et al. (1984) first demonstrated that the observed data require the presence of some X-ray opacity in the photosphere. They discussed the role of "metals" (but they consider only C, N, and O), and concluded that these elements cannot be supported, according to the theoretical diffusion calculations by Vauclair, Vauclair, & Greenstein (1979). Therefore, they concluded that it is most likely helium which provides the missing opacity. Subsequent studies either elaborated this idea (e.g., Paerels & Heise 1989), or refined it by considering H-He stratified models (Koester 1989; Vennes & Fontaine 1992).

It soon became clear, however, that homogeneous models or even the sophisticated stratified H-He models do not provide a satisfactory explanation of the observed EUV and X-ray flux. The most dramatic demonstration of this effect was given by Barstow et al. (1993) who have analyzed ROSAT fluxes for about 30 DA white dwarfs and have shown that virtually all DA's with effective temperature hotter than about 40,000 K exhibit substantially lower EUV flux than predicted by pure hydrogen models. They also convincingly demonstrated that helium alone cannot provide sufficient EUV opacity and that the heavier elements have to be included. The opacity from several light elements up to $Z = 20$, mainly C, N, O, or Si, were considered in earlier studies (Paerels et al. 1986; Vennes et al. 1989; Vennes et al. 1991; Vennes 1992; Wilkinson et al. 1992).

Later, heavier elements were detected, namely Fe (Sion et al. 1992; Vennes et al. 1992), and very recently Ni (Holberg et al. 1994). Finally, several extremely metal rich DA's were discovered (Holberg et al. 1993). In other words, the presence of heavy metals in the hot DA white dwarf atmospheres seems now to be the rule rather than the exception.

In order to determine the metal abundances accurately, one needs a reliable model atmosphere and a satisfactory computational strategy to produce line profiles (or, at least, equivalent widths) to be compared to observations. Theoretical work in this area reflected faithfully the improvement in the observations associated with new data. Originally, since the heavier elements were considered as genuine trace elements, the model atmospheres were calculated assuming a simple chemical composition (mostly pure hydrogen, or a stratified H-He composition), while the heavier elements were considered only for spectrum synthesis. In other words, the metals were not allowed to influence the atmospheric structure (temperature).

When constructing a model atmosphere, an important question to ask is whether the models can be calculated under the assumption of local thermodynamic equilibrium (LTE). This assumption was traditionally adopted in view of the high surface gravity, and therefore high atmospheric densities, in the atmospheres of white dwarfs. Nevertheless, a high atmospheric density does not guarantee the validity of the assumption of LTE. For very high temperatures, the radiation field is very strong, and consequently the radiative rates of many atomic transitions may dominate over the corresponding collisional rates—a signature that the atmosphere may be susceptible to

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non-LTE effects. Auer & Shipman (1977) first discussed this problem in the context of analyzing EUV spectrum of the hot DA star HZ 43 and concluded that non-LTE effects are negligible. Wesemael et al. (1980) calculated an extensive grid of pure hydrogen model atmospheres and demonstrated that the non-LTE effects are indeed almost completely negligible for the UV and visible continua. Nevertheless, they found some non-LTE effects in the line centers of the first members of the Lyman and Balmer series. However, it is important to note that they computed the so-called NLTE/C models, wherein the lines are assumed to be in detailed radiative balance, and therefore their results for the hydrogen line profiles must be considered with caution.

Following the demonstration of Wesemael et al. (1980) that non-LTE effects are unimportant in the atmospheres of hot DA white dwarfs, most workers in the field have been using LTE models. Subsequent refinements in modeling proceeded in the direction of developing adequate approaches for computing models with self-consistent diffusion and helium stratification (Jordan & Koester 1986; Vennes & Fontaine 1992), rather than investigations of the non-LTE effects.

When it became clear that the heavier elements must absorb a large fraction of the EUV flux in the very region where the pure H models predict the maximum flux, it also became clear that this blocked flux must be redistributed to longer wavelength portions of the spectrum, thus invalidating the assumption that the heavy elements do not influence the atmospheric structure. This point is not only of academic interest; instead, it may be crucial in view of the need for accurate determinations of the basic stellar parameters (effective temperature, surface gravity, chemical abundances), for instance, for studying late stages of stellar evolution. Moreover, hot DA white dwarfs, like G191-B2B, are being used as radiometric standards for UV spectrophotometry, for instance with IUE and HST/FOS.

Since most of the important opacity sources are located near or shortward of the flux maximum, the corresponding ions which provide the opacity may be significantly influenced by non-LTE effects. This may be expected from the analogy with other stellar classes, as for instance the main-sequence early A-type stars (see Hubeny 1986). For this stellar class the non-LTE effects for hydrogen and consequently for the predicted visible and near-UV continua, were found to be negligible, while the far-UV opacity sources like C I are significantly influenced by non-LTE effects.

