On the Chemical Composition of Metal-Poor Stars

Impact of Stellar Granulation and Departures from Local Thermodynamic Equilibrium on the Formation of Spectral Lines

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Dissertation presented at Uppsala University to be publicly examined in Polhemsalen, Ångström Laboratory, Uppsala, Friday, September 22, 2006 at 13:15 for the degree of Doctor of Philosophy. The examination will be conducted in English.

Abstract

The information about the chemical compositions of stars is encoded in their spectra. Accurate determinations of these compositions are crucial for our understanding of stellar nucleosynthesis and Galactic chemical evolution. The determination of elemental abundances in stars requires models for the stellar atmospheres and the processes of line formation. Nearly all spectroscopic analyses of late-type stars carried out today are based on one-dimensional (1D), hydrostatic model atmospheres and on the assumption of local thermodynamic equilibrium (LTE). This approach can lead to large systematic errors in the predicted stellar atmospheric structures and line-strengths, and, hence, in the derived stellar abundances. In this thesis, examples of departures from LTE and from hydrostatic equilibrium are explored. The effects of background line opacities (line-blocking) due to atomic lines on the statistical equilibrium of Fe are investigated in late-type stars. Accounting for this line opacity is important at solar metallicity, where line-blocking significantly reduces the rates of radiatively induced ionizations of Fe. On the contrary, the effects of line-blocking in metal-poor stars are insignificant. In metal-poor stars, the dominant uncertainty in the statistical equilibrium of Fe is the treatment of inelastic H+Fe collisions. Substantial departures of Fe abundances from LTE are found at low metallicities: about 0.3 dex with efficient H+Fe collisions and about 0.5 dex without. The impact of three-dimensional (3D) hydrodynamical model atmospheres on line formation in red giant stars is also investigated. Inhomogeneities and correlated velocity fields in 3D models and differences between the mean 3D stratifications and corresponding 1D model atmospheres can significantly affect the predicted line strengths and derived abundances, in particular at very low metallicities. In LTE, the differences between 3D and 1D abundances of C, N, and O derived from CH, NH, and OH weak low-excitation lines are in the range -0.5 dex to -1.0 dex at [Fe/H]=-3. Large negative corrections (about -0.8 dex) are also found in LTE for weak low-excitation neutral Fe lines. We also investigate the impact of 3D hydrodynamical model stellar atmospheres on the determination of elemental abundances in the carbon-rich, hyper iron-poor stars HE 0107-5240 and HE 1327-2326. The lower temperatures of the line-forming regions of the 3D models compared with 1D models cause changes in the predicted spectral line strengths. In particular we find the 3D abundances of C, N, and O to be lower by about -0.8 dex (or more) than estimated from a 1D analysis. The 3D abundance of Fe is decreased but only by -0.2 dex. Departures from LTE for Fe might actually be very large for these stars and dominate over the effects due to granulation.

Keywords: late-type stars, stellar abundances, stellar atmospheres, spectral line formation, convection, hydrodynamics, Galactic chemical evolution

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ISSN 1651-6214
ISBN 91-554-6641-9
urn:nbn:se:uu:diva-7121 (http://urn.kb.se/resolve?urn=urn:nbn:se:uu:diva-7121)
If you find yourself on the side of the majority, it's time to pause and reflect.

—Mark Twain
List of Papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals.

    “Effects of line-blocking on the non-LTE Fe I spectral line formation”,  
    *Astronomy & Astrophysics*, 442, 643–650

    “Three-dimensional hydrodynamical simulations of surface convection in red giant stars – Impact on spectral line formation and abundance analysis”,  
    *Astronomy & Astrophysics* (submitted)

    “The chemical compositions of the extreme halo stars HE 0107−5240 and HE 1327−2326 inferred from three-dimensional hydrodynamical model atmospheres”,  

Papers not included in the thesis:

    “A probable stellar solution to the cosmological lithium discrepancy”,  

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1. Introduction

In the short story “The golden apples of the Sun”, Ray Bradbury imagines that a group of astronauts is sent on a mission to the Sun to collect a sample of solar material from its interior and bring it back to Earth. If such a mission were possible, we could study the chemical composition and possibly other physical properties of the Sun by means of direct measurements. In reality, we obviously cannot travel to the Sun nor to other stars and perform similar experiments. In order to quantitatively study the properties of stars, we have to rely on telescope and satellite observations of their emitted light. Nearly all the information we can access about stars comes, in fact, encoded in their starlight. By analysing the emitted stellar radiation, we can retrieve this information and deduce physical properties of stars. Accurate measurements of stellar brightness oscillations, for instance, can give us remarkable insight on the structure of stellar interiors even deep below the visible surfaces of stars. Also, a wealth of information can be extracted from stellar spectra about the physics, the origin, and the history of stars. Analyses of stellar spectra allow us to estimate important parameters, such as effective temperatures and gravities, investigate physical processes such as stellar winds, pulsations, and magnetic fields, as well as determine the evolutionary stages of stars. Furthermore, stellar spectra also carry the signatures of the chemical compositions of stars in form of absorption (or emission) lines at characteristic wavelengths corresponding to transitions between energy states of ions and molecules. Quantitative estimates of the elemental abundances in stars can be derived by means of spectroscopic analyses. Such information is of particular interest in astrophysics as it can be used to investigate fundamental aspects of stellar nucleosynthesis as well as of stellar, galactic, and cosmic chemical evolution. The determination of stellar chemical compositions therefore plays a central role in our understanding of the origin of elements and, ultimately, of the formation and evolution of galaxies, stars, and planetary systems.

Elemental abundances, however, cannot be directly measured from observed stellar spectra. In fact, the task of deriving accurate spectroscopic elemental abundances is not straightforward, but requires knowledge of the physical structure of the stellar layers responsible for the formation of the emergent stellar radiation. The light we receive from stars comes from a

\[\text{\footnotesize\footnote{However, it is noteworthy to mention NASA's Genesis Discovery probe (Burnett et al. 2003) which recently returned samples of solar wind material for high-precision measurements of their isotopic compositions in terms of oxygen, nitrogen, and noble gases. The data are currently being analysed.}}\]
relatively thin region at the stellar surface known as the photosphere. In the photosphere of the stars, photons experience their last interactions with the stellar plasma before escaping into space. The distribution of photons at the different wavelengths in the emitted stellar radiation depends not only on the chemical composition of the star but also on the physical structure of its atmospheric layers. In order to quantitatively decipher the information about elemental abundances contained in stellar spectra, it is therefore necessary to construct realistic models of the stellar atmospheric layers where the processes leading to the formation of the emergent fluxes are taking place. Such models can then be used to theoretically study the propagation of radiation through the photosphere and predict the strengths of spectral lines as a function of the chemical composition. Synthetic and observed spectral lines can then be compared to derive elemental abundances.

