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Abundances of light elements in metal-poor stars

II. Non-LTE abundance corrections*

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Abstract. We present non-LTE corrections to abundances of Fe, O, Na, and Mg derived from LTE analyses of F-K stars over a broad range of gravities and metal abundances; they were obtained using statistical equilibrium calculations and new model atoms. Line opacity was considered by means of an empirical procedure where it was attributed to a veil of weak Fe I lines; in the case of solar-type dwarfs, results were compared with those obtained using (LTE) mean intensities computed from OSMARCS models. We think that the empirical procedure produces better results for metal-poor stars, while mean intensities should perhaps be preferred for the Sun (where departures from LTE are anyway not very large). Collisions with both electrons and H I atoms were considered. Since cross sections for this second mechanism are very poorly known, we calibrated them empirically by matching observations of RR Lyrae variables at minimum light (discussed in Clementini et al. 1995). These stars were selected because non-LTE effects are expected to be larger in these stars than in those usually considered in the study of the chemical evolution of the Galaxy (cool main sequence and red giant branch stars). We found that different non-LTE mechanisms are important for the different species and transitions considered; on the whole, our calculations yielded moderate corrections to LTE abundances for high excitation O lines in warm dwarfs and giants, Na and Mg lines in giants and supergiants, and Fe I lines in F-supergiants (where corrections becomes very large for IR O lines). Non-LTE corrections were found to be negligible in the other cases studied.

Key words: stars: abundances – stars: atmospheres – stars: Population II – Sun: abundances

1. Introduction

In the present series of papers, we are studying the abundances of light elements (C, N, O, Na, and Mg) in metal-poor stars, a basic constraint for models of the chemical evolution of our Galaxy (Wheeler et al. 1989). An important concern in the derivation of accurate abundances for these (and other) elements is the possible presence of systematic errors related to the usual assumption of Local Thermodynamic Equilibrium (LTE). This could be tested by appropriate determinations of statistical equilibrium (SE), that should eventually substitute LTE abundance analysis. However, as extensively discussed by Bruls et al. (1992), the interpretation of the results of SE requires consideration of a variety of physical processes, including line scattering and photon loss, photon suction, ultraviolet overionization, infrared overrecombination, and ultraviolet line pumping. The relevance of each of these mechanisms for a given species depends on the atomic structure, on the cross-section for the most relevant transitions, and on the intensity of the radiation field at the corresponding wavelengths. Their complex interplay may cause a large variety of behaviours, which are difficult to predict *a priori*, and determines the size of the model atom required for realistic SE computations. Furthermore, the reliability of SE calculations for late-type stars is still not adequate, mainly for two reasons:

- It is difficult to describe realistically the UV ionizing flux due to the large number of atomic and molecular lines present. This concern heavily hampered old determinations of SE (as well as theoretical calibrations of UV and blue colours); however, important progresses have been achieved by use of the very extensive line list prepared by Kurucz (1992). Model atmospheres computed using this line list reproduce the observed solar flux distribution (Kurucz 1992; Edvardsson et al. 1993) rather well, although problems still exist (see e.g. Bell et al. 1994).
- Steenbock & Holweger (1984) have shown that in several cases, the most important thermalizing process in cool stars is collision with neutral H atoms; unfortunately, cross sections for this process are known only at an order of magnitude level.

For these reasons, it is not easy to disentangle non-LTE effects from other sources of uncertainties in abundance analyses. Occasionally, various authors underlined the relevance of depar-

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* The Tables 1 to 12 are available only in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsweb.u-strasbg.fr/Abstract.html

tures from LTE in the formation of lines in the atmospheres of solar and late-type stars: e.g. O permitted IR lines, that can be easily observed in metal-poor dwarfs, likely form in non-LTE conditions when they are rather strong (Baschek et al. 1977, Eriksson and Toft 1979). However, no reasonably consistent discussion for stars having a wide range of atmospheric parameters has been carried out, so reliable use of existing SE results in the analyses of stars spanning a range in the fundamental parameter is difficult. We try to address this point in this second paper of this series, where we discuss the effects of possible departures from LTE in the formation of lines of Fe, O, Na, and Mg in dwarfs, giants and RR Lyrae variables of various metal abundances.

Our non-LTE corrections are based on SE solutions obtained by using MULTI code of Carlsson (1986, v. 1.3); this code is based on the operator perturbation method by Scharmer & Carlsson (1985). The model atoms used in this paper are described in Sect. 2. Critical aspects in our calculations are examined in some detail: in Sect. 3 we compare the results obtained using our empirical line opacities, based on fits of the flux distribution of the Sun and Arcturus, with those obtained using theoretical computations of mean radiation intensities in model atmospheres. In Sect. 4 we discuss the relevance of collisions with HI atoms, and envisage an empirical parametric procedure to estimate their cross sections based on results obtained from the analysis of RR Lyrae variables (Clementini et al. 1995). The main features of our determinations of SE are described in Sect. 5, while in Sect. 6 we estimate the corrections to the LTE abundances for a number of spectral features due to Fe, O, Na, and Mg, often used in abundance analysis of cool stars.

Our SE calculations are mainly aimed to the determination of corrections to abundances obtained assuming LTE. For this purpose mainly relatively weak spectral lines, formed in the photospheres, are used. Therefore, our discussion is focussed on results obtained for the photospheres (for various reasons, our results are not adequate to discuss chromospheric features). Throughout this paper we generally used the latest version of Kurucz (1992) model atmospheres[1]. However, other model atmospheres (mainly the new version of MARCS model atmospheres: Edvardsson et al. 1993) were used when discussing the contribution of lines to opacity, because tables of mean radiation intensities throughout the atmospheres were available in a suitable format. Note that all these models were computed assuming LTE. While of course this assumption is not consistent with the results presented in this paper, realistic non-LTE model atmospheres for late-type stars are beyond current computational capabilities, and are then not available.

2. Model atoms

In this section we describe the model atoms used in our analysis. Most features were common to all models. Each level was collisionally coupled with all other levels. Coupling with the continuum occurred through photoionization/recombination and collisions. Radiative bound-free transitions are considered in detail. Lines were computed using a Voigt profile; radiative broadening was obtained from lifetimes, while the van der Waals broadening was computed from the Unsöld (1955) formula, with enhancement factor E given by:

$$E = 1 + 0.67 EP$$

(Simmons & Blackwell 1982), where EP is the lower excitation potential in eV. Stark broadening (not very important, anyway) was also included. Save when explicitely mentioned, radiative data were from the OPACITY project (Seaton 1987), as available at the Strasbourg CDS (Cunto et al. 1993). Collisional ionization cross sections were determined using the formula by Bely & Van Regemorter (1970), using the (generalized) oscillator strengths obtained from photoionization cross sections. For permitted transitions, cross sections for collisional excitation were obtained using the formula by Van Regemorter (1962); for forbidden transitions, they were arbitrarily set equal to one tenth the value for an allowed transition.

2.1. The Fe I model atom

Fe I has a complicate atomic structure, having more than 100 levels with an excitation energy below 5 eV. We used a model atom similar to that considered by Takeda (1991). Takeda's model originally included 50 levels and 84 bound-bound transitions; we however added 9 more arbitrarily equispaced levels between the highest energy level of Takeda and the continuum. Due to the small energy difference (about 700 cm^{-1}), these levels are strongly collisionally coupled each other and with the continuum. Hence, they simulate the *quasi*-continuum of high energy levels. To test the impact of the size of the model atom on the results of our computations, we also performed calculations with smaller model atoms. Results provided by our extended 60-level model atom closely reproduced those obtained with a 40-level one, while departures from LTE were much larger in models with less than 40 levels; we then concluded that 60 levels should be enough to adequately describe excitation and ionization of Fe in the photosphere of the programme stars. The energy levels of our Fe model atom are listed in Table 1 (available only in electronic form), while the bound-bound transitions treated in details are listed in Table 2 (available only in electronic form).

Opacity Project data for neutral and singly ionized Fe are not available at CDS. Hence, our model atom was constructed using data gathered from the literature. While oscillator strengths for several Fe I transitions are well determined, few experimental and theoretical determinations of photoionization and electron collision cross sections existed. Threshold cross section for photoionization A_0 from the ground level of Fe I has been determined experimentally to be $A_0 = 5.0 \times 10^{-18}$ cm^2 (Lombardi et al. 1978); this value is larger than that computed by Kelly & Ron (1971, 1972) by means of Hartree-Fock and many-body pertubation approximations ($A_0 = 2.2 \times 10^{-18}$ cm^2). The experimental value was preferred, since large uncertainties are present in the theoretical estimates for a complicate atomic system like Fe. The experimental cross section is not much different from the value adopted by Athay & Lites (1972:

[1] CD-ROM 13 version

$A_0 = 6.3 \times 10^{-18}$ cm^2). Whenever possible, cross sections for photoionization from excited levels were taken from Athay & Lites (1972); for the other levels they were obtained using the hydrogenic approximation.

Accurate oscillator strengths gf's for bound-bound Fe I transitions were obtained by means of an experimental absorption technique by the Oxford group (see e.g. Blackwell et al. 1979), and by combining lifetimes and branching ratios by Bard et al. (1991), Bard & Kock (1994), and O'Brian et al. (1991). Whenever possible, these gf's were adopted. They were complemented with emission data from May et al. (1974), and semiempirical gf's computed by Kurucz & Peytremann (1975). These last gf's display large errors, which are functions of the multiplet. Therefore, for each individual multiplet they were corrected for the average difference with values given by the cited experiments.

The adopted collisional cross sections for Fe are about one order of magnitude smaller than those adopted by Saxner (1985), which were taken from Athay & Lites (1972). However, they are in fair agreement with the only experimental data we are aware of (Kolosov & Smirnov 1983).