The only way to determine whether the metals influence the atmospheric structure, and whether the metal lines and continua are in turn influenced by the non-LTE effects, is to calculate a set of fully consistent non-LTE models in which the metals are allowed for explicitly; in other words, to calculate non-LTE line-blanketed model atmospheres. We note that the LTE line-blanketed model atmospheres for the DAO star Feige 55 were recently presented by Bergeron et al. (1993); they found that the effects of line blanketing on the atmospheric structure and the predicted Balmer line profiles are indeed quite important. However, as we demonstrate in § 2, the LTE line-blanketed models may overestimate the effects of EUV metal opacity, and therefore these results should be viewed with caution.

The only previously calculated non-LTE metal line-blanketed model atmospheres for white dwarfs are those by Dreizler & Werner (1992, 1993). Their models were also used by Holberg et al. (1993). Dreizler & Werner used the accelerated lambda iteration (ALI) method, applied first to model atmosphere construction by Werner (1986) and later refined by Werner (1989). Werner and collaborators then used the method extensively to compute model atmosphere for the PG 1159 stars, which are believed to be precursors of white dwarfs (for a review, see Werner 1992). The method, its advantages, drawbacks, and extensions, were discussed extensively in the previous paper in this series (Hubeny & Lanz 1995; hereafter Paper I), where we also presented details of our hybrid complete linearization/ALI method.

In their work published to date, Dreizler & Werner have concentrated on analyzing individual stars, and on presenting some representative models. In the present paper we adopt a different philosophy. We chose a single model to represent a typical hot, metal-rich DA white dwarf, $T_{\text{eff}} = 60,000$ K, log $g = 7.5$, with the two typical "trace" elements—carbon and iron. We then vary the abundances of these two species and calculate a number of LTE and non-LTE models, taking into account the effect of numerous lines of these elements on the atmospheric structure (§ 2). We also present a number of synthetic spectra (§ 3).

We do not intend to compare our results to observations of any particular star. Instead, the basic aim of this paper is to define the best strategy for future detailed analyses of the individual stars. Specifically, we will discuss the two following questions. First, under what conditions can the so-called trace elements be left out of the construction of the model atmosphere and included only in the spectrum synthesis. Second, is whether LTE a viable approximation, or, analogously, when does a detailed non-LTE description become necessary.

2. NON-LTE LINE-BLANKETED MODEL ATMOSPHERES

2.1. Method and Assumptions

We have calculated several model atmospheres under the assumptions of a plane-parallel geometry, and the radiative and hydrostatic equilibrium. In all these models we assume a homogeneous chemical composition. We do not assume the local thermodynamic equilibrium (LTE); instead, several selected energy levels of selected atoms and/or ions are allowed to depart from their LTE populations.

Since the aim of this paper is to investigate possible non-LTE effects, we adopt a relatively simple chemical composition, namely, an atmosphere composed of hydrogen, carbon, and iron. We vary the carbon and iron abundances all the way from zero to very high (large value, see the next subsection). Dreizler & Werner (1992, 1993) have used a "mean iron-peak element," which lumps together all the species between scandium and nickel. However, since the total abundance of all iron-peak elements except iron is about 10% of the iron abundance, the effect of missing iron-peak elements may be somewhat compensated by increasing the iron abundance by that amount. In any case, the mean iron peak element approach forces all elements to have the same ionization balance as iron, and therefore the results may be misleading.

We use the new numerical method developed in Paper I, called the hybrid complete linearization/accelerated lambda iteration (CL/ALI) method. It combines the advantages of both its constituents; its convergence rate (i.e., the number of iterations required to reach a given accuracy) is virtually as high as for the standard CL method, while the computer time per iteration is almost as low for the standard ALI method. The method formally resembles the standard complete linearization (Auer & Mihalas 1969; Hubeny 1988; Hubeny & Lanz
2.2. Calculated Model Atmospheres

We have computed a series of model atmospheres for the parameters $T_{\text{eff}} = 60,000$ K and $\log g = 7.5$ (cgs) that are representative of hot DA white dwarfs with trace metal lines in their spectrum. These models have either a pure hydrogen composition or they include carbon and/or iron with various abundances. Table 1 describes the H, H-C, H-Fe, and H-C-Fe models that we have considered. We stress that all models, with the exception of two pure H models, are the so-called NLTE/L models, wherein the lines are considered explicitly. The adopted abundances encompass typical values found in the literature, derived from LTE analyses. A few additional pure hydrogen model atmospheres have been computed for higher effective temperatures ($T_{\text{eff}} = 65,000$, 80,000, and 100,000 K). Table 1 also lists the number of non-LTE levels, transitions, lines, and frequencies which are included in the models.