During the past three decades, the rapid advancements in observational technology have dramatically improved the quality and accuracy of spectroscopic data. The dominating uncertainties in most of the stellar abundance analyses carried out today are primarily due to inadequacies in the determination of stellar parameters, the model atmospheres, the spectral line formation calculations, or the atomic and molecular data, rather than to the limitations on signal-to-noise and resolution that can be achieved with the existing observational facilities (Gustafsson 2004a). In fact, nearly all spectroscopic analyses of late-type stars are currently still based on classical model atmospheres constructed under the simplifying assumptions of a stationary, 1D, homogenous, hydrostatic stratification, a rudimental treatment of convective energy transport, and local thermodynamic equilibrium for the radiative transfer and spectral line formation calculations. Given the numerous approximations involved, this approach can often lead to systematic errors in the predicted stellar atmospheric structures and line-strengths, and therefore in the derived stellar abundances. In order to use high-precision spectroscopic data at their full potential for abundance analyses, improvements in the realism of the modelling of stellar atmospheres and of spectral line formation are necessary. In the present work, I will discuss some examples of situations where such improvements can be done. In particular, in chapter 2, I will summarize the main aspects of spectral line formation outside local thermodynamic equilibrium, while, in chapter 3, I will briefly dwell upon hydrodynamical modelling of stellar atmospheres. In chapter 4 (Paper I), I will describe a study of the effects of line-blocking on the formation of neutral iron lines, and, in chapters 5 and 6, I will present the results of state-of-the-art three-dimensional, hydrodynamical simulations of red giant stars and their application to spectral line formation (Paper II) and to the abundance analysis of extreme halo stars (Paper III). Finally, future prospects will be discussed in chapter 7.
1.1 Definitions
In the following chapters I will make extensive use of some concepts which I define here below.

1.1.1 Source function and optical depth
The variation of monochromatic intensity in a given direction across a stellar atmosphere is described by the radiative transfer equation:

\[
\frac{dI_\nu}{ds} = j_\nu - \alpha_\nu I_\nu \tag{1.1}
\]

where \(j_\nu\) and \(\alpha_\nu\) are the emissivity and extinction coefficient at frequency \(\nu\), respectively, and \(s\) is the geometrical distance measured along the beam. The ratio of the extinction coefficient and the gas density defines the extinction cross-section per unit mass or opacity \(\kappa_\nu = \alpha_\nu/\rho\).

Equation Eq. 1.1 is normally re-written in the form:

\[
\frac{dI_\nu}{\alpha_\nu ds} = S_\nu - I_\nu \tag{1.2}
\]

where \(S_\nu = j_\nu/\alpha_\nu\) is the source function. According to Eq. 1.2, the formation of the emergent intensity at the stellar surface is determined by the variation of two parameters as a function of depth in the stellar atmosphere: the extinction coefficient, which measures the transparency of the medium, and the source function, which depends on the thermodynamic properties of both radiation and matter at a given location.

When studying radiative transfer through a stratified stellar atmosphere, it is convenient to introduce the concept of monochromatic optical depth, that is the integral of extinction with geometrical depth:

\[
\tau_\nu = \int_0^\infty \alpha_\nu dz \tag{1.3}
\]

The concept of optical depth is fundamental for spectral line formation. It makes it possible to quantitatively distinguish between transparent, optically thin (\(\tau_\nu < 1\)) and optically thick (\(\tau_\nu > 1\)) layers of a stellar atmosphere at frequency \(\nu\).

Finally, the disk-averaged flux emitted by a star per unit area on its surface is defined as the outgoing intensity \((I_\nu^+)\) in the direction of the observer averaged over the apparent stellar disk:

\[
F_\nu^{\text{surf}} = \int_{\text{disk}} I_\nu^+ d\Omega = \int_0^\pi \int_0^\pi I_\nu^+(\theta, \phi) \sin \theta d\theta d\phi \tag{1.4}
\]

where \(\theta\) and \(\phi\) are the polar coordinates on the surface of the star.
1.1.2 Equivalent width and curve-of-growth

Spectroscopic elemental abundances can be usually determined in two different ways. The first method consists in fitting observed spectral lines with theoretical (synthetic) ones by varying the elemental abundances in the spectral line formation calculations (assuming that the other relevant parameters of the model stellar atmosphere have been determined). This is the preferred method when spectral lines are severely blended. The second method, suitable mainly for unblended features, consists in comparing the theoretical equivalent widths of spectral lines with the observed ones. The equivalent width of a spectral line is defined as the integrated dip of the emergent flux profile of a spectral line normalized with respect to the continuum:

\[
W_{\lambda} = \int_{\text{line}} \frac{F_{\lambda}^{\text{cont}} - F_{\lambda}}{F_{\lambda}^{\text{cont}}}
\]

(1.5)

It corresponds to the width of a rectangular portion of spectrum completely blocking the emergent flux (Fig. 1.1). The main advantage of using equivalent widths for abundance determinations is that they are essentially insensitive to certain broadening mechanisms (such as rotational and instrumental broadening).

The equivalent width of a spectral line of a certain element naturally depends on the number density of absorbing particles in the stellar atmosphere and therefore on the elemental abundances; it also depends on the parameters of the transition, such as excitation potential of the lower level of the line and \(gf\)-value.\(^2\) The variation of the equivalent widths of spectral lines with elemental abundances also depends strongly on how the source function changes with depth. In particular, if the source function decreases monotonically outwards in the line formation layers of the atmosphere (as it normally does for typical photospheric lines), the equivalent width becomes larger as the elemental abundance increases. A graph specifying the dependence of the equivalent width on the elemental abundance is called curve-of-growth. The qualitative behaviour of the curve-of-growth for a typical transition is illustrated in Fig. 1.2). At relatively low abundances, the spectral line appears weak and the curve-of-growth follows a linear trend. As the abundance increases, the curve-of-growth approaches a saturation level and flattens; then, at even larger abundances, the line equivalent width begins to grow again, although less steeply than for weak lines\(^3\) (e.g. Gray 1992).