2.2. O I

Our O I model atom is similar to that of Kiselman (1991, 1993), which, in turn, was based upon the much larger model atom of Carlsson & Judge (1993, hereafter CJ93). Our final model consists in 13 bound levels plus the continuum (see Table 3, available only in electronic form). According to Kiselman (1993), a decrease from 44 to 13 bound levels does not significantly affect the strength of the 777 nm triplet (the change is ∼3% in the EWs), which is the main feature we are interested in. 28 radiative transitions (see Table 4, available only in electronic form) among the levels were treated in detail. Energies and statistical weights were from the compilation of Bashkin & Stoner (1975).

Electron collisional cross sections for excitation and ionization from the ground level were from the critical compilation of experimental work by Laher & Gilmore (1990). Cross section for the $2p^4\,{}^1$D – $2p^4\,{}^1$S^o transition were derived from the theoretical formulae of Sawada & Ganas (1973).

According to Bahcall & Wolf (1968), collisions with protons can have at least the same relevance as electron collisions for transitions among the fine structure levels of the ground term, while they are negligible for the other transitions (see CJ93). We computed these proton collisional rates using the formulae quoted by Haisch et al. (1977); we then added to these values the rates due to electron collisions computed using the theoretical formulae given by Saraph (1973).

Since the charge-exchange reaction:

$$O^0(2p^4\,{}^3P) + H^+ \rightarrow O^+(2p^3\,{}^4S) + H^0({}^2S) \qquad (1)$$

can dominate over photoionization and ionization by electron impact under some conditions (Field & Steigman, 1971), we computed the rate of this reaction, using the values tabulated in Osterbrock (1974). The rate was then summed to the ionization rate for electron collisions.

2.3. The Na I model atom

Several model atoms for Na I have been presented in the literature. A rather simplified model was adopted by Kelch (1975) and Kelch and Miller (1976) to study Na overionization in the Sun and in other late-type stars. A more extensive and accurate model atom was used by Gehren (1975) and Caccin et al. (1980) to investigate the use of Na lines as probes of the solar chromosphere. Sakhibullin (1987) extended this model to 19 levels plus the ground level of Na II to investigate departures from LTE in the Sun and in late type population I stars. More recently, Bruls et al. (1992) made an extensive discussion of non-LTE effects for the resonance lines using an 18-levels model atom; this topic has been also investigated by Caccin et al. (1993) with a very simplified atom but updated collisional cross sections. Finally, Drake et al. (1992) used a very extended model atom (47 levels plus the Na II continuum) to discuss the observed Na excesses in some globular cluster giants.

The model we adopted has the same levels of the model by Sakhibullin (see Table 5, available only in electronic form); we however considered a larger number (=32) of radiative transitions between these levels (see Table 6, available only in electronic form). Laboratory and theoretical data for sodium are very abundant, due to its rather simple atomic structure and the possibility to accurately test the computational methods used. It is then possible to prepare a rather realistic model atom.

Experimental data about collisional ionization cross sections are available only for the ground level (McFarland and Kinney 1965; Zapesochnyi and Aleksakhin 1969). They agree with theoretical predictions based on the Born approximation (Peach, 1966; Bates et al. 1965).

Both theoretical and experimental data on electron collision excitation of Na atoms are rather abundant. For excitation from the ground level, we selected whenever possible the experimental results by Phelps and Lin (1981), except for the 3S-3P and 3S-3D transitions, for which more accurate data exist (Stumpf and Gallagher 1985). For the remaining transitions, we used the (empirically corrected) theoretical results by Park (1971). In the case of forbidden transitions, rates were set at one tenth the value for an allowed transition.

2.4. The Mg I model atom

Recently, there have been various calculations of SE for Mg; they were motivated by the use of the recombination line at 457.1 nm as a diagnostic for the solar chromosphere (Mauas et al. 1988), by the observation that Mg I Rydberg lines are in emission in the solar spectrum (Carlsson et al. 1992), and by the relevance of Mg in the atmospheres of A-type stars (Gigas 1988). While our motivation is different, these papers were used as sources of data in the construction of the model atom and as a guide in the interpretation of the results of our own calculations.

Our calculations of SE for Mg were based on a rather extended model atom, including 43 levels plus the continuum (i.e. all levels up to a principal quantum number of n=9 listed by Bashkin & Stoner 1975), and 30 bound-bound radiative transitions (see Tables 7 and 8, available only in electronic form). For the purposes of this paper, this model atom should be a fair representation of the Mg atom: in fact we found that the results provided by this extended model atom were qualitatively very similar to those obtained with a smaller model atom including only 17 levels, departures from LTE being reduced by roughly a factor of two.

Line parameters and photoionization cross sections were taken from the Opacity Project data. For the intercombination $3s^1\mathrm{S}{-}3p^3\mathrm{P}$ transition we adopted the experimental value determined by Kwong et al. (1982); for the $3s^1\mathrm{S}{-}4p^3\mathrm{P}$ and $3p^3\mathrm{P}{-}4s^1\mathrm{S}$ transitions, the values determined by Laughlin & Victor (1974) were considered.

3. UV opacity

3.1. Empirical line opacities

UV radiation field within the upper layers of the atmospheres of late type stars, computed without consideration of the line opacity, is severely overestimated. From the point of view of determination of ionization and excitation equilibria, the net result of neglecting line opacity is to overestimate photoionization events, producing departures from LTE more severe than those likely to occur in real stellar atmospheres. Throughout this paper we included the effect of line opacity by means of an empirical approach that is described in this subsection. As noticed by the referee, the approach used in this paper (while a clear improvement with respect to computations where the line opacity is neglected) is still quite rough. In the next subsection we discuss the drawbacks of this approach, and compare the results obtained with this technique with those provided by a fully theoretical approach, in which radiation intensities were computed at each optical depth, taking into account the line opacity by means of an opacity-sampling method. While we acknowledge limitations in the present approach, we think their impact is not large for the stars considered in the present series of papers mainly because errors possibly present are largely offset by our use of a multiplicative factor to collisional cross sections adjusted in order to match observations (see next section).

In our primary approach, observed monochromatic fluxes from stars were matched with those computed from model atmospheres with parameters appropriate for the observed stars, considering known continuum opacity sources, but with an extra opacity due to a veil of metal lines of excitation potential χ_l (in eV) (a similar approach was used by Magain 1983). Iron was taken as a representative metal in this respect. At each optical depth, the contribution c_l of this last source to the total opacity (per cm^{-3}) was given by:

$$c_l = 10^{-14.825}\, c_{l,0}\, \frac{1}{(m_\mathrm{H}\mu)}\, \frac{n(\mathrm{Fe\,I})}{n(\mathrm{H})}\, \frac{10^{-\chi_l\theta}}{Q(T)}, \qquad (2)$$

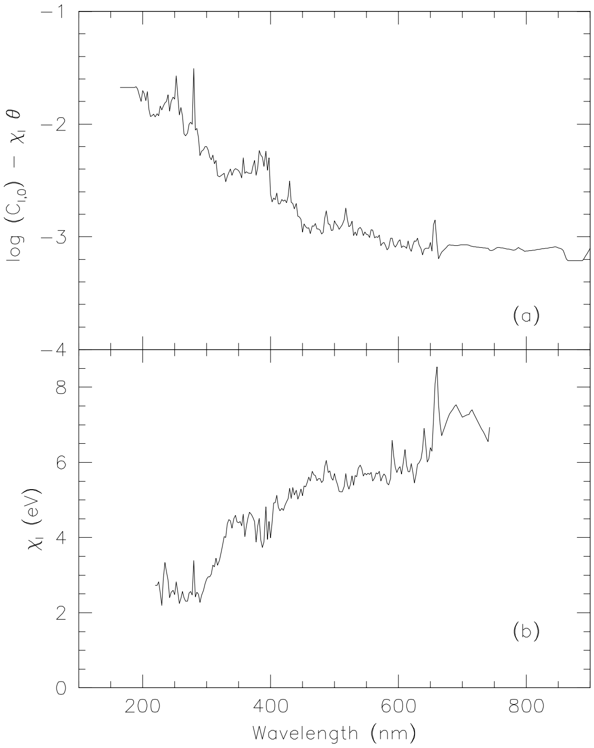

Fig. 1a and b. Run of the empirical line opacities parameters with wavelength: **a** excitation potentials χ_l and **b** constant terms $c_{l,0}$. In the run for the constant term, the Boltzmann term for a temperature $\theta = 5040/T = 1$ is included

where $c_{l,0}$ was a constant (dependent on wavelength), T was the temperature ($\theta = 5040/T$), $Q(T)$ was the partition function (for Fe I), n(Fe I) and n(H) were the number of neutral iron and the total number of hydrogen atoms, m_H was the hydrogen atom mass, μ was the mean molecular weight, and the numerical factor was used for consistency with the usual expression for line opacity (where $c_{l,0}$ is replaced by the oscillator strength gf times the line profile $\phi(\lambda)$).

At this step, the value of the excitation potential χ_l was arbitrary. In fact, for any value of χ_l, the observed flux might be reproduced by an appropriate value of $c_{l,0}$. However, the slope of the line of solutions in the plane $(\chi_l, \log c_{l,0})$ was an estimate of the excitation temperature for typical (Fe I) lines in the stellar spectrum. Therefore, solution lines for stars having different temperatures have different slopes, and the intersection between two such lines provides an estimate of the value of the excitation potential of Fe I lines adequate to describe the temperature dependence of the line opacity at the considered wavelength. We repeated this procedure averaging fluxes over a set of equally spaced (2 nm) wavelengths, providing a table of values of the excitation potentials χ_l and of the coefficients $c_{l,0}$.

Fig. 1 displays the runs of the excitation potentials χ_l and of the constant terms $c_{l,0}$ obtained using the observed monochromatic solar center intensities (Labs & Neckel 1967; Kohl et al. 1973, 1974), and the monochromatic fluxes from Arcturus (Honeycutt et al. 1977; Strecker et al. 1979; Carpenter et al.