Hydrogen is treated essentially exactly in the model atmospheres calculations. The first eight lowest levels are classical non-LTE levels, and all 28 lines between these levels are considered explicitly. All higher levels are lumped into a merged level within the occupation probability formalism, as described by Hubeny, Hummer, & Lanz (1994). The highest members ($n \geq 9$) of the Lyman and Balmer line series are then represented by the transitions from the first two levels to this merged level and are represented by appropriate opacity distribution functions (Hubeny et al. 1994). These two “superlines” are thus represented by a limited number of frequencies, 12 and 16 for the Lyman and Balmer superlines, respectively.

We have adopted a model atom for carbon with 12 non-LTE levels of C III, 12 non-LTE levels of C IV plus one level of C V. The C III model includes all singly excited levels 2s $n$l up to $n = 3$ (i.e., all levels with $E < 300,000$ cm$^{-1}$). The atomic data for C III have been extracted from the model atom described by Dreizler (1993) and updated by oscillator strengths from Allard et al. (1990). The C IV model atom includes all levels up to $n = 4$, and averaged levels for $n = 5, 6, 7$. We have extracted the data from a more detailed model atom built by Werner (1988), who has kindly made the data available to us.

Iron is treated as described in detail in Paper I. We consider four ions of iron, Fe IV to Fe VII. Fe IV is represented by 21 superlevels and 109 superlines, which represent 7897 genuine lines; Fe V is represented by 19 superlevels and 82 superlines, which represent 3670 genuine lines; Fe VI is represented by 11 superlevels and 31 superlines, which similarly represent 1100 genuine lines. Fe VII is considered as a one-level ion. The model atoms for these three ions have been built considering all the observed energy levels. However, an inspection of the Grotrian diagrams plotted in Figure 1 of Paper I reveals that we will miss many high-energy levels. At the studied temperature range ($T > 50,000$ K), the population of these levels may be significant. We treat these levels through the “upper sums” calculated by means of the appropriate partition function, as described by Hubeny (1988). For the iron partition functions, we use tables by Sparks & Fischel (1971). To verify the reliability of this approach, we have set up extended model atoms with two additional superlevels per ion, with one superlevel for each parity, representing all the higher (predicted) levels. The data for predicted levels were taken from Kurucz (1991). We have performed several test calculations and verified that the populations of the two additional superlevels are consistent with the predictions based on Sparks & Fischel partition functions, and that the computed atmospheric structure is insensitive to different treatments of the higher levels. The photoionization cross sections are taken from the detailed Opacity Project tables (Sawey & Berrington 1992), kindly made available to us by Sultana Nahar and Anil Pradhan.

2.3. Results

Table 1 lists the computed models. There are four groups of model atmospheres for $T_{\text{eff}} = 60,000$ K, $\log g = 7.5$: pure hydrogen models (LTE, NLTE/C and NLTE/L); H-C models (NLTE/L) with various carbon abundances; H-Fe models with various iron abundances; and H-C-Fe models, assuming the same abundance for carbon and iron, and varying this abundance. We have also calculated one H-Fe model (HFE4H) assuming all photoionization cross sections for iron given by the hydrogenic values, to demonstrate the effects of more accurate cross sections on the ionization balance of iron and the predicted spectrum.

The upper panel of Figure 1 shows the effect of various combinations of the carbon and iron opacity on the calculated temperature structure. Model H (pure-H) exhibits the classical non-LTE temperature rise at the surface, first discovered by Auer & Mihalas (1969; see also Mihalas 1978), and explained as an indirect effect of hydrogen lines on the heating rate in the dominant heating continuum. They discussed the effect in the
Comparing the H-C and H-C-Fe model, we see that the additional backwashing due to the presence of iron is very weak (less than 1000 K for log $m > -2$), while the surface cooling is much more pronounced than in the case of H-Fe model. This is explained by the fact that the presence of the carbon far-UV and EUV opacity decreases the non-LTE underpopulation of Fe$^{4+}$ (driving the ionization balance closer to LTE); therefore the efficiency of the iron line cooling increases.

The lower panel of Figure 1 compares various H-C-Fe models. We see that the iron opacity is almost inconsequential for $N$(Fe)/$N$(H) $\lesssim 10^{-5}$, while its importance determining the temperature structure dramatically increases for higher abundances. For $N$(Fe)/$N$(H) $= 10^{-3}$, the predicted temperature is higher by 1000 K for the whole range of depths where observed features originate (log $m < -1$); consequently, this will be reflected as a systematic error in determining the effective temperature.