The detailed behaviour of the theoretical curve-of-growth for a given spectral line depends in general on the thermal structure of the adopted model stellar atmosphere, and on the approximations involved in the solution of the

\(^2\)The \(gf\)-value is the product of the statistical weight \(g\) of the lower level of the transition and the oscillator strength \(f\).

\(^3\)The equivalent width of strong lines scales approximately as the square root of the number density of the absorbing species while the strength of weak lines is linearly proportional to it.
Figure 1.1: The equivalent width of a spectral line corresponds to the width of a rectangular portion of fully blocked spectrum with the same area as the integrated flux absorbed by the line.

radiative transfer problem. This also implies that, in spectroscopic analyses, abundances derived comparing theoretical and measured equivalent widths are sensitive to the details of the model atmosphere and of the specific assumptions made in the spectral line formation calculations. Most of the work presented in this thesis consists in evaluating how different assumptions and approximations in the modelling of stellar atmospheres and line formation affect the behaviour of curves-of-growth and the determination of elemental abundances.
Figure 1.2: The curve-of-growth specify the dependence of the equivalent width $W_{\lambda}$ of a spectral line as a function of elemental abundance $\varepsilon$. Incidentally, it is customary in stellar astronomy to define the abundance of a certain element X in stellar atmospheres as $\log \varepsilon(X) \equiv \log N(X)/N(H) + 12$, where $N(X)$ and $N(H)$ are the number density of nuclei element X and hydrogen, respectively.
2. Spectral line formation

In stellar interiors, where the plasma reaches high densities and temperatures, collisions between particles occur at very high rates and fully control the energy partitioning of matter. All processes of excitation, ionization, and dissociation of particles in the gas are in equilibrium with each other and with the corresponding reverse processes. The distributions of velocities, excitation energies, and ionization fractions for not too dense gases follow, respectively, the Maxwell, Boltzmann, and Saha laws at the local kinetic temperature and are independent of the radiation field. When these conditions are fulfilled, local thermodynamic equilibrium (LTE) is said to hold.

Deep within stars, where opacities are high, the mean free paths of photons are small compared with the scales over which the thermodynamic state of the medium varies appreciably; under these conditions, photons are continuously emitted, re-absorbed, and thermalized, fully participating of the thermodynamics of the gas particles. At large optical depths, collisional processes dominate the expression of the source function which can then be approximated by the Planck distribution at the local temperature of the medium: \( S_\nu = B_\nu(T) \). Nonetheless, even deep in stellar interiors, the intensity of radiation is not exactly isotropic, making the net radiative flux different from zero and photons to slowly diffuse and carry energy outwards. As photons approach the stellar surface, where matter becomes increasingly more transparent to radiation, they begin to travel over larger distances, eventually reaching the optically thinnest layers of the photosphere and escaping into space. Because of the non-local nature of radiative transfer, the source function at a given location in the stellar atmosphere is not necessarily described by the Planck function at the local temperature. At the same time, as the temperature and density of the gas are lower in the upper layers of stellar photospheres, excitation, ionization, and dissociation processes in the gas are no longer exclusively controlled by collisions with other particles but are also directly affected by the interaction with radiation originating from deeper and hotter layers. Under these circumstances, the distributions of energy states and ionization stages are, in general, found to be out of equilibrium and do not follow the Saha-Boltzmann laws at the local kinetic temperature. The general cases in which energy distributions for matter depart from LTE are normally referred to with the term non-LTE.

In non-LTE, the variation with time and space of the number densities (or populations) \( n_i \) of gas particles (e.g. atoms, ions, molecules) in a certain state (excitation state and/or ionization stage) \( i \), at a given location in a stellar at-
mosphere, can be written in terms of a system of coupled equations of the following form:

$$\frac{dn_i}{dt} = \frac{\partial n_i}{\partial t} + \nabla \cdot (n_i u) = \sum_{j \neq i}^{N} n_j P_{ji} - n_i \sum_{j \neq i}^{N} P_{ij} \quad (2.1)$$

where $u$ is the bulk velocity of the gas and the $P_{ij}$ terms represent the transition rates from state $i$ to state $j$, per particle in state $i$. Naturally, beside fulfilling the rate equations Eq. 2.1, the populations $n_i$ must also satisfy the equations for conservation of charge and of the total number of nuclei of each element.

The transition rates $P_{ij}$ account for both radiative and collisional processes:

$$P_{ij} = R_{ij} + C_{ij} = A_{ij} + B_{ij} J_\nu + C_{ij} \quad (2.2)$$

where $A_{ij}$, $B_{ij}$, and $C_{ij}$ respectively denote the Einstein coefficients for spontaneous radiative emission, radiative absorption/stimulated emission, and collisional excitation/de-excitation, and $J_\nu$ represents the intensity averaged over the whole solid angle and over the profile of the radiative transition from state $i$ to $j$. The radiative transition rates ($R_{ij}$ in Eq. 2.2) therefore depend on the value of the intensity at all angles and virtually all frequencies, which is computed by solving the radiative transfer equation. The solution of the latter equation, in turn, depends on the expression of the source function $S_\nu$ which, in non-LTE conditions, is a function of the populations $n_i$. This situation demonstrates the complexity of the general non-LTE problem that requires the simultaneous solution of a non-linear system of time-dependent rate equations fully coupled with each other and with the radiative transfer equation.

In most cases, the problem of determining the populations $n_i$ is usually simplified by considering a steady state solution ($\partial / \partial t = 0$) and neglecting the advective terms ($u = 0$), so that the rate equations Eq. 2.1 become:

$$\sum_{j \neq i}^{N} n_j P_{ji} - n_i \sum_{j \neq i}^{N} P_{ij} = 0 \quad (2.3)$$

which is the so-called statistical equilibrium approximation. Even with the assumption of statistical equilibrium, the complexity of the system remains very large due to the non-linearities involved and the strong coupling between rate equations and the radiative transfer equation. Incidentally, LTE can be considered as an extreme case of statistical equilibrium in which collisional rates $C_{ij}$ dominate over radiative rates $R_{ij}$. When LTE holds, the rate equations Eq. 2.3 and the radiative transfer equation de-couple from each other and can be solved independently. Under the assumption of LTE, the strength of a given spectral line can be directly computed from the parameters of the line and of the corresponding absorbing species (element or molecule) alone, once the continuous opacities and the temperature structure of the model atmosphere (and therefore the source function) are known. In general, however, the radiative rates for transitions in the visible and the UV are often comparable or even
much higher than the collisional ones, implying that the assumption of LTE fails. Outside LTE, populations and frequency-dependent variables all depend on each other and the solution of the non-LTE problem cannot be derived straightforwardly, but normally requires an iterative numerical approach.