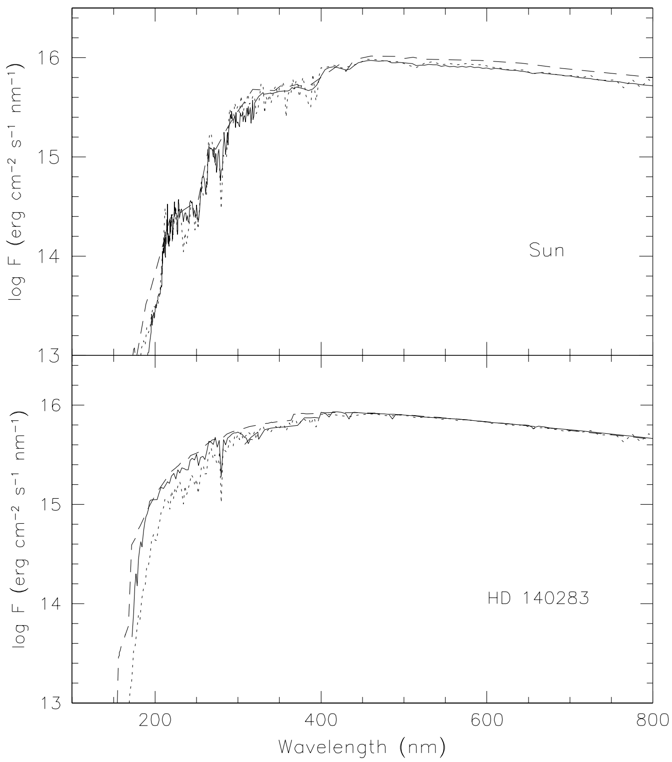

Fig. 2a and b. Comparison between observed and computed fluxes for the Sun (panel **a**) and HD 140283 (panel **b**). Solid lines are observations; dotted lines are fluxes computed with theoretical line opacities; dashed lines are fluxes computed with empirical line opacities. OSMARCS model atmospheres were adopted when preparing this figure

1985). For the Sun, the Holweger and Müller (1974) model atmosphere was used here. In the case of Arcturus, we used the MARCS model atmosphere presented by Frisk et al. (1982), and the apparent diameter of $\beta = 20.0 \pm 0.3$ milliarcsec given by Augason et al. (1980)[2].

The dependence of χ_l shown by Fig. 1b indicates that typical transitions have upper levels close to the ionization continuum for Fe I (exceptions are due to a few strong features, like H_α, the Mg II and Ca II resonance doublets, or the CN violet system). This is precisely the expected trend if most of the line opacity is due to weak lines of the Fe-group elements.

Fig. 2 compares the observed distribution of fluxes with wavelength with those computed through our empirical consideration of line opacity for the Sun and the metal-poor subgiant HD 140283. Observations were from the compilation by Vernazza et al. (1976) (Sun); and Oke & Gunn (1983) and Cacciari (1985) (HD 140283). The atmospheric parameters for HD 140283 were as follows: effective temperature $T_{\rm eff}$=5690 K, surface gravity $\log g = 4$, metal abundance [A/H]=-2, and microturbulent velocity $v_t = 1.5$ kms^{-1}. The value of the effective temperature was taken from Gratton & Sneden (1991), while a somewhat larger gravity than that find in that paper (from Fe equilibrium of ionization) was adopted, since we expected some Fe overionization in this metal-poor subgiant[3]. For the same reason, we adopted a metal abundance slightly larger than that provided by Fe I lines. The agreement between observed and computed fluxes is good. However this result is obvious for the Sun, while we note that line opacity in the atmosphere of HD 140283 is so small that it barely affects the computed fluxes even at UV wavelengths.

3.2. Comparison with results provided by theoretical mean radiation intensities

The above described empirical approach has several weak points, including attribution of the whole line opacity to a single agent (Fe I atoms), and possible errors either in the atmospheric parameters or in the structure of the model atmospheres adopted for the standard stars. Extensive calculations suggested us that these sources of uncertainty have not a large impact on present computations. However, use of mean opacities over a certain spectral range might introduce systematic errors in the determination of SE when the wavelength step in the binning procedure is larger than the Doppler width of lines, since line opacity usually displays large variations in even narrow spectral ranges. Therefore, (i) photons with wavelengths corresponding to spectral regions between lines have a large mean free path, and produce non-local effects; and (ii) mean values for the line opacity determined over large spectral ranges may be underestimated, due to saturation of strong lines. Errors are not expected to be large in the atmospheres of extremely metal-poor stars, where line opacity is however small and fluxes are reduced roughly in proportion to the mean opacity; yet they have a significant impact on the size of departures from LTE determined in the atmospheres of metal-rich stars.

The combined effects of wavelength binning and saturation are difficult to estimate accurately, due to lack of basic atomic data and limitations in computing facilities. The best we could do was to compare the results obtained with our empirical approach with those that could be obtained using mean radiation intensities computed by means of an opacity sampling (OS) technique. This was done for the cases mentioned above (the Sun and the metal-poor subgiant HD 140283). Both models were extended up to $\log \tau_{\rm Ross} = -4$, and they did not include any chromosphere; this is not a basic limitation here, since we aim at addressing the non-LTE effects on the abundance analyses that are based on lines formed at great photospheric depths. The comparison between fluxes computed using OSMARCS models and observations is also shown in Fig. 2. The agreement is fully satisfactory for the Sun, while the observed UV flux is larger then the predicted one for HD 140283 by 0.25 dex below 300 nm. Monochromatic fluxes computed using OS opacities better reproduce observations in the range 300–400 nm,

[2] We regarded as minor the inconsistency generated by the use of model atmospheres different from those of Kurucz (1992) used elsewhere in this paper

[3] This value of gravity for HD140283 is actually too large when compared to the Hipparcos parallax for this star, that definitely set it as a subgiant; a more appropriate value is indeed that used by Gratton & Sneden 1991, or in Paper I. However, the impact of the small difference in gravity on the flux distribution is at most marginal

where those obtained using empirical opacities are too large by ~ 0.05 dex. Note that fluxes in this wavelength range are from ground observations (Oke & Gunn, 1983).

We verified that differences between old MARCS and OSMARCS models (albeit not entirely negligible) are not the cause of the discrepant results in the far UV; in fact fluxes computed with the empirical method with the two models are within 3% (note that OSMARCS model for HD 140283 has a rather different temperature structure than the old MARCS model computed with the same atmospheric parameters, the surface temperature being lower by about 200 K; it is however warmer in the line forming region by about 20÷40 K).

The discrepancy between observed and computed UV-fluxes for HD 140283 may be ascribed to various sources:

1. theoretical fluxes may be wrong for several resons: a) If there are too few lines in the line list, and intensity of strong (saturated) lines is overestimated, the correct flux may still be obtained for the solar spectrum, but line opacity may be overestimated in metal-poor stars (see Balachandran & Bell 1997). b) Departures from LTE are neglected in the computation of opacities (both from lines and continuum). This might lead to an overestimate of opacity if either lines or photoionization of metals are important opacity sources and the most important non-LTE effect is overionization (see the discussions in Rutten & Kostik 1982, and Rutten 1988; we note here that H^- reacts in the opposite direction; however, since most metals are ionized, even a large overionization does not appreciably change the amount of free electrons). c) The present atmospheric model does not include any chromosphere, which may show-up in the UV-spectra of metal-poor stars (Kurucz, private communication). d) The non-local convection may produce thermal inhomogeneities which would lead to a UV-excess (see e.g. Gustafsson and Bell, 1979, and Magain 1983)
2. the calibration of UV (IUE) data may be wrong: the agreement between ground and satellite observations is good in the small overlapping region; however, there may be saturation in the extreme long wavelength range of satellite observations.
3. the observed UV excess might be due to an insofar unrecognized companion: this is not confirmed by other observations (e.g. the radial velocity seems constant to within 1 kms^{-1}).
4. rather different values of the effective temperature have been obtained even very recently for HD 140283. Nissen et al. (1994) obtained a value of $T_{\rm eff}$=5540 K from a theoretical calibration of $b-y$ colours based on the OSMARCS model atmospheres, where the zero points were set by the solar $b-y$ value as estimated from solar analogue stars (details in Edvardsson et al. 1993). A much larger average value of $T_{\rm eff}$=5755 K was obtained in Paper I using various colour indices (most weight being given to $V-K$) exploiting the theoretical colour-metallicity dependences given by the K92 model atmospheres, and empirical calibrations for population I stars based on $T_{\rm eff}$'s from the infrared flux method. The value adopted in the present context ($T_{\rm eff}$=5690 K) is closer to the upper value; however, an even larger $T_{\rm eff}$ would be required to match the observed UV flux.

On the whole, we think that convection effects are the most likely explanation for the discrepancy. However, it should also be mentioned that the present theoretical procedure is not fully consistent, since the radiative transport equation is not solved simultaneously with the SE equations, the radiation field being computed assuming that excitation and ionization follows Boltzmann and Saha equations. A consistent approach requires that results of SE are re-entered in the radiative transport equation, and the whole procedure is iterated until convergence is reached. The present approach would be adequate for a trace element, but Fe cannot be considered as a trace element, since its abundance significantly affect opacities. Results obtained with the empirical approach (which iterates the solution of SE and of the transfer equation up to convergence, although still mantaining the LTE temperature structure) are then perhaps preferable for metal-poor star, while those obtained with the theoretical approach are perhaps best for the metal-rich stars (where departures from LTE are rather small, and LTE may be considered as a rather good zero-order approximation). In the rest of this paper we will generally use the empirical approach for line opacity; in a few cases we will comment about results obtained with the theoretical approach.