Figure 2 displays the iron ionization balance for several calculated model atmospheres. The results are qualitatively similar to those by Dreizler & Werner (1993), their Fig. 5. The upper panel plots the LTE ionization fractions calculated for the pure H model; the other two panels show the non-LTE ionization fractions; the middle panel for the H-Fe model (HFE4); and the lower panel for the H-C-Fe model (HCFE4). The middle panel also shows the ionization fractions computed context of B stars, in which case the heating is driven by the Balmer lines, which provide an efficient channel to increase the $n = 2$ level population. In the case of very hot stars, an analogous effect was reported by Werner (1986). In this case, it is dominated by the Lyman lines and their influence on the Lyman continuum.

Including carbon with an abundance $N$(C)/$N$(H) $= 10^{-4}$ increases the temperature in the temperature minimum region by about 3000 K (due to the backwashing by carbon lines). We have found only a marginal cooling due to the C IV resonance lines, because the temperature is rather high and the dominant stage of ionization is C$^{4+}$. Consequently, a cooling due to the C IV resonance lines around log $m = -4$ is small compared to the direct cooling in the Lyman-$\alpha$ line (by a factor of 4–10).

A hydrogen-iron model (HFE4) exhibits classical features to be expected for a metal line-blanketed model—the backwashing (for log $m = -4$), and the surface cooling (for log $m < -4$). However, the effect is relatively small because the iron ions which provide most of the "blocking effect" (mainly Fe v) are underpopulated by non-LTE effects. The underpopulation is essentially driven by an imbalance of ionizations (given by a strong radiation field which originates at deep layers) and recombinations (which are determined by the local Planck function). This effect is usually called the "non-LTE ionization shift."
for model HFE4H, i.e., calculated assuming hydrogenic photoionization cross sections for iron. As discussed above, the basic non-LTE effect is the shift of the ionization balance toward Fe\(^{3+}\), so that the Fe\(^{4+}\) and Fe\(^{5+}\) ionization fractions are lower than in LTE. As pointed out above, the inclusion of carbon tends to drive the iron ionization fractions closer to LTE (compare the two lower panels). Finally, the effect of exact photoionization cross sections is important: they increase the ionization fractions of Fe\(^{3+}\) and Fe\(^{4+}\) by almost an order of magnitude for \(\log m = -1\), while they decrease the Fe\(^{5+}\) ionization fraction around \(\log m \approx -2\) by a factor of 3. The differences between LTE and non-LTE ionization fractions of iron are reflected in predicted line profiles, which will be discussed in the next section.

3. THEORETICAL SPECTRA

3.1. UV Continuum and the Hydrogen Lyman Lines

Figure 3 shows the short-wavelength portion of the Balmer continuum, the region of Lyman lines, and the Lyman discontinuity. The flux is normalized to that for the pure hydrogen NLTE/L model (model H) at \(\lambda = 5500\) Å. The upper panel shows a comparison of the pure-H LTE and non-LTE models. In agreement with previous studies (e.g., Wesemael et al. 1980), the effects of non-LTE were found to be rather small. A more interesting result is a comparison of the UV continua for models with varying iron abundance (middle panel). The flux in this wavelength region increases with increasing iron abundance, which is a consequence of the iron line backwarming. For comparison, we present in the lower panel a flux calculated for pure hydrogen models with higher effective temperatures. In order to predict the same UV continuum flux for a pure H model as for model HCFE4 (both the carbon and iron abundances equal to \(10^{-6}\)), we need to increase the effective temperature of the pure H model by about 7000 K. Therefore, neglecting the metal opacity in the model construction may lead to important systematic errors in the effective temperature determination.

Figure 4 shows a detailed profile of the hydrogen Ly\(\alpha\) line, which is traditionally used to determine the basic stellar parameters (Holberg, Wesemael, & Basile 1986). The upper left-hand panel shows the comparison of the LTE and non-LTE profiles. Non-LTE has an important effect in the line core, but in practice it is always obscured by the interstellar absorption. We show this effect in the lower left-hand panel, where the Ly\(\alpha\) profile is displayed for three values of the hydrogen column density \(10^{17}\), \(10^{18}\), and \(10^{19}\) cm\(^{-2}\). For typical values of \(N_H\) for nearby white dwarfs, \(10^{18}\), the interstellar absorption dominates in the line core. The lower right-hand panel shows the Ly\(\alpha\) profile for several metal line-blanketed models. In this case, there are some differences in the predicted line wings, which are, in principle, measurable. As in the previous case, we present also the profiles for the hotter pure H models. Similarly as in the case of the continuum flux, the hotter pure H models are able to simulate the blanketed models. The effective temperature must be increased by the same order of magnitude, several thousand degrees.

In conclusion, the influence of metals in determining the atmospheric structure is more important than non-LTE effects for metal abundances around or above \(10^{-5}\). In such cases, spectroscopic analyses based on pure-hydrogen models overestimate the effective temperature.