The introduction of the approximated lambda operator and accelerated lambda iteration techniques (e.g. Scharmer 1981; Scharmer and Carlsson 1985; Olson et al. 1986; Rybicki and Hummer 1991) has made it possible to perform non-LTE calculations with very large and complex model atoms. In particular, the non-LTE calculations presented in this thesis have been carried out with the statistical equilibrium code MULTI by Carlsson (1986) which is based on the numerical scheme developed by Scharmer and Carlsson (1985). The code iteratively solves the radiative transfer and statistical equations and allows the computation of detailed non-LTE spectral profiles for lines of a given element within the framework of 1D plane-parallel model stellar atmospheres. The code implicitly assumes that the element under consideration is a trace element; this means that the results of the statistical equilibrium calculations do not feed back into the structure of the model atmosphere nor affect significantly the continuous opacities.

2.1 Non-LTE mechanisms

As mentioned above, LTE is actually a limiting case of statistical equilibrium, holding under very specific conditions. However, as it simplifies enormously the solution of the radiative transfer, the assumption of LTE is commonly used in spectral line formation calculations and has therefore become the standard method of abundance analysis for late-type stars. This can create the false impression that departures from LTE rarely occur in reality and that a full treatment of non-LTE is required in rather exceptional cases only. Given the intrinsic non-locality of radiative transfer and the non-linear coupling with the statistical equilibrium equations, one could instead expect LTE to be the exception. In practice, however, it is customary to talk about non-LTE effects, with LTE implicitly considered as the reference point. In the following, I will briefly discuss the most common mechanisms leading to departures from LTE in late-type stars.

If the mean intensity is higher than the Planck function \( J_\nu > B_\nu \) at frequencies where important bound-free transitions are located, the photo-ionization (i.e. radiatively induced ionization) rates can become sufficiently large to produce significant over-ionization with respect to the LTE expectation. For species which are ionized to a considerable degree in stellar atmospheres, over-ionization can lead to a significant reduction of line opacities and, in turn, of line strengths. The condition \( J_\nu > B_\nu(T) \) required by over-ionization occurs when \( B_\nu(T) \) increases rapidly inwards with optical depth. In this case, the mean intensity in the optically thin regions of the
stellar atmosphere reflects the higher temperatures of the layers deeper in, so that \( J_\nu \) becomes larger than the local value of \( B_\nu \). According to the Eddington-Barbier approximation (e.g. Rutten 2003), the mean intensity at the stellar surface can in fact be approximated as

\[
J_\nu(\tau_\nu = 0) \approx \frac{1}{2} S_\nu(\tau_\nu = 1/2) \tag{2.4}
\]

This shows that, if the source function increases too rapidly inwards then the mean intensity \( J_\nu \) in the uppermost photospheric layers will locally exceed \( S_\nu \) and, in practice, also \( B_\nu \).\(^1\) In late-type stars, the gradient of \( B_\nu \) with respect to optical depth may become sufficiently steep at ultraviolet (UV) frequencies for the above condition to occur. The efficiency of the over-ionization mechanism depends on the characteristic parameters of the stellar atmosphere. In particular, over-ionization is expected to be stronger at higher effective temperatures, lower surface gravities, or in metal-poor\(^2\) stars. Naturally, efficient collisional processes in stellar atmospheres can, on the other hand, counteract the mechanism of over-ionization (e.g. Asplund 2005; Collet et al. 2005). The opposite of over-ionization is over-recombination, which takes place when the gradient of the Planck function with optical depth is relatively shallow so that \( J_\nu < B_\nu \), as in the infrared (IR) region of late-type stellar spectra.

The analogue of over-ionization for bound-bound transitions is over-excitation or photon-pumping. In this case, the condition \( J_\nu > B_\nu(T) \) at the line frequency can cause over-population of the upper level of the transition. As a consequence of this, stimulated emission increases and the line tends to become weaker than in the LTE case. The opposite mechanism is called under-excitation and, similarly as for over-recombination, can take place when \( J_\nu < B_\nu \).

An interesting non-LTE mechanism is also photon suction (Bruls et al. 1992), which can occur in presence of a direct sequence of resonance transitions with large oscillator strengths from close to the ionization limit down to lower energy levels. The combined effect of photon losses in these resonance lines can lead to \( J_\nu < B_\nu \), causing a replenishment of lower levels from a large population reservoir in the next ionization stage (see also Asplund 2005).

Finally, a typical effect of the non-locality of radiative transfer in stellar atmospheres is resonance scattering. For strong resonance lines, a usual simplification of this process is to treat the absorbing ions or molecules as two-level systems. Under this approximation, the source function at the resonance frequency can be written as:

\[
S_\nu = \epsilon_\nu B_\nu + (1 - \epsilon_\nu) J_\nu \tag{2.5}
\]

\(^1\)Under the two-level approximation illustrated later in this section, \( J_\nu > S_\nu \) implies \( S_\nu \geq B_\nu \).

\(^2\)In astronomy, it is customary to refer to all elements heavier than hydrogen and helium as “metals”.
where $\varepsilon_\nu$ is the photon \emph{destruction probability}, i.e. the probability that photons be absorbed and thermalized when they interact with gas particles. Strong resonance lines experience a shallow Planck function gradient with monochromatic optical depth; this implies that the mean intensity $J_\nu$ remains below $B_\nu$ in the line formation region and that $S_\nu < B_\nu$, making the line stronger than when scattering is neglected.