4. Collisions with H I atoms

In the stars under consideration, collisions with neutral H atoms may dominate over collisions with electrons, since neutral H atoms outnumber free electrons by several orders of magnitude. In the case of bound-bound transitions, this result can be demonstrated by comparing the rate found from the formulae given by Steenbock & Holweger (1984) for transitions induced by collisions with neutral H atoms (based on order of magnitude formulas due to Drawin 1968, 1969), with that by Van Regemorter (1962) for transitions induced by collisions with electrons. After some simplification (which is justified since these formulas only give order of magnitude), we obtain the following expression for the ratio between collisional excitation rates with H atoms $C_{\rm H}$ and with electrons $C_{\rm e}$:

$$\frac{C_{\rm H}}{C_{\rm e}} = 1.23\times10^{-4}\,\frac{m_{\rm A}}{m_{\rm H}}\,(\chi\theta)^{0.66}\,\left(1+\frac{0.95}{\chi\theta}\right)\,\frac{n_{\rm H}}{n_{\rm e}} \qquad (3)$$

where $m_{\rm A}$ and $m_{\rm H}$ are the mass of the atom to be considered and of H, χ is the energy jump (in eV), $\theta = 5040/T$, T being the temperature (in K), and $n_{\rm H}$ and $n_{\rm e}$ are the number of H atoms and free electrons (per cm^{-3}). This expression is valid for $m_{\rm A} \gg m_{\rm H}$, and for $0.1 < (\chi\theta) < 10$.

The analogous expression for the ratio between collisional ionization rates by hydrogen atoms $D_{\rm H}$ and by electrons $D_{\rm e}$ is:

$$\frac{D_{\rm H}}{D_{\rm e}} = 9.36\times10^{-4}\,\frac{m_{\rm A}}{m_{\rm H}}\,f\,\left(1+\frac{0.95}{\chi\theta}\right)\,\frac{n_{\rm H}}{n_{\rm e}} \qquad (4)$$

where f is an effective oscillator strength (of the order of 1).

If these approximate expressions hold, collisions with H atoms dominate over collisions with electrons insofar $n_{\rm H} >$

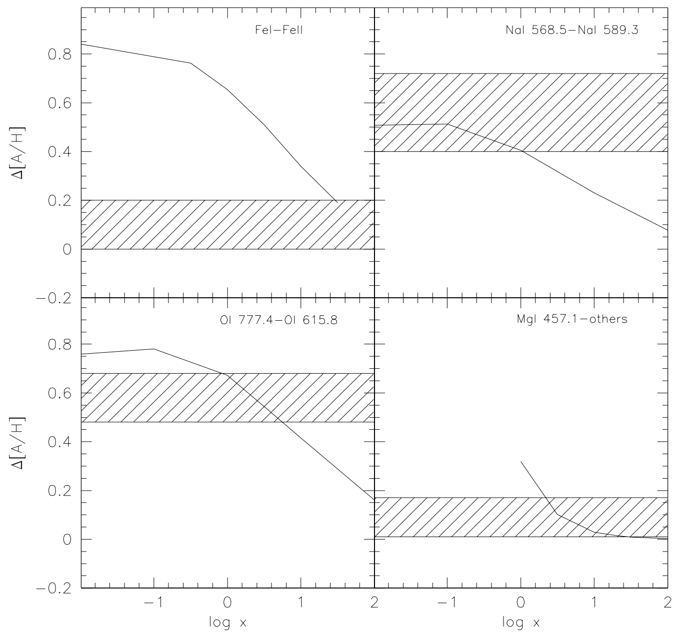

Fig. 3a–d. Calibration of collisional cross sections. Differences between abundances obtained from various spectral indices for RR Lyrae variables at minimum light are shown as a function of the factor x multiplying cross sections for H I collisions. Spectral indices used are: Fe I and Fe II lines for Fe (panel **a**); triplets at 777.4 and 615.8 nm for O (panel **b**); doublets at 568.5 and 589.3 nm for Na (panel **c**); intercombination line at 457.1 nm and higher excitation lines for Mg (panel **d**). The dashed regions represent range of values allowed by observations

$500n_{\rm e}$. However, Caccin et al. (1993) compared the cross sections for HI collisions for a Na model atom derived from Drawin formulae with more detailed estimates by Kaulakys (1984, 1985), and found that in that case Drawin formulas overestimate the cross sections by two orders of magnitude. Given the large uncertainties in these cross sections, we employed a parametric approach, where collisional cross sections are estimated by matching observed non-LTE features in stars where they are expected to be larger than in the programme stars, and for which accurate atmospheric parameters are available. In Clementini et al. (1995) it was shown that the spectra of RR Lyrae variables at minimum light are well suited to this purpose: explorative SE computations showed that in several cases departures from LTE are expected to be much larger than in cooler and/or lower gravity stars, due to the simultaneous presence of a rather large ionizing flux, low pressure (and hence small collisional rates), and trasparent atmospheres (due to the low metal content); furthermore, accurate temperatures and gravities could be determined exploiting the stellar pulsation. While some concern exist about possible (and likely) deviations of the atmospheres from flux constant, static models, Clementini et al. found that K92 model atmospheres succesfully describe most of the observed features (flux distribution, Balmer line profiles, etc) for variables close to minimum light, at least for the deep atmospheric layers, where not too strong lines form.

Our approach was then to multiply the cross sections for HI collisions by a factor of x, which was changed until we got agreement between abundances provided by different features in the spectra of RR Lyrae variables at minimum light (see Clementini et al. 1995). The features we exploited in our empirical calibration of collisional cross sections were as follows:

- Fe: the main non-LTE effect for Fe in RR Lyrae is overionization; we then forced agreement between average abundances provided by Fe I and Fe II lines. In this way we obtained only a lower limit: $\log x \geq 1.5$ (see Fig. 3a); as a conservative approach we adopted $\log x = 1.5$. In the next sections we will explore the effects of adopting different values of $\log x$ within those allowed by our estimate for the lower limit.
- O: for O, we found rather large non-LTE effects for the IR triplet; we then forced agreement between average abundances provided by this feature and the much weaker triplet at 615.6–615.8 nm. In this way we obtained a value of $\log x = 0.5 \pm 0.5$ (see Fig. 3b).
- Na: departures from LTE are rather large for the D resonance doublet in RR Lyrae, while they are negligible for weak subordinate lines. We obtained an upper limit: $\log x \leq 0$ (see Fig. 3c); the adopted value is $x = 0.01$, in agreement with Caccin et al. (1993). Again, in the next sections we will explore the effects of adopting different values of $\log x$ within those allowed by our estimate for the upper limit.
- Mg: we matched abundances provided by the resonance intercombination line with those given by higher excitation lines. We obtained a rather large value of x ($\log x > 0.3$) (see Fig. 3d); a value as small as $\log x = 0$ is in clear disagreement with observations, since in that case the high excitation line at 552.8 nm would be expected to be in emission, while it is observed as an absorption line in the spectra of RR Lyrae stars at minimum light. The adopted value is $\log x = 0.5$.

It should be noticed here that our estimates of the cross sections for collisions with HI atoms are model dependent for at least two reasons:

1. Drawin formulae give cross sections for HI collisions as a linear function of collisions with electrons; hence any uncertainty in e-collision cross sections yields an error in the HI collision cross sections. In our parametric approach, this is partly compensated for by the empirical comparison with observed features: therefore, the value of x might be interpreted as a correction to the whole collisional cross sections.
2. our estimate for the value of x rests on the applicability of the analysis of Clementini et al. (1995) to the spectra of RR Lyrae stars; to include possible errors in the analysis, we adopted rather generous error bars. The effects of forcing x to the extremes of these error bars are discussed later.

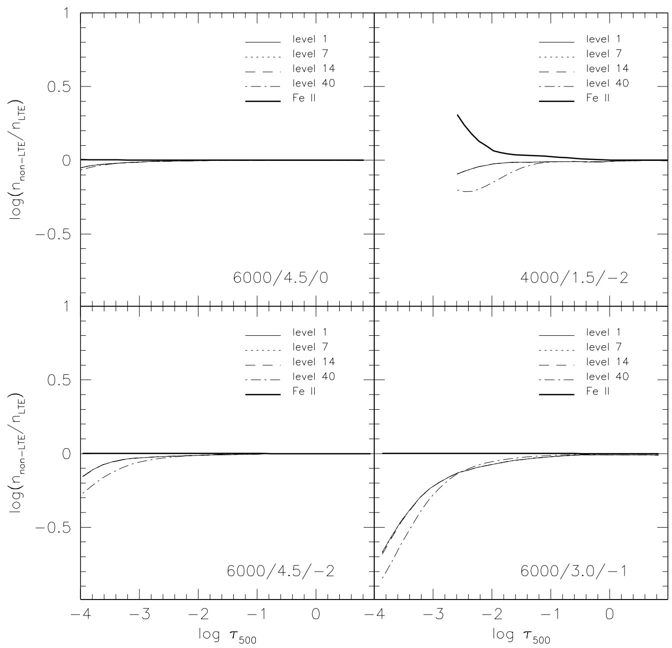

Fig. 4. Run of departure coefficients for selected levels of the Fe model atom with optical depth in model atmospheres having parameters typical for a metal-rich dwarf, a metal-poor dwarf, a metal-poor giant, and an RR Lyrae variable. These departure coefficients were computed with our empirical line opacities and collisional cross sections. Lines for levels 7 and 14 are virtually identical to those for level 1. Note the moderate overionization occurring in the upper layers of the low gravity model atmospheres; depopulation is larger for levels of intermediate energy due to photon suction

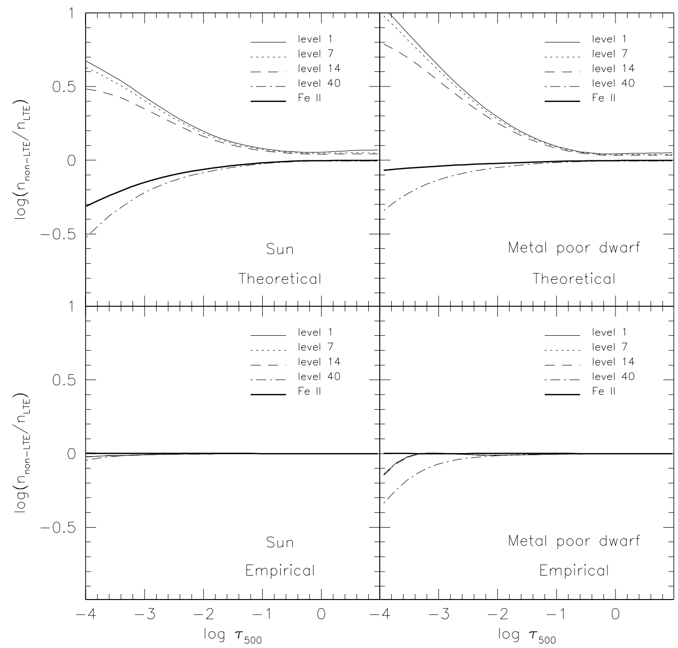

Fig. 5. Run of departure coefficients for the selected levels of the Fe model atom with optical depth in model atmospheres having parameters typical for the Sun and HD 140283. These departure coefficients were computed with theoretical radiation intensities (upper panels) and empirical (bottom panels) line opacities and empirical collisional cross sections. When compared to the results obtained with our empirical approach for line opacities, departures from LTE are much larger and occur deeper in the atmospheres when using theoretical line opacities

5. Results of statistical equilibrium computations

5.1. Fe

In this section, we describe the main results of our SE computations; in the next section we will discuss their effects on abundance analysis.