3.2. H\(\alpha\) Line

We consider separately the H\(\alpha\) line because this is the only feature which exhibits a striking non-LTE effect for pure H models, namely an appreciable central emission—see Figure 5. The effect was discovered observationally by Reid & Wegner (1988) for G191-B2B. They suggested several possible explanations, but not the correct one—the non-LTE effects. The only existing non-LTE models available at the time, those of Wesemael et al. (1980), where NLTE/C models for which the lines are assumed to be in detailed radiative balance. The correct explanation was given by K. Werner (1988, private communication) and Vennes, Thejll, & Shipman (1991), who have shown that the central emission is a consequence of a non-LTE temperature rise (see Fig. 1), which is produced only for NLTE/L models, where the lines (in particular the Lyman lines) are taken into account explicitly.

The upper left-hand panel of Figure 5 shows the LTE, NLTE/C, and NLTE/L profiles of H\(\alpha\). They illustrate the aforementioned effect—neither LTE nor NLTE/C models produce the central emission, because only the NLTE/L model exhibits the surface temperature rise. The upper right-hand panel displays the profiles for NLTE/L pure H model of various temperatures and shows that the effect increases with increasing effective temperature. However, the most interesting effect is shown in the lower panels of Figure 5, namely that the
Fig. 4.—Predicted Lyz profiles for various model atmospheres. Upper left panel: a comparison of the pure-hydrogen non-LTE (thick line) and LTE (dotted line) models. Lower left panel: an effect of interstellar absorption. Thick line: unattenuated stellar non-LTE profile for a pure-H atmosphere. Thin lines: profiles for column densities $N_H = 10^{12}$, $10^{14}$, and $10^{16}$ cm$^{-2}$ (progressively deeper profiles). Lower right panel: a comparison of the pure-H model and various H-C-Fe models. In the order of increasing flux are shown H, HCFe6, HCFe5, and HCFe4. Upper right panel: a comparison of several pure-H models with various effective temperatures: $T_{\text{eff}} = 60,000$ K (lower curve), 65,000 K (middle curve), and 80,000 K (upper curve). The spectra are convolved with a Gaussian (instrumental) profile with FWHM = 0.1 Å.

Fig. 5.—Predicted Hz profiles for various model atmospheres. Upper left panel: a comparison of the pure-hydrogen NLTE/L (thick line), NLTE/C (dashed line), and LTE (dotted line) models. Upper right panel: a comparison of several pure-H models with various effective temperatures: $T_{\text{eff}} = 60,000$ K (lower curve), 65,000 K (middle curve), and 80,000 K (upper curve). Two lower panels: a comparison of the pure-H model and various H-C-Fe models. In the order of increasing flux at the Hz center are shown H, HCFe6, HCFe5, and HCFe4. The right panel displays the enlarged central portion of the line.
height of the central emission increases with increasing metallicity! At first, one might expect that the central emission would decrease with increasing metallicity because the non-LTE temperature rise is diminished by the presence of metal lines. However, the non-LTE source function in the center of Hα is given roughly as \( S \approx (b_2/b_1)B_r \), where \( b_2 \) and \( b_1 \) being the non-LTE departure coefficients for the \( n = 2 \) and \( n = 3 \) levels of hydrogen, and \( B_r \) the Planck function at the Hα center. While \( b_2 \approx 1 \) for all models, \( b_1 \) is smaller for the metal line-blanketed model than for the pure H model (having values of the order of 1.04 for the former and 1.1 for the latter) at the depth of formation of the Hα center. Even such a seemingly small difference is able to override the difference in temperature (and therefore the value of \( B_r \)) between the two models. Finally, the decrease of \( b_2 \) in the metal-rich models is caused by a decrease of the photoionization rate in the Balmer continuum, due to the surface cooling and direct metal line blocking.

Similarly, a weak emission is predicted in the core of the Hβ line, while higher lines of the Balmer series do not show any central reversal for this effective temperature and gravity. In addition, their behavior is analogous to that of the Lyman lines and the UV continuum. When comparing the predicted line profiles of Hβ, Hγ, and Hδ calculated with pure hydrogen models and with metal line-blanketed models, we find that the wings are slightly narrower for blanketed models and that they can be reproduced with pure-hydrogen models with higher effective temperature. The predicted wings for the most metal rich model (HCFE4) are quite similar to the wings calculated with a pure hydrogen model with \( T_{\text{eff}} = 65,000 \) K.

3.3. Carbon Lines

The carbon lines were first detected in the spectra of DA white dwarfs in the high-resolution IUE spectra obtained by Dupree & Raymond (1982) and Bruhweiler & Kondo (1983). Henry, Shipman, & Wesemael (1985) have calculated a grid of LTE equivalent widths for a number of lines, including the C ii \( \lambda 1176 \) and C iv \( \lambda 1549 \) lines. These predicted equivalent widths were later used to derive carbon abundances for several DA stars (e.g., Vennes et al. 1991; Sion et al. 1992), but the authors found discrepancies between the abundance derived from the C ii and C iv lines. This was interpreted either as an argument in favor of a nonphotospheric origin of carbon, or as a consequence of non-LTE effects.