\section{2.2 Non-LTE line formation}

The strength of a given spectral line of a trace element computed in non-LTE can differ from the value predicted in LTE because of two reasons. The first one is that the opacity in the line may be different in the two cases. A different line opacity in non-LTE compared with LTE directly reflects a change in the density of absorbers in the line. It is convenient to define the \emph{departure coefficient} for level $i$ as the ratio of non-LTE to LTE number densities of particles in state $i$: $b_i = n_i/n_{i,\text{LTE}}$. If the departure coefficient for the lower excitation level of a line is $b_l < 1$ then the non-LTE line formation region is shifted inwards compared with the LTE case. In practice, this usually means that the line becomes stronger under the assumption of LTE than in non-LTE. In this particular case, this also implies that a lower abundance is required in LTE to reproduce a given equivalent width. Naturally, the opposite can also occur, and for $b_l > 1$ the non-LTE line formation region is shifted outwards with respect to LTE. A change in line opacity, however, does not always necessarily translate into an appreciable change of line strength: differences between the non-LTE and LTE source functions have also to be considered. The second reason why the strength of a line may be different in non-LTE compared with LTE is, thus, that the line source function deviates from the Planck function (LTE). Assuming complete redistribution,\footnote{“Complete redistribution” means that a photon resulting from de-excitation is not correlated with the photon that was responsible of the excitation (Rutten 2003).} the non-LTE line source function, i.e. the ratio of emissivity and extinction coefficient in the line, can be written as:

\begin{equation}
S_\nu = \frac{2h\nu^3}{c^2} \frac{1}{b_l b_u e^{h\nu/kT} - 1}
\end{equation}

If, for a weak spectral feature, the non-LTE line source function is larger than the Planck function in the line formation region, then the line becomes weaker in non-LTE. In this case, the elemental abundance derived in non-LTE from the measured equivalent width of a line is larger than the one predicted under the assumption of LTE.

In practice, one has to take into account both the changes in line opacity and source function to interpret the differences between non-LTE and LTE spectral line formation calculations and abundance analyses.
3. Stellar convection

3.1 The role of convection in stars

In stellar interiors and envelopes, energy can be carried outwards not only by means of radiation transfer but also by convection, i.e. by bulk motions of matter. Convection zones are expected to be present in regions of the star where energy transport by radiation alone would require the temperature gradient to be exceedingly steep, creating the conditions for an instability. As the variation of pressure with depth is largely determined by quasi-hydrostatic equilibrium, in order to compensate for a steep temperature gradient, the gas density should decrease rather slowly outwards, or possibly even increase, leading to an unstable stratification. Let’s assume now that the structure is perturbed and that an element of gas is displaced outwards, expanding adiabatically to respond to the change in pressure. If the vertical density gradient is too shallow the density in the element might end up being lower than in the surrounding gas: instead of returning to its original position, the element would keep moving outwards driven by buoyancy. Similarly, elements of gas rapidly cooling and becoming denser than the surroundings would keep sinking because of buoyancy in such a stratification. This is the so-called convective instability (Schwarzschild 1906). By displacing warm material upwards from the interior and bringing cooler gas down from upper layers, convective motions effectively produce a net outward flux of heat. In the presence of convection, the amount of flux that radiation has to carry outwards to maintain the stellar structure in a quasi-equilibrium configuration is consequently reduced and the thermal stratification can adjust in favour of a shallower mean temperature gradient.

Besides being a fundamental mechanism of energy transport in stars, convection also plays an important role in many other aspects of stellar structure and evolution (see e.g. Stein and Nordlund 1998). Convection constitutes an efficient way of thoroughly mixing material in stellar interiors and transporting angular momentum outwards. Convective motions modulate and alters the frequency of $p$-mode oscillations that can be used to probe stellar interiors by means of asteroseismology. Furthermore, convection can also generate magnetohydrodynamic waves supplying energy to stellar chromospheres. Also, its interaction with rotation is believed to drive stellar dynamos responsible for the evolution of magnetic fields in solar-like stars.

In late-type stars, the convection zone extends over a significant fraction of the stellar radius, reaching the stellar surface and overshooting beyond the
convectively unstable deeper layers into the upper photosphere. Convection therefore significantly affects the temperature-density structure and the dynamics of gas flows in those layers of the star ultimately responsible for the emergent stellar flux.

3.2 Signatures of stellar convection

A glimpse at the surface of the Sun in fact immediately reveals that the solar photosphere is dominated by granulation (e.g. Title et al. 1990; Spruit et al. 1990; Carlsson et al. 2004) which is the observable manifestation of the bulk flows of matter in the convection zone deeper inside: a complex, continuously evolving pattern of broad, bright regions (the granules) with warm upflowing material in the midst of narrow, cool, dark downdrafts (intergranular lanes). Observational diagnostics of stellar convection and granulation in general are limited by the fact that direct imaging of the surfaces of most other stars is still beyond the capabilities of present instruments. Nonetheless, other characteristic observational signatures of surface convection in late-type stars can be found by looking at high-resolution stellar spectra (e.g. Dravins 1982, 1987a,b; Allende Prieto et al. 2002). The presence of velocity fields and correlated temperature and density inhomogeneities in the photospheres of late-type stars influences thus the shapes of absorption lines and their positions in the observed spectra. Observed spectral line profiles are the result of the integrated contribution to radiative flux in the absorption line from all points across the stellar disk. Lines tend to be stronger in the granules than in the intergranular lanes because the temperature structure is typically steeper in the upflows than in the downdrafts (see discussion in Asplund 2005, and references therein). The flux in the continuum is also higher in the granular regions since the gas in the upflows is warmer at the level of the optical surface. Furthermore, lines forming within granular regions appear blue-shifted relatively to their rest-frame wavelengths as the ascending gas is moving away from the stellar surface; on the contrary, lines forming in connection with downflows appear red-shifted. As a consequence of the inhomogeneities and the different area coverage of granules and intergranular lanes, observed disk-integrated spectral line profiles in solar-like stars are characterized by asymmetries and wavelength shifts that provide a sensitive probe of the temperature and velocity structures in stellar atmospheres.

1Among the few notable exceptions, apart the Sun, is Betelgeuse (α Ori) whose surface was resolved for the first time using the Hubble Space Telescope.
3.3 Stellar convection and 1D model atmospheres

The vast majority of spectroscopic abundance analyses of late-type stars carried out today involve theoretical 1D model atmospheres constructed under the assumptions of plane-parallel geometry or spherical symmetry, hydrostatic equilibrium, and flux constancy. Examples of widely used numerical codes for 1D modelling of stellar atmospheres include the MARCS (Gustafsson et al. 1975; Plez et al. 1992; Asplund et al. 1997, Gustafsson et al. 2006, in preparation); ATLAS (Kurucz 1993a), and PHOENIX/NEXTGEN (Hauschildt et al. 1999) programs. The assumption of a 1D stratification implies that all physical variables are treated as a function of depth or distance from stellar centre only and that inhomogeneities across surfaces of constant depth are neglected. Also, magnetic fields and their effect on the atmospheric structure are commonly neglected. The requirement of flux constancy throughout the atmosphere is introduced to prevent energy from piling-up in layers and to maintain the structure of the model in a stationary configuration. The simplifying approximation of LTE concerning the interaction between radiation and matter is also normally adopted, although theoretical 1D non-LTE statistical equilibrium model atmospheres have been recently developed for solar-type and red giant stars (Anderson 1989; Hauschildt et al. 1999; Short and Hauschildt 2003).