Fig. 4 shows the run of the departure coefficients for selected levels of the Fe I model atom, as a function of optical depths, in some typical model atmospheres: a metal-rich dwarf (not much different from the Sun), a metal-poor dwarf, a metal-poor giant (near the tip of the red-giant branch), and an RR Lyrae variable. Note that lines for levels 1, 7 and 14 (typical of low excitation levels, potential energy < 2.5 eV) are virtually undistinguishable. On the whole, we found negligible departures from LTE in high gravity stars, insofar our empirical approach for line opacity was adopted (most lines form at optical depths in the range $\log\tau_{\rm Ross} \sim -2 \div -1$).

A quite different result was obtained when using theoretical radiation intensities. This is illustrated by Fig. 5, where we compare departure coefficients obtained using both descriptions of the radiation field for model atmospheres appropriate for the Sun and HD 140283. Departures from LTE are significant even at optical depths $\log\tau_{\rm Ross} > -2$ when using theoretical radiation intensities. It should, however, be noticed that in this case collisions were likely underestimated in the SE calculations: in fact, we expect larger non-LTE effects for RR Lyrae variables too, and hence we should have adopted a larger value for x in order to match the observed good agreement between abundances provided by Fe I and Fe II lines for these stars. Explorative computations showed that mean non-LTE corrections to abundances given by Fe lines in HD 140283 decrease from 0.21 dex to 0.09 dex if $\log x$ is raised from 1.5 to 2.0; for the Sun, they decrease from 0.14 to 0.06 dex. We conclude that our SE based on theoretical radiation intensities may be considered an upper limit to real departures from LTE in stellar atmospheres.

In our calculations, departures from LTE are more pronounced in low gravity stars, where the thermalizing effect of collisions is not as strong. In the case of RR Lyrae variables, the main non-LTE effect is overionization from low energy levels by the rather strong UV flux, while other effects (resonance line scattering, photon suction) play a minor role, as indicated by the close similarity of the departure coefficients from different levels. Overionization is however not very large due to the residual collisional coupling of high energy levels to the continuum: overionization was expected to be much larger in SE computations using very simplified model atoms (Athay & Lites 1972; Saxner 1985, Bikmaev et al. 1990).

The reduced UV radiation field is able to support only a moderate overionization for stars near the tip of the red giant branch (upper right panel of Fig. 4). In this case collisions are unsufficient to mantain the excitation equilibrium, so that there

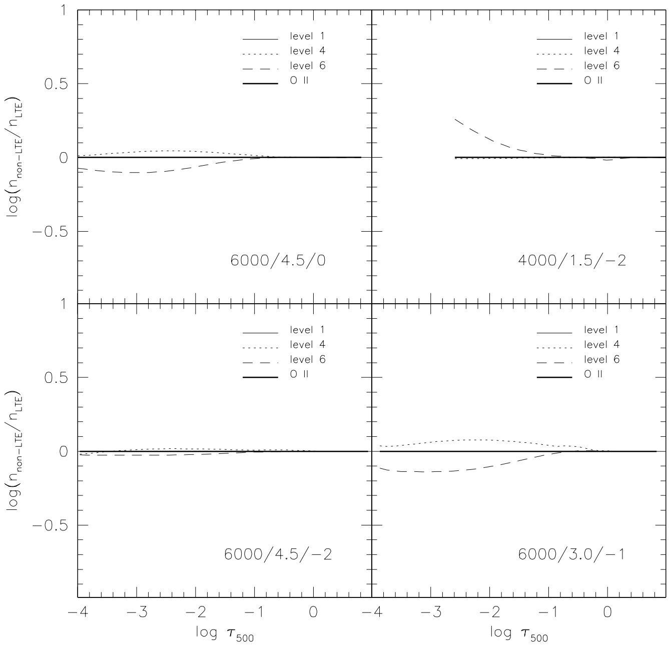

Fig. 6. Same as Fig. 4, but for our O I model. Levels 6 and 4 are the upper and lower levels of the IR triplet respectively

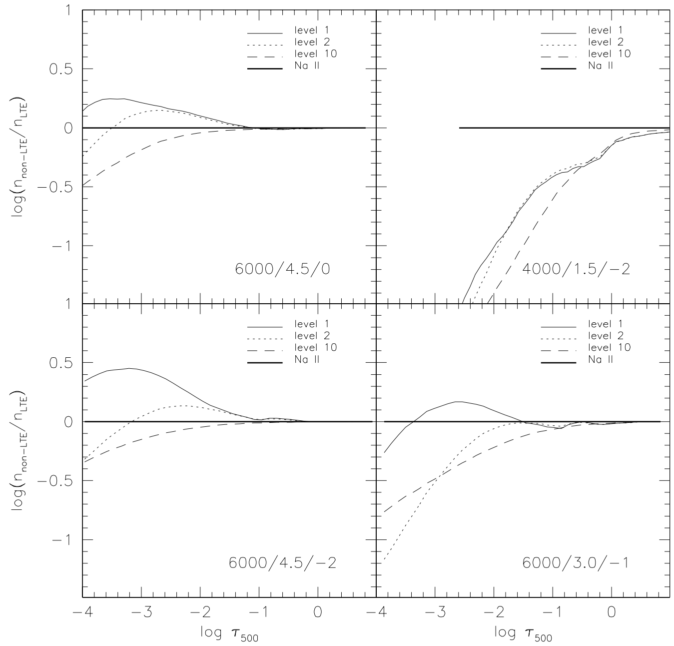

Fig. 7. Same as Fig. 4, but for our Na I model. Note the large overionization occurring in low gravity stars, and the overpopulation of the ground level in high gravity ones due to photon suction

is a radiative cascade from higher to lower energy levels (photon suction), an effect already described for alkaly atoms in the Sun (Bruls et al. 1992). Therefore, the larger depopulation (anyway moderate) occurs for levels of intermediate energy.

5.2. O

Although not very large, departures from LTE are more important for O (see Fig. 6). Overionization is generally unimportant, due to the large ionization energy. Most O is in the OI ground state, which is then very close to LTE. The large gap between the two levels of lowest energy and levels of higher energy makes collisions unefficient to mantain LTE, though they help to keep the Boltzmann equilibrium within high energy levels, which is however not perfect in the outer part of the atmospheres. Since the upper level of the IR triplet is more depopulated than the lower one, the source function is smaller than the Planck function (and the IR triplet is then expected to be stronger than in LTE).

5.3. Na

Results of our SE computations for Na reproduce the main features discussed by Bruls et al. (see Fig. 7). Three competing effects are important:

1. due to the low ionization energy of Na, there is a large overionization even in the coolest stars.
2. Na overionization is a function of gravity due to competition with collisional recombination to the levels of higher energy from the Na II reservoir (most Na is in the ground state of Na II even in cool stars): it occurs deep in the atmospheres of giants, while it is appreciable only in the outer part of the atmospheres of dwarfs.
3. depopulation of Na I levels is selective, owing to the small collisional cross sections; there is a recombination cascade to the ground level which has a very small photoionization cross section (photon suction: Bruls et al. 1992). The ground level is less underpopulated than levels of higher energy (and it is actually overpopulated in high gravity stars).

5.4. Mg

Fig. 8 illustrates our result for Mg. They share various features with those obtained for Fe: departures from LTE are negligible in dwarfs, while the decreased efficiency of collisions make it more pronounced in stars of lower gravity (although they are anyway quite small). A moderate overionization by the strong UV flux occurs in the atmospheres of RR Lyrae variables due to photoionization from the two first excited levels ($3p^3$P and $3p^1$P); photoionization from the ground level ($3s^1$S) is less important, because there is not much flux at short wavelengths. Higher excitation levels are closer to LTE, due to collisional recombination and cascades from levels with energies close to the continuum. Photon suction causes a relative overpopulation of the levels of lowest energy in cool giants, where overionization is much less efficient due to the smaller UV flux. It must be noticed that the two levels of lowest energy are collisionally coupled due to the very small value of the oscillator strength of the resonance intercombination line; hence they share the same departure coefficients throughout all the model atmospheres considered here.