Our models include carbon self-consistently, so we may study the question of non-LTE effects on the carbon lines in detail. Table 2 lists the computed equivalent widths, and Figure 6 shows the theoretical curve of growth for the C ii \( \lambda 1176 \) and the C iv \( \lambda 1549 \) lines. We see that while the equivalent widths of the C iv lines are virtually unaffected by non-LTE effects, the predicted C ii \( \lambda 1176 \) multiplet is much weaker in non-LTE. Consequently, the LTE abundance determinations based on these lines will systematically underestimate the carbon abundance by about an order of magnitude (for \( T_{\text{eff}} \approx 60,000 \) K). This ionization shift points to the right direction to solve the previously reported abundance discrepancies.

The conclusion that the equivalent widths of the C iv resonance lines are not influenced by the non-LTE effects does not tell the whole story, however. When we compare the detailed line profiles, calculated assuming LTE and non-LTE for carbon, we see that they are very different—see Figure 7. The line cores are deeper in non-LTE, while the wings are shallower. We show two different LTE profiles. First, we calculate an LTE profile using a previously calculated LTE pure H atmosphere (which is analogous to the approach of Henry et al. 1985); and, second, an LTE profile for the non-LTE pure hydrogen model atmosphere. The latter profile shows a central reversal, which is a consequence of the above mentioned non-LTE temperature rise. This exercise illustrates two important conclusions. First, non-LTE effects are very important for...
describing the carbon resonance line formation and are able to explain previously found discrepancies in abundance determination based on the C\textsc{iii} and C\textsc{iv} lines. Second, inconsistent models (i.e., those assuming LTE line formation of carbon in a non-LTE atmosphere) may give misleading results.

3.4. UV Iron Lines

We present in Figures 8–10 synthetic spectra in the region between $\lambda = 1269$ and 1274 Å, which is rich in iron lines, and which moreover contains lines of three ionization degrees—Fe\textsc{iv}, Fe\textsc{v}, and Fe\textsc{vi}. Figure 8 shows a comparison of line profiles produced with various model atmospheres. The upper panel compares the predicted non-LTE and LTE line profiles; the line identifications are shown in Figure 10. Non-LTE line profiles are calculated for model HCFE4, and the LTE profiles are produced for the pure H LTE model (model HLTE). The differences between the LTE and non-LTE predictions are dramatic. The Fe\textsc{vi} lines are significantly stronger because the non-LTE ionization balance favours Fe$^{+}$ (see Fig. 2). The Fe\textsc{v} lines are weaker, again due to the non-LTE ionization shift toward Fe$^{+}$; and the Fe\textsc{iv} line at $\lambda = 1270.8$ Å almost disappears, because for Fe$^{+}$ the non-LTE underpopulation is even greater (Fe$^{+}$ is underpopulated with respect to Fe$^{+}$, and Fe$^{+}$ is underpopulated with respect to Fe$^{+}$).

The middle panel of Figure 8 compares the predictions for the H-Fe and the H-C-Fe models, both assuming non-LTE iron line formation. While the Fe\textsc{vi} lines are not influenced by the presence of carbon because Fe$^{+}$ is the dominant ionization degree, the Fe\textsc{v} lines are stronger for the H-C-Fe model because, as discussed in § 2.3, the ionization balance is closer to LTE when the carbon EUV opacity is considered.

This result dramatically demonstrates that the usual strategy, namely computing first a model atmosphere (either LTE or non-LTE) with a simplified chemical composition (typically pure H), and then determining abundances of individual elements, may be quite inaccurate because varying the abundance of one element (in this case carbon) influences the ionization balance, and therefore the predicted line strengths, of another element, such as iron.

The lower panel of Figure 8 compares the predictions using the accurate photoionization cross-sections for iron (model HFE4—full line), and the hydrogenic cross sections. As we have already discussed in § 2.3 (see also Fig. 2), the photoionization cross sections have an important effect on the ionization balance and therefore on the predicted line profiles. The Fe\textsc{iv} and Fe\textsc{v} lines are weaker in the case of the hydrogenic cross sections, due to an even higher underpopulation of these ions (see Fig. 2). The case of Fe\textsc{vi} lines is more interesting. Although the hydrogenic cross sections produce a somewhat larger population of Fe\textsc{vi} around the depth of formation (log $m \approx -2$), they produce a lower population in the upper layers. Therefore, the lines are formed deeper in the atmosphere where the temperature is higher; and the lines are therefore weaker.