As mentioned previously, convective flows can reach the surface of late-type stars and significantly affect the photospheric thermal stratification. Therefore, it is essential to take into account the effects of convection for properly modelling the structure of late-type stellar atmospheres and accurately understanding the formation of stellar spectra. Convection, however, is a complex, highly non-linear, non-local, chaotic, and intrinsically multi-dimensional process. The treatment of convection in the framework of 1D models of stellar structure is inevitably plagued by fundamental limitations and can only rely on rudimentary and incomplete descriptions. In 1D model stellar atmospheres, convective energy transport is normally accounted for by means of some approximate scheme such as the mixing length theory (Biermann 1932; Böhm-Vitense 1958) or other local convection models (Canuto and Mazzitelli 1991). The central assumption behind these 1D formulations is that warm, ascending material in the convectively unstable regions of the star must completely mix with cooler, descending gas over a certain distance $\ell$ (commonly referred as the mixing length) that is normally assumed to be proportional to the pressure scale height $H_P \equiv (d \ln P/dz)^{-1}$. In the mixing length formulation, the convective energy flux can be directly expressed as a simple function of $\ell$. The proportionality constant relating $\ell$ to $H_P$ is not supplied in a self-consistent way by the theory and is therefore necessarily regarded as a free tunable parameter. Empirical calibration of

\textsuperscript{2}Incidentally, the mixing length theory and its derivatives also rely on a number of other adjustable parameters beside the proportionality factor between $\ell$ and $H_P$.  

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the proportionality factor is possible for stellar interior calculations where the stellar radius is a function of the mixing length; the latter is found to be approximately equal to 1.5 pressure scale heights. Calibrations for stellar atmospheres are less straightforward, thus values of the order of 1.5 pressure scale heights are also typically adopted (Gray 1992).

3.4 1D spectral line formation: micro- and macro-turbulence

Even though the mixing length theory and its analogues might provide a crude estimate of the fraction of energy flux transported by convection, classical, hydrostatic, 1D model atmospheres still cannot self-consistently predict temperature-density inhomogeneities nor reproduce the complexity of the convective velocity fields present in the photospheres of late-type stars. Such velocity fields not only are responsible for the asymmetries observed in the absorption profiles, but also contribute significantly to non-thermal broadening of spectral lines associated with Doppler shifts. Accounting for such non-thermal broadening is necessary in order to derive accurate elemental abundances based on the analysis of partially saturated spectral lines (on the non-linear part of the curve-of-growth). Two additional fudge parameters, micro- and macro-turbulence, are introduced in 1D spectral line formation calculations in order to compensate for the shortcomings of classical 1D hydrostatic model atmospheres and their lack of internally consistent velocity fields.

Micro-turbulence enters 1D spectral line formation as a convolution of the local distribution of thermal velocities in the gas with an additional velocity distribution generally assumed to be isotropic and Gaussian. In essence, this implies that the Doppler width, i.e. wavelength dispersion due to Doppler shifts of a line absorption profile, is adjusted as:

$$\Delta \lambda_D = \frac{\lambda}{c} \sqrt{\frac{2kT}{m} + \xi^2}$$  \hspace{1cm} (3.1)

where $\lambda$ is the central wavelength of the absorption line, $2kT/m$ is proportional to the root-mean-square thermal velocity of the absorbing particles with mass $m$, and $\xi$ is the dispersion of the micro-turbulence velocity distribution. The main effect of adding micro-turbulence in 1D line formation calculations is to increase the equivalent widths of saturated or partially saturated lines while leaving unaltered the overall strength of weak lines. In 1D spectroscopic analyses, trends of elemental abundances as a function of line strength can be eliminated or significantly reduced by appropriately tuning the value of the micro-turbulence parameter. Macro-turbulence is instead defined as a convolution of the emergent flux (or intensity) profile with a random (usually Gaussian) velocity distribution. The parameter is normally introduced to account for blurring processes due to large-scale photospheric flows in which
the equivalent width of spectral line profiles is essentially conserved (e.g. Gray 1992).

Contrary to what their names seem to suggest, these two parameters are most probably not at all related to turbulence in its conventional physical meaning (Asplund et al. 2000). According to a more physical interpretation, the micro-turbulence parameter accounts, at least for solar-type stars, for non-thermal velocity gradients along the line of sight in the line formation region, i.e. variations of the convective flow velocity occurring on scales that are small compared with unit optical depth (Dravins and Nordlund 1990). The macro-turbulence instead is supposed to model the effects of the variations of the convective velocity component in the line of sight over scales that are large compared with unit optical depth.

The use of free adjustable parameters (mixing length, micro- and macro-turbulence) in 1D line formation calculations casts doubts on the accuracy of elemental abundance analyses based on 1D model atmospheres. As these parameters are not based on a robust theoretical foundation, they generally require to be specifically calibrated for individual observed stellar spectra by means of a semi-empirical procedure. Errors in the calibration of the free parameters can directly translate into uncertainties in the derivation of effective temperatures, surface gravities, and chemical compositions of stars. More importantly, calibration of micro-turbulence and macro-turbulence parameters can erroneously mask shortcomings in the approximations used for solving the radiative transfer equation, in the treatment of non-thermal broadening mechanisms (e.g. hyperfine splitting), or in 1D modelling of stellar atmospheres. Also, classical 1D line formation calculations using standard micro-turbulence and macro-turbulence parameters completely fail in reproducing asymmetries and wavelength shifts of spectral line profiles arising from the correlation between temperature and velocity structures. Furthermore, the observable manifestations of stellar surface convection suggest that the assumptions of flux constancy and hydrostatic equilibrium force the atmospheric structure into an unrealistic and unstable stationary configuration. The use of 1D model atmospheres as a tool for quantitatively interpreting observational data is therefore questionable and can lead to systematic errors in the derivation of elemental abundances.