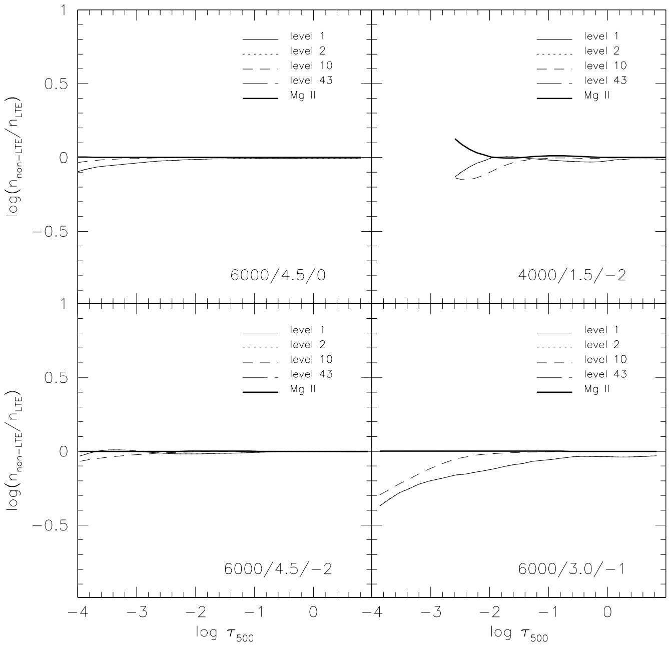

Fig. 8. Same as Fig. 4, but for our Mg I model. Lines for level 2 are virtually undistinguishable from those of level 1, since these levels are collisionally coupled each other

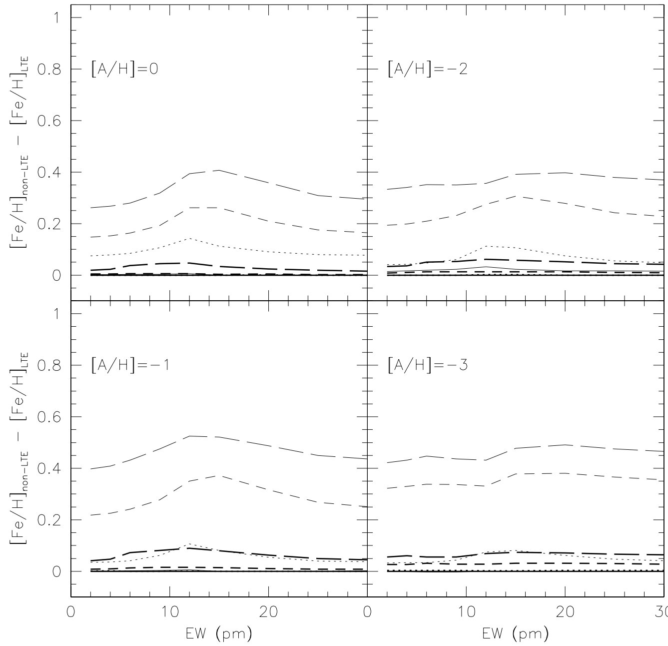

Fig. 9. Non-LTE corrections to the Fe abundances derived for the $a^5D - z^7F^0$ transition (representative of a low excitation line: EP=0 eV) as a function of line strength computed in K92 model atmospheres with different values of $T_{\rm eff}$, $\log g$, and overall metal abundance. Solid, dotted, short-dashed, and long-dashed lines are for models with $T_{\rm eff}$=4000, 5000, 6000, and 7000 K respectively. Thin lines are for low gravity models ($\log g = 1.5$ for $T_{\rm eff}$=4000, 5000, 6000; $\log g = 2.25$ for $T_{\rm eff}$=7000 K), while thick lines are for high gravity models ($\log g = 4.5$). Microturbulent velocities used in these computations are a function of gravity (see text)

6. Corrections to LTE abundances

In this section we present non-LTE corrections to abundances as estimated using our SE calculations for calculating equivalent widths of selected spectral lines from Fe, O, Na, and Mg. The corrections are simply the difference between abundances obtained assuming LTE, and those we obtained multiplying the LTE population of the lower level of the transition for the departures coefficients given by MULTI code and the source function (a Planckian) for the ratio between the departure coefficients for the upper and lower levels. This approximation is not adequate when stimulated emission is important, e.g. for far infrared transitions; however it is reasonably correct for the lines considered here.

In the figures of this section, we display the non-LTE corrections to LTE abundances as a function of equivalent width for various features in a number of atmospheric models, extracted from the grid by Kurucz (1992). The equivalent widths and the corrected abundances plotted roughly correspond to the ranges of equivalent widths consistent with the initial [A/H]. The following relation between microturbulent velocity $v_{\rm t}$ and surface gravity was adopted:

$$v_{\rm t} = -0.322 \ \log g + 2.22 \quad {\rm km\,s^{-1}} \qquad (5)$$

(Paper I).

6.1. Fe I features

For Fe, we give non-LTE abundance corrections for lines belonging to the $a^5D - z^7F^0$ transition (RMT 2, representative of low excitation lines: EP=0 eV) (Fig. 9), and the $y^5D^0 - u^5F$ transition (representative of high excitation Fe I lines: EP=4.10 eV) (Fig. 10). These data are also given in tabular form in Table 9, available only in electronic form. We remind that in the case of Fe we conservatively adopted for x a value which is the minimum allowed by the analysis of RR Lyrae variables: hence the abundance corrections of Fig. 9 and 10 must be considered as upper limits.

As it should be expected from the plots relative to the departure coefficients, non-LTE corrections for Fe lines are very small in dwarfs of any $T_{\rm eff}$ (in the range explored in this paper), and only small corrections (< 0.1 dex) are expected for stars on the red giant branch. This result is highly welcome, since it validates hundreds of LTE abundance analyses, and supports current views on galactic evolution.

On the other hand, we found that our upper limit for non-LTE corrections is large in the case of warm, low gravity stars, where collisions are less important and there is a large overionization due to the strong UV flux: we found values as large as 0.3–0.7 dex (depending on excitation) for stars with $T_{\rm eff}$=7000 K and log g=2.25, these values being only weakly dependent on EWs (note that our non-LTE corrections for a dwarf of similar $T_{\rm eff}$ are negligible). This result occurs because in these warm, low gravity stars we found that departure coefficents are quite different from unity even at rather large optical depths (see Fig. 11). It is not easy to reconcile such large corrections with

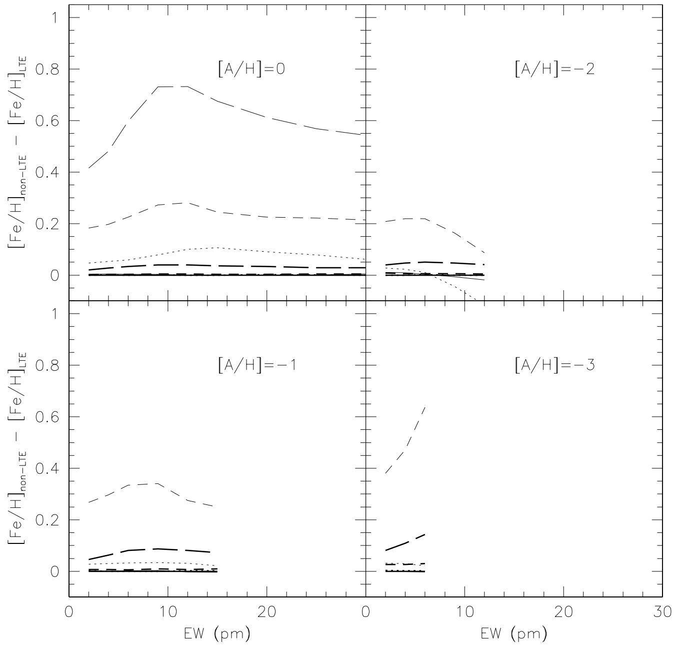

Fig. 10. The same as Fig. 9, but for the $y^5D^0 - u^5F$ transition (representative of a high excitation Fe I line: EP=4.10 eV)

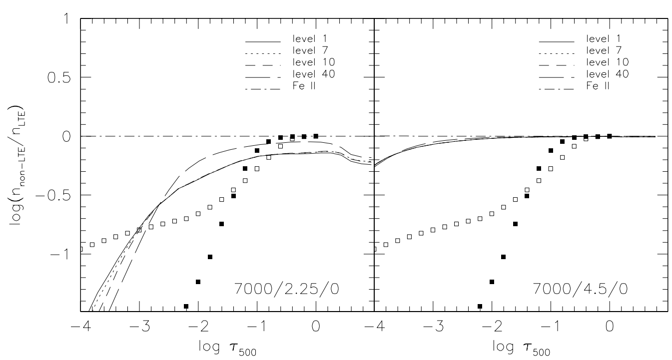

Fig. 11. Run of departure coefficients for selected levels of the Fe model atom with optical depth in model atmospheres for a warm dwarf and giant ($T_{\rm eff}$=7000 K, log g=4.5 and 2.25 respectively). These departure coefficients were computed with our empirical line opacities and collisional cross sections. Overlaid are the overionization factors ϕ computed by Nissen & Gustafsson (1978) for a warm dwarf, using a simple 12-level model atom (open squares) and with no consideration of HI collisions; and those empirically determined by Lyubimkov & Boyarchuk (1983) for F stars (filled squares)

spectroscopic data for F-supergiants, where significant non-LTE corrections seem required only for rather strong lines: e.g. Spite et al. (1989) successfully eliminated trends of abundances derived from Fe I lines with equivalent widths using the overionization factors ϕ computed by Nissen & Gustafsson (1978; to make comparisons with our results easier, these are also plotted in Fig. 11). Although adoption of these overionization factors, computed for dwarfs using a small 12-level Fe I model atom, is clearly inadequate in that context, Spite et al. result suggests that the upper limits to non-LTE corrections we obtain for Fe are indeed larger than those really required.

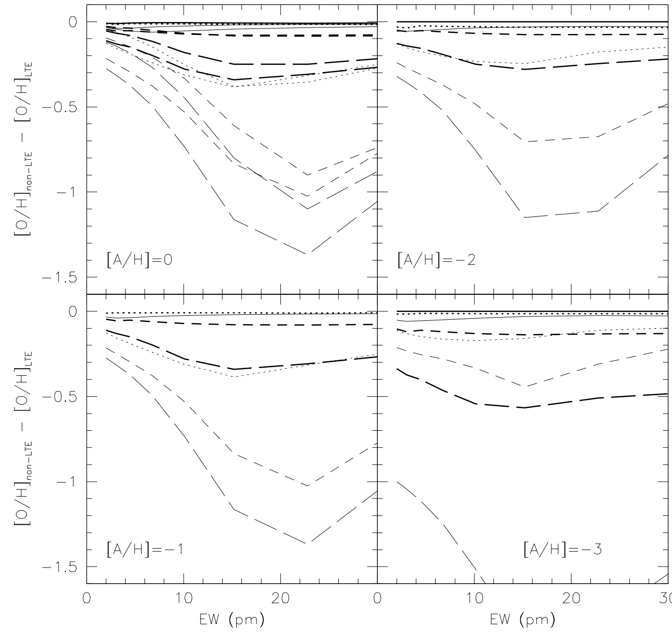

Fig. 12. The same as Fig. 9, but for lines of the O I IR triplet (777.1–777.4 nm)

We conclude that non-LTE corrections are not required in the analysis of Fe lines in the spectra of the stars studied in this series of papers (they are on the main sequence or the red giant branch). Hence for Fe we will simply adopt the results of the LTE analysis. Anyway, our SE solutions suggest that much caution should be exerted when considering results for warm, low gravity stars, like some of the post-AGB stars (Bond 1991): in that case we propose that the extreme Fe underabundances obtained for some post-AGB stars may in part be due to departures from LTE.