Figure 9 compares the LTE and non-LTE predictions for various iron abundances. The upper panel is identical to the upper panel of Figure 8. Finally, Figure 10 compares the iron line profiles obtained by the self-consistent metal line-blanketed non-LTE models and the LTE iron line profiles computed for pure H non-LTE atmospheres of various temperatures. As we have already shown for the case of UV continuum and the hydrogen line profiles, predictions for hotter pure H models roughly mimic results for cooler, blanketed atmospheres. In the case of iron line profiles, the effects are much stronger. In order to obtain the LTE Fe\textsc{vi} lines of similar
strength as predicted with non-LTE, we have to go to an effective temperature as high as 80,000 K!

To conclude, the non-LTE effects are much more important for iron than for hydrogen. Our results indicate that for obtaining consistent line profiles for several ionization stages, and/or for attempting to constrain the temperature structure via the iron ionization balance, a non-LTE treatment is mandatory. We have also shown that the use of accurate photoionization cross-sections is important.

3.5. EUV Spectrum

We first study the influence of carbon on the EUV spectrum. Figure 11 displays a part of the EUV spectrum, \( \lambda < 450 \, \text{Å} \), for pure H and H-C models, both LTE and non-LTE. The carbon continuum opacity is very important; the C IV photoionization edges from the ground state and the first excited state at \( \lambda = 192 \) and 220 Å, respectively, are clearly visible already at \( N(\text{C})/N(\text{H}) = 10^{-6} \); and they remove almost all the flux below \( \lambda = 220 \, \text{Å} \) for \( N(\text{C})/N(\text{H}) = 10^{-4} \). Differences between the LTE and non-LTE predictions for the EUV carbon continua are apparent, but are not critical.

Figure 12 shows the influence of iron on the predicted EUV spectrum for several H-Fe models with different iron abundance. For comparison, we also show the flux for the pure H non-LTE model. The effects of iron opacity, as well as the influence of non-LTE are now quite dramatic. For \( N(\text{Fe})/N(\text{H}) = 10^{-4} \), the iron continuum opacity removes practically all the flux for \( \lambda < 180 \, \text{Å} \), where many ionization edges for low-lying states of Fe\textsuperscript{2+} are located. Even at relatively low iron abundance, \( N(\text{Fe})/N(\text{H}) = 10^{-6} \), a strong edge at \( \lambda = 130 \, \text{Å} \) (corresponding to photoionization from low-lying levels of Fe\textsuperscript{2+}), previously invisible, now appears to be important.
Strong line-like features at \( \lambda = 190, 200, 208 \, \text{Å}, \) etc., correspond to strong photoionization resonances in the iron cross sections. In the upper panel, we also display the spectrum computed assuming the hydrogenic cross sections, where the resonance features are obviously missing. Both the shape of the spectrum, as well as the detailed predicted features, are significantly different for \( \lambda < 230 \, \text{Å}, \) which shows that the use of detailed (e.g., Opacity Project) photoionization cross sections is mandatory for interpreting the EUV observations. We also note that the position of the flux maximum is displaced to longer wavelengths with increasing metallicity. Such a prediction should be readily verified on EUVE spectra.

Differences between LTE and non-LTE predictions in the EUV region are also dramatic. LTE predicts much lower flux, in particular for \( \lambda < 260 \, \text{Å}, \) This wavelength represents the position of several edges from mildly excited levels of \( \text{Fe}^{4+} \) and low-lying levels of \( \text{Fe}^{3+}, \) whose LTE populations are much larger than the non-LTE ones. The lower flux for \( \lambda > 260 \, \text{Å} \) follows from the fact that the LTE spectrum is calculated for a pure H model structure, which has a lower temperature in the continuum-forming layers. In order words, the metal-rich models have larger flux for \( \lambda > 200 \, \text{Å} \) because the flux below 200 Å is blocked by the iron and carbon opacity, and the absorbed flux must be redistributed to a longer wavelength region. This example shows dramatically the inadequacy of treating iron as a trace element, even for as low an iron abundance as \( 10^{-6}. \) As Figure 12 clearly indicates, the total integrated flux for LTE models is significantly lower than the flux stipulated by the effective temperature, simply because in the trace element approach, the flux is allowed to be absorbed at a certain wavelength region but is not allowed to be redistributed elsewhere. Self-consistent LTE line-blanketed models would solve this particular problem, but the resulting blanketing effect would be exaggerated due to an incorrect ionization balance of iron.