3.5 Hydrodynamical simulations of stellar convection

During the past two or three decades, advances in computer technology and the development of efficient numerical algorithms have made it possible to perform realistic 3D hydrodynamical simulations of stellar surface convection (Dravins et al. 1981; Nordlund 1982; Nordlund and Dravins 1990; Stein and Nordlund 1998; Asplund et al. 1999; Freytag et al. 2002; Ludwig et al. 2002; Carlsson et al. 2004; Vögler 2004). In these numerical simulations, the
assumptions of a homogeneous 1D stratification, hydrostatic equilibrium, and flux constancy are relaxed, and the dynamics and evolution of bulk flows in the convectively unstable layers as well as in the overshooting regions are studied in detail as a function of time in full 3D geometry. State-of-the-art numerical modelling of stellar surface convection typically solves the standard equations for conservation of mass, momentum, and energy together with the 3D radiative transfer equation using realistic equation-of-state and opacities; much work has been devoted in recent years to also include magnetic fields and study their interaction with convection. The radiative-hydrodynamical equations are generally solved for a representative volume of the stellar surface (box-in-the-star models) encompassing several pressure scales vertically and covering several granules horizontally. Simulations of supergiants (Freytag et al. 2002) require instead the whole atmosphere to be included in the computational domain (star-in-the-box models) as the characteristic scales of the largest convective elements at the stellar surface are comparable to the radii of these stars.

Three-dimensional convection simulations open up new possibilities for stellar spectroscopy where they can be used as time-dependent model stellar atmospheres to study the impact of inhomogeneities and velocity fields on the formation of spectral lines and on abundance analyses. Recent spectroscopic analyses based on state-of-the-art 3D time-dependent simulations of surface convection in the Sun (Asplund et al. 2005, and references therein) have led to a systematic downward revision of the solar photospheric abundances by almost a factor of two compared with the widely used compilation of Anders and Grevesse (1989). Line formation calculations based on 3D hydrodynamical model atmospheres of dwarfs and subgiants (e.g. Asplund et al. 1999; Asplund and García Pérez 2001; Nissen et al. 2002) indicate that the structural differences between 3D simulations and 1D hydrostatic model stellar atmospheres can have a significant impact on the predicted strengths of synthetic spectral lines and hence on the derivation of elemental abundances. The effects are particularly severe for very metal-poor stars where the differences between the 1D and mean 3D stratifications are largest.

Carrying out 3D time-dependent simulations of surface convection is inherently a more computationally demanding task than modelling stellar atmospheres in 1D. While extended grids of 1D model atmospheres exist covering a wide range of combinations of stellar parameters, the availability of 3D model atmospheres suitable for spectral line formation calculations and abundance analyses is still rather limited. So far, 3D hydrodynamical model atmospheres have been constructed for main sequence stars and subgiants of spectral types A to M at different metallicities, with much attention devoted in particular to the Sun and solar-like stars. Convection simulations of red giants are, however, currently being developed (Collet et al. 2006a,b; Kucinskas et al. 2006). In this thesis, I will present recent results on 3D hydrodynamical modelling of red giant stellar atmospheres with varying metallicities and
effective temperatures and discuss some of their applications to spectral line formation calculations and, in particular, to abundance analysis.

3.6 Stellar surface convection simulations: ingredients

The simulations of surface convection in red giant stars discussed in this thesis have been carried out using the 3D, time-dependent, radiative-hydrodynamical, compressible, code by Stein and Nordlund (1998). The simulations are of the box-in-the-star type (see Sec. 3.5): the hydrodynamical equations of mass, momentum, and energy conservation are solved for a representative cubic volume of stellar surface extending from the optically thin photospheric layers down to the upper part of the convectively unstable zone. The dimensions of the computational domain are chosen to be sufficiently large to typically cover $\gtrsim 10$ pressure scales and about 10 granules at the surface. In terms of continuum optical depth at $\lambda = 5000$ Å, the simulations extend from $\log \tau_{5000} \approx -5$ down to $\log \tau_{5000} \approx 7$. The fluid in this domain is highly stratified: the gas density and pressure vary with depth by several orders of magnitude between the upper and lower boundaries of the simulations. For the purposes of the numerical discretization, it is convenient to formulate the hydrodynamical equations in terms of the logarithmic derivatives of gas density $\rho$ and pressure $P$:

\begin{align}
\frac{\partial \ln \rho}{\partial t} &= -\mathbf{u} \cdot \nabla \ln \rho - \nabla \cdot \mathbf{u} \quad (3.2) \\
\frac{\partial \mathbf{u}}{\partial t} &= -\mathbf{u} \cdot \nabla \mathbf{u} + \frac{P}{\rho} \nabla \ln P + \nabla \cdot \mathbf{\sigma} \quad (3.3) \\
\frac{\partial e}{\partial t} &= -\mathbf{u} \cdot \nabla e - \frac{P}{\rho} \nabla \cdot \mathbf{u} + Q_{\text{rad}} + Q_{\text{visc}} \quad (3.4)
\end{align}

where $\mathbf{u}$ is the flow velocity and $e$ the internal energy per unit mass; $g$ is the acceleration of gravity, $\mathbf{\sigma}$ the viscous stress tensor, and $Q_{\text{rad}}$ and $Q_{\text{visc}}$ represent the radiative heating/cooling and viscous dissipation rates per unit mass, respectively. Magnetic fields have been neglected in the present simulations, as the scope of this study is primarily to investigate the difference between hydrostatic and hydrodynamical model atmospheres. Also, magnetic fields are expected to be weak in giant stars such as the ones considered in the present work.

The hydrodynamical equations 3.2–3.4 are discretized and solved on a non-staggered Eulerian rectangular mesh with $100 \times 100 \times 125$ grid-points in the simulations of red giants presented here. Spatial derivatives are calculated using third-order splines representations of the hydrodynamical variables. A third-order leapfrog predictor-corrector explicit scheme (Hyman 1979) is used to integrate the equations with respect to time. A hyper-viscosity is introduced to stabilize the numerical solution and to
remove spurious short-wavelength oscillations without damping modes with longer wavelengths (Stein and Nordlund 1998).

An accurate representation of the processes of energy exchange between matter and radiation is needed in order to produce a realistic description of the structure of the stellar surface layers. The radiative heating/cooling rate is calculated from the integral

\[ Q_{\text{rad}} = \int_{\lambda} \int_{\Omega} \kappa_\lambda (I_{\lambda,\Omega} - S_{\lambda}) d\Omega d\lambda \]  

(3.5)

In order to compute the monochromatic intensity \( I_\lambda \) as a function of wavelength and estimate \( Q_{\text{rad}} \), the 3D radiative transfer equation is solved at each time-step and for each point at the surface along eight inclined rays and the vertical using a Feautrier-like long-characteristic method. A shorter but finer depth grid, extending down to optical depth \( \tau \approx 2.5 \), is used to achieve a higher numerical accuracy for the solution; the results are subsequently interpolated back to the original grid. At larger optical depths, radiative transfer is computed instead under the diffusion approximation. In order to ease the computational burden, LTE without scattering terms in the source function \( S_\nu = B_\nu \) is assumed throughout the calculations. Line-blanketing is accounted for using an opacity binning technique (Nordlund 1982). Wavelengths are sorted into four groups (bins) representing lines with varying strengths plus the continuum; for each bin, pseudo-Planck functions are computed and stored in a look-up table together with the opacities and the equation-of-state. In spite of all the simplifications involved, it is worthwhile to mention that the solution of the radiative transfer still remains the most time-consuming part of the simulations.