6.2. *O I features*

Non-LTE abundance corrections for lines of the O I IR triplet (777.1–777.4 nm) are given in Fig. 12. These data are also given in tabular form in Table 10, available only in electronic form. Generally, abundance corrections are negative (i.e. non-LTE abundances are smaller than LTE ones), as found by many other authors (see e.g. Baschek et al. 1977). These abundance corrections are due to differences between departure coefficents for individual levels, causing significant deviations of source functions from Planckians in the outer atmospheric regions: therefore, corrections are function of equivalent widths (as expected, since saturated lines form outer in the atmospheres), of gravity, and of temperature.

For dwarfs, commonly used when discussing galactic chemical evolution, corrections are quite small (≤ 0.1 dex) if $T_{\rm eff}<6000$ K; however, corrections increase for warmer stars and are as large as 0.4 dex for stars with $T_{\rm eff}$=7000 K. While these corrections cannot by themselves explain the very large overabundances obtained e.g. by Abia & Rebolo (1989), they should be included in accurate abundance analysis. Corrections are even

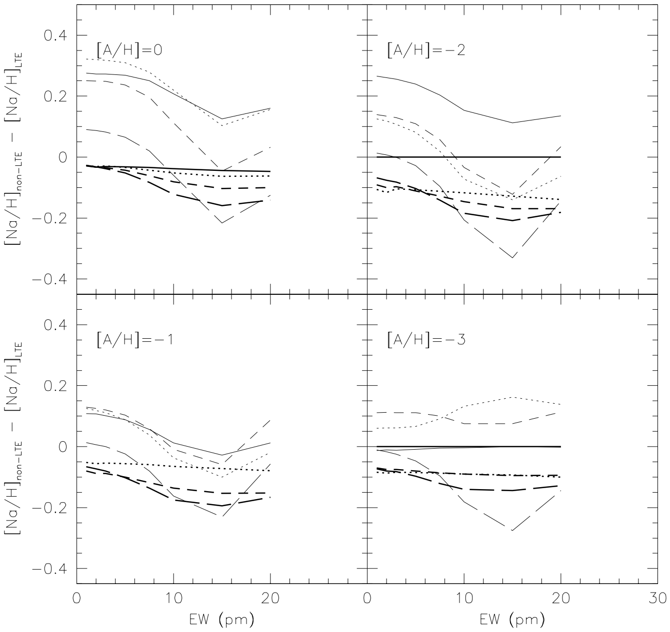

Fig. 13. The same as Fig. 9, but for Na I doublet at 568.2–568.8 nm

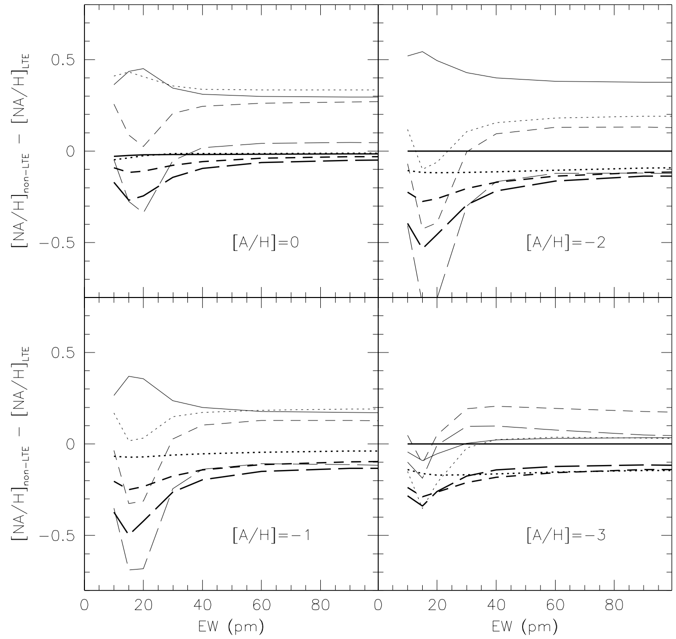

Fig. 14. The same as Fig. 9, but for Na I resonance doublet at 589.0–589.6 nm

larger for warmer giants, like RR Lyrae variables (where typical values are ~ 0.6 dex), and may be extremely large ($\gg 1$ dex) for the warmest, low gravity stars considered here ($T_{\rm eff}$=7000 K and log g=1.5). Our results agree with the well known large O overabundances found from LTE analysis of IR lines in A-type stars (see e.g. Reimers 1969), at variance with the nearly solar abundances provided by weak lines in the visible. Thus, caution should be excercised in the interpretation of abundance analysis for post-AGB stars (Bond 1991). We notice that application of present non-LTE corrections would substantially reduce the very large O overabundances found in some post-AGB stars.

6.3. Na I features

Non-LTE abundance corrections for lines of the Na I doublets at 568.2–568.8 nm, 589.0–589.6 nm (D lines), and 615.4–616.0 nm are given in Figs. 13, 14, and 15 respectively. These data are also given in tabular form in Table 11, available only in electronic form.

Non-LTE corrections for the subordinate lines considered here are generally positive, since the lower level ($3p^2{\rm P}^0$) is the most depleted by overionization and cascade; they have only moderate sensitivity on line strength. Corrections are small (< 0.1 dex) in high gravity stars, but they are not negligible (up to 0.3 dex) for giants, depending on metal abundance. Furthermore, we find that for these stars SE is quite sensitive to the adopted values for collisional cross sections. In order to test this issue, we repeated our SE computations for a model with parameters characteristic of those of a metal-poor giant (HD 122956) with different values of x ($x = 0.001$, $x = 0.01$, $x = 0.1$). As expected, we found that non-LTE corrections are negligible for large values of x; however, they are rather large (~ 0.4 dex) for $x = 0.001$. This value of x is very low even when compared to

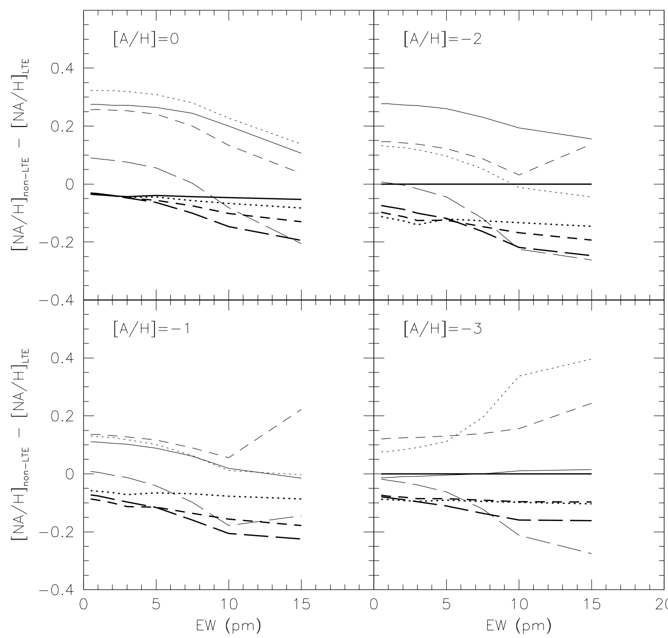

Fig. 15. The same as Fig. 9, but for Na I doublet at 615.4–616.0 nm

the estimates by Kaulakys (1984, 1985); however, it would yet be compatible with the observations of RR Lyrae stars. A better determination of x would be welcome.

Non-LTE abundance corrections for D-lines show a more complicate pattern: their absolute value is larger for EWs in the range 15–20 pm, as observed in very metal-poor stars, since these are saturated lines with only weak wings: in this case rather large negative corrections are expected for warm stars (e.g. RR Lyrae variables), where photoionization is very important, while corrections are positive for red giants, where the ef-