In Figure 13, we compare the EUV flux predicted for various H-C-Fe non-LTE models. For model HCFE4, with \( N(\text{Fe})/N(\text{H}) = N(\text{C})/N(\text{H}) = 10^{-4}, \) the effect of additional carbon opacity (the \( \text{C}^{3+} \) jump at \( \lambda = 220 \, \text{Å}, \) in particular) is large (cf. Fig. 11). For model HCFE5 (both C and Fe abundances 10 times lower), the effect of both \( \text{C}^{3+} \) jumps from the two lowest levels is still clearly visible, while the effect of carbon is marginal at \( N(\text{C})/N(\text{H}) = 10^{-6}. \)

4. CONCLUSIONS

We have calculated several pure hydrogen and metal line-blanketed hydrogen-carbon-iron model atmospheres for representative parameters of a hot, metal-rich DA white dwarf, \( T_{\text{eff}} = 60,000, \log g = 7.5, \) and various values of the carbon and iron abundances. The aim of this paper was to discuss two important issues: (1) for which features are the non-LTE effects important; and (2) to what extent do the trace elements influence the atmospheric structure; in other words, whether the usual strategy of computing first a simple (typically pure hydrogen) model atmosphere, and considering metals only in the spectrum synthesis, is reliable. To put it another way, are non-LTE metal line-blanketed model atmospheres really necessary for spectroscopic studies of these stars?

We have found, in agreement with previous studies, that the non-LTE effects are rather small in the context of pure hydrogen models. The only significant non-LTE effect is a central emission in Hz. However, this does not mean that non-LTE is
unimportant altogether for hot white dwarfs, as one might conclude. In contrast, non-LTE effects are crucial in predicting the profiles of the C \textsc{iii} and C \textsc{iv} resonance lines. Likewise, non-LTE effects on the iron ionization balance are quite dramatic. In addition, we have demonstrated that the iron ionization balance is significantly influenced by the opacity of light elements, as for instance carbon, if its abundance \( N(\text{C})/N(\text{H}) \geq 10^{-4} \).

The general conclusion of this study is that for low abundances of the "trace elements," i.e., below \( 10^{-6} \) relative to hydrogen by number, it is a reasonable approximation to calculate first a pure hydrogen model and then to include trace elements in the spectrum synthesis. However, for higher abundances, it is increasingly important to calculate self-consistent non-LTE line-blanketed model atmospheres. This procedure becomes mandatory if the abundances of the trace elements are above \( 10^{-5} \). The effective temperature of metal-rich DA white dwarfs derived with pure hydrogen models is indeed overestimated by several thousand degrees. A similar conclusion has been reached very recently by Bergeron et al. (1994) who studied the implications of the presence of small traces of helium in the atmospheres of DA white dwarfs. We stress also that the non-LTE line-blanketed model atmospheres should have a realistic overall chemical composition: the abundance of heavier elements in DA white dwarfs cannot be derived completely reliably with simple models including only one species at a time in addition to hydrogen. Finally, we have found that the accurate photoionization cross sections (including photoionization resonances), such as those provided by the Opacity Project, are very important for reliable predictions of the iron ionization balance. However, the Opacity Project data still need improvement, and work is underway to calculate more accurate data for all ions of iron (A. Pradhan, private communication).

In this exploratory study, we have made two major approximations. First, we have considered only carbon and iron. In future studies, we will consider also other light elements (N, O, Si, Al, etc.), and at least one other separate iron-peak element, namely nickel. We expect that although the inclusion of these elements will not influence the predicted UV and visible features significantly, it may strongly influence the predicted EUV spectrum.

The second major approximation is that of a homogeneous abundance distribution. Ideally, one needs to formulate an approach in which the elemental diffusion equation is solved self-consistently with the atmospheric structure, taking into account detailed non-LTE metal line-blanketing. Several years ago, such an undertaking would have seemed hopeless, but now, thanks to the development of fast and efficient numerical methods, such as the scheme introduced in Paper I, this problem may be investigated in the near future.

![Figure 12](image12.png)

**Fig. 12**—Predicted EUV spectrum for H-Fe models with various iron abundances (including Fe/H = 0, i.e. a pure-H model). Thick lines: non-LTE predictions; dotted line: LTE predictions; dashed line (upper panel): non-LTE predictions using the hydrogenic photoionization cross sections for iron (model HFE4H); thin full line: pure-H model. Upper panel: Fe/H = 10^{-4}. Middle panel: Fe/H = 10^{-3}. Lower panel: Fe/H = 10^{-5}. Small triangles at the top indicate the positions of averaged photoionization edges for the superlevels of Fe iv (uppermost row), Fe v (middle row), and Fe vi (lower row). The spectra are convolved with a Gaussian profile of FWHM = 2 Å, corresponding roughly to the EUVE instrumental profile.

![Figure 13](image13.png)

**Fig. 13**—A comparison of predicted EUV spectra for non-LTE H-C-Fe models (heavy lines), and non-LTE H-Fe models (thin lines), with various carbon and iron abundances, as indicated in the corresponding panels. The spectra are convolved with a Gaussian profile with FWHM = 2 Å.
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