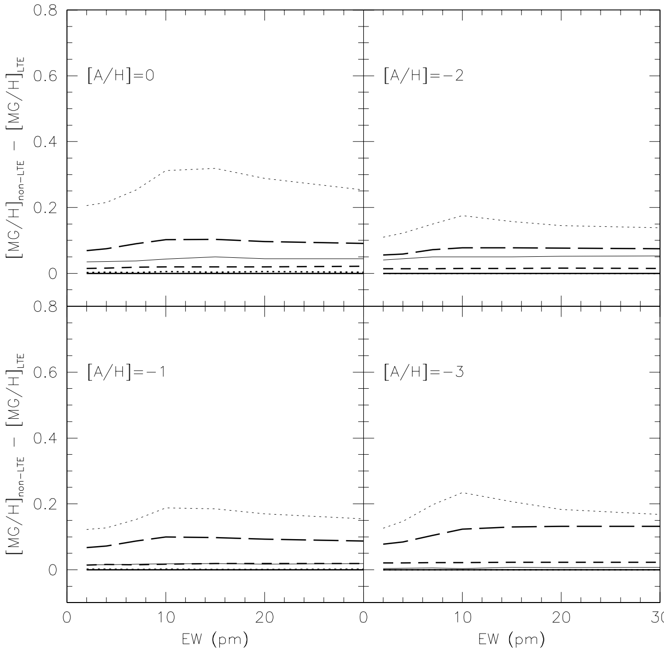

Fig. 16. The same as Fig. 9, but for the Mg I intercombination line at 457.1 nm

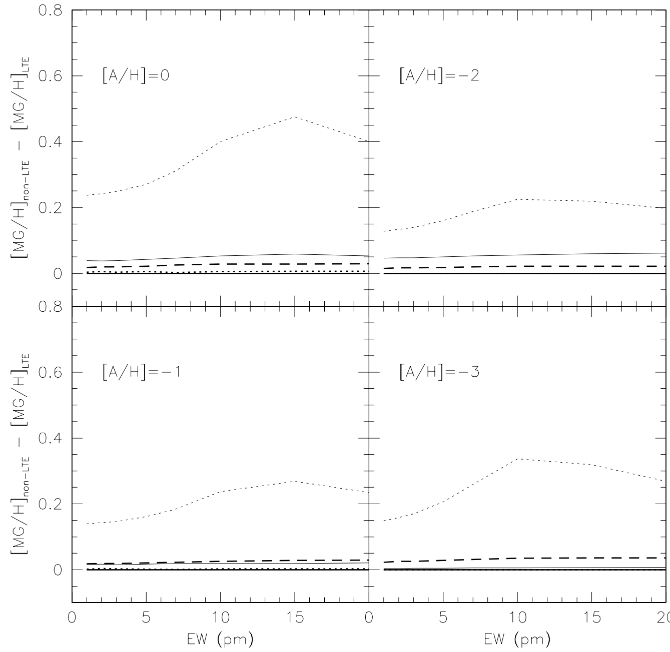

Fig. 17. The same as Fig. 9, but for the Mg I high excitation line at 473.0 nm

fects of photon suction dominate. For stronger, wing-dominated lines (like those observed in population I stars), corrections are usually moderate (< 0.2 dex) for dwarfs, but they may be as large as 0.35 dex in giants, since in that case departures from LTE occur deep in the atmospheres.

Our non-LTE corrections may explain part of the large Na overabundances found in population I F-K giants and supergiants (see e.g. Sasselov 1986). As an example, we consider the case of three supergiants analyzed by Gratton et al. (1989): the average Na overabundance reduces from [Na/Fe]=+0.35 to [Na/Fe]=+0.22 after application of non-LTE corrections. As mentioned above, smaller values of x may perhaps be adopted: in this case non-LTE corrections are expected to be larger in cool giants, where collisions with H I may still be the major thermalizing mechanism. More extensive comparisons will be presented in Carretta et al. (1999).

6.4. Mg I features

Non-LTE abundance corrections for the Mg I intercombination line at 457.1 nm, the weak line at 473.0 nm (assumed to be representative of high excitation lines), and lines of the $b-$triplet (516.7–518.3 nm) are given in Fig. 16, 17, and 18 respectively. These data are also given in tabular form in Table 12, available only in electronic form.

The source function for the 457.1 nm transition, connecting the metastable $3p^3$P level and the ground state ($3s^1$S), is in LTE because the transition is dominated by collisions (see Mauas et al. 1988). On the other hand, the source function for the other transitions considered for the RR Lyraes is smaller than 1, because departure coefficients are much smaller for the lower level ($3p^1$P) than for the high excitation levels close to

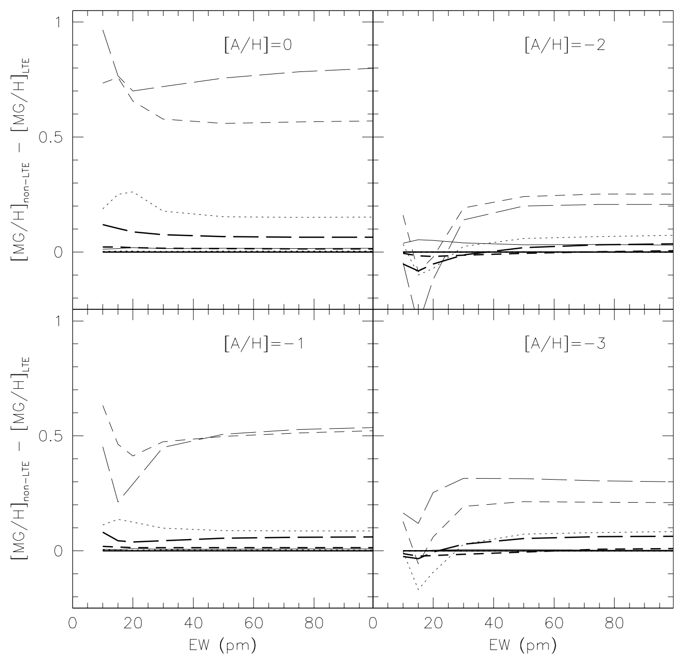

Fig. 18. The same as Fig. 9, but for the Mg I b triplet at 516.7–518.3 nm

the continuum. This fact is not unexpected: in fact, some IR Mg lines are seen in emission in the solar spectrum, precisely due to this effect (see e.g. Rutten & Shchukina 1992). Our SE computations reproduce all these features quite well.

Since the dominating non-LTE effect for Mg is overionization, non-LTE abundance corrections are generally positive. Corrections for the 457.1 nm line are small in cool dwarfs ($T_{\rm eff} \leq 6000$ K); however, they are not negligible (~ 0.15 dex) in the warmer dwarfs. Corrections are larger in giants, where collisions less efficiently compete with photoionization; we get larger corrections (up to ~ 0.3 dex) in the warmer stars due to the larger UV flux.

LTE is a good approximation also in the analysis of higher excitation lines, insofar cool dwarfs are considered; in warm giants, however, non-LTE corrections may become large for high excitation Mg lines, and in a few extreme cases emissions are predicted by our SE calculations, in analogy with the IR lines in the solar spectrum: as discussed in Sect. 4, this result is very sensitive to the adopted value of x, which is then well constrained to large values.

7. Conclusions

In this paper we have presented determinations of the SE of Fe, O, Na, and Mg in model atmospheres for stars with $T_{\rm eff}$ in the range 4000–7000 K. These SE calculations aimed at estimating corrections to abundances provided by LTE analysis, and hence were limited to photospheric regions. Two important aspects of SE calculations were discussed in some detail:

1. Estimates of the radiation field within the atmospheres need consideration of the line opacity. This was first obtained by an empirical procedure: monochromatic theoretical fluxes from atmospheres adequate to describe the Sun and Arcturus were computed by considering known continuum opacity sources and a veil of weak Fe I lines, the parameters (excitation energy and line strengths) of which were adjusted to match observations. We compared the results provided by this technique with those obtained by using mean intensities determined by means of an OS method (Edvardsson et al. 1993) based on the very extended line list prepared by Kurucz (1992). We found that our empirical approach yielded smaller departures from LTE than the theoretical one, at least partly reflecting the fact that it underestimates the non-local effects of photons with wavelengths corresponding to regions between lines (pseudo-continuum). Mean intensities of radiation in the theoretical approach were computed assuming LTE, and were then inconsistent with the solution of SE equations. We think that results obtained through the theoretical approach may perhaps be preferable when departures from LTE are small, while those obtained with the empirical line opacities are better when they are large, and the line opacity is small. Since these are the cases we are most interested in, the empirical method was adopted throughout this paper.
2. We found, not unexpectedly, that the largest source of uncertainty in the present computations is the poor knowledge of cross sections for collisions with H I atoms, which is the most important thermalizing mechanism in late type stars. We tried to overcome this problem by parametrizing these cross sections by means of a multiplicative factor x. Empirical values for x were obtained by matching abundances provided by different spectral indices in the spectra of RR Lyrae variables at minimum light. These stars were selected because departures from LTE were expected to be large (owing to the high temperatures, low gravities and metal abundances), and because gravities could be accurately determined from the light curve. While there might be some concern related to the applicability of static model atmospheres to the analysis of variable stars, in a separate paper (Clementini et al. 1995) it was found that Kurucz (1992) models seem adequate for this purpose if spectra at minimum light are considered. While the values of x determined by this procedure are model dependent, our SE calculations should be rather robust for models of old stars on the main sequence and the red giant branch, if the value of x is allowed to vary within its considerable ranges of error in order to test the significance of the corresponding uncertainties in the collision cross sections. The calculations still present rather good first approximations to the statistical equilibria in the real photospheres of these stars, at least as long as the other basic assumptions of the models are adequate - in particular the assumption of plane-parallel stratification and mixing-length convection.

Using these methods, we performed a consistent and extensive set of SE calculations over a wide range of atmospheric parameters (4000$\leq T_{\rm eff} \leq$7000 K, $1.5\leq \log g \leq$4.5, $-3 \leq$[A/H]≤ 0), derived tables of corrections to LTE abundances as a function of equivalent widths for a number of features of Fe, O, Na, and Mg, and briefly compared them with a few, selected observations. In general, we found that non-LTE corrections are small in dwarfs and red giants, moderate in RR Lyrae stars, while they may be large in F supergiants; however, each element shows its own peculiarities. The dominating non-LTE effect for Fe and Mg is overionization by UV photons, photon suction being of some relevance in the coolest stars; source functions are often much different from the Planck function for O; while in the case of Na both overionization and photon suction are important in all stars, causing a more complicated pattern. For Fe, we found that non-LTE corrections may be neglected in most cases, validating LTE analyses for stars on the main-sequence, red giant branch, and even for RR Lyrae stars; only in the case of F-supergiants non-LTE effects may significantly change results obtained by LTE analysis. Non-LTE corrections should be included in accurate analysis of the OI IR lines in warm stars, and of all Na lines in giants of any $T_{\rm eff}$; for Mg, they must be considered in the analysis of giants and supergiants.

We conclude that progress in computational methods and facilities make realistic estimates of non-LTE effects possible for a variety of atomic species in the atmospheres of G- and K-stars. Close comparisons with high quality observations of stars with carefully determined parameters are valuable tools when judging the relevance of the data used in SE computations. The results discussed here suggest that non-LTE corrections are small but not negligible for elements having a rather large ionization potential, even in extremely metal-poor stars, where line opacity is small. A number of small but significant effects revealed by high quality analyses in the last decade can now be explained as due to non-LTE effects. Similar computations should be extended to other important elements like C, Si and Ca.

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