State-of-the-art input physics is used in order to make the simulations as realistic as possible. The equation-of-state is adopted from Mihalas et al. (1988) and accounts for ionization, excitation, and dissociation of 15 of the most abundant elements plus the \( \text{H}_2 \) and \( \text{H}_3^+ \) molecules. Continuous opacities come from the Uppsala package (Gustafsson et al. 1975, and subsequent updates), while line opacities are adopted from Kurucz (1992, 1993b). We employ transmitting boundaries at the top and bottom of the simulation domains and periodic boundaries horizontally. The latter condition is acceptable for box-in-the-star type simulations if effects of curvature at the surface are negligible with respect to the width and depth of the domain. At the same time, one implicitly assumes also that the computational domain is sufficiently large so that the stellar surface structure and the convection pattern are well-represented by the sampled volume. The upper boundary is placed as high as possible to minimize the effects of numerical artefacts on the structure of the optically thin layers of the simulations. The lower boundary is located at sufficiently large depth to ensure that the inflowing gas at the bottom be isentropic. The input parameters of the simulations are the surface gravity, the overall chemical composition, and the entropy of the inflowing material at the lower boundary.
Contrary to what is assumed for classical, 1D, hydrostatic model atmospheres, the effective temperature is not a constant, but fluctuates with time, depending on the evolution of the photospheric granulation structure.

3.7 The on-set of convection

Hydrodynamical simulations of the solar surface clearly illustrate the fundamental importance of radiative cooling as the driving mechanism of surface convection (Stein and Nordlund 1998). As the ascending, isentropic gas approaches the optical surface, radiation starts to escape, which leads to cooling. In the outer layers of the Sun and late-type stars in general, the opacity is very temperature sensitive; this means that lowering the temperature causes a significant reduction of the continuous opacities, allowing, therefore, radiation to escape more easily and gas temperature to decrease even further. This positive feedback produces a sudden drop in the gas temperature from about 10000 K to less than 5000 K within a relatively narrow region in the photosphere. By cooling, the gas loses entropy, becomes negatively buoyant, and is eventually accelerated downwards. Almost all the buoyancy work is in fact done by downflowing material, with the upflowing gas being pushed towards the surface because of mass conservation. This description of convection is valid not only for the Sun but also for late-type stars, including the red giant simulations presented in the following chapters.

3.8 3D spectral line formation

The simulations are carried out for sufficiently long time to allow for thermal relaxation and follow the evolution of the granulation pattern for several turnover time-scales. The resultant physical structure from the simulations can then be used as time-dependent 3D hydrodynamical model atmospheres to study the formation of spectral lines.

The full convection simulations extend well down below the visible layers of the photosphere; for the purpose of spectral line formation, they are therefore interpolated to a finer vertical depth-scale with the same number of points but extending only down to log $\tau_{5000} \geq 2.5$ in the continuum. At the same time, the horizontal resolution of the 3D simulations is decreased to $50 \times 50$ to reduce the computational burden, without, however, significantly compromising the accuracy of the results.

The 3D line formation calculations presented here are performed under the assumption of LTE, with the source function given by the Planck function and scattering implemented as true absorption. The assumption of LTE is certainly a major simplification for line formation calculations when dealing with the structural complexity and the inhomogeneities of 3D model stellar
atmospheres. However, as briefly discussed in Chapter 2, the assumption of LTE is often questionable. A 3D non-LTE approach is in general required to make realistic predictions about the strengths of spectral lines for the purposes of high-precision abundance analyses. A full 3D non-LTE analysis, however, goes beyond the scope of the present work, and is postponed to a future study.

Another issue is the treatment of scattering as true absorption. Scattering (in particular Rayleigh scattering of H I) can contribute significantly to the total continuous extinction in the UV and blue part of the spectrum. At these wavelengths, a large contribution of scattering to continuous extinction implies that the radiation field in the continuum forming regions reflects the physical conditions in deeper and hotter layers (see Sec. 2.1); treating scattering as true absorption in the UV therefore could underestimate the flux in the continuum and the strength of spectral lines. This approximation is further discussed in Sec. 5.4. Spectral line profiles are calculated for typically 60 to 100 wavelength points; opacities and source function are computed in detail for each wavelength point, at all depth points in the 3D model atmospheres. The 3D radiative transfer equation is solved numerically for all wavelength points along nine directions (including the vertical) using a Feautrier-like method similarly as for the convection simulations. Test calculations performed using a larger number of rays (32 plus the vertical) indicate that the procedure is accurate enough in reproducing disk-averaged profiles: the differences between elemental abundances determined with our procedure and the test cases are typically less than 0.01 dex (Paper II). The line formation calculations are performed for a number of representative snapshots selected from the full time sequences in order to take into account the effects of the temporal evolution. Test calculations ensure that 10 to 30 snapshots are typically sufficient to obtain statistically significant predictions for the strength of spectral lines and for the purposes of abundance determinations.

From the spatially resolved intensity profiles at the different angles and for the different snapshots, temporally averaged disk-integrated flux-profiles are computed from which the equivalent widths of spectral lines are predicted. The underlying assumption here is that temporal averaging over several snapshots of a box-in-the-star simulation are equivalent to spatial averaging over the whole disk of the star. It is noteworthy that none of the ad-hoc adjustable parameters hampering 1D line formation calculations (i.e. micro- and macro-turbulence) are necessary in 3D: Doppler shifts caused by the velocity fields inherent to the hydrodynamical simulations are fully accounted for in the 3D calculations and are sufficient to reproduce non-thermal broadening and asymmetries of spectral lines associated with convective motions, at least in convection simulations of solar-type stars.

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3It is also possible to take into account rotational and instrumental broadening, although they affect only on the shapes of line profiles, leaving equivalent widths unaltered.
Figure 3.1: Normalized flux profiles of a neutral iron line (Fe I 3727.6 Å) predicted using 3D hydrodynamical (black line) and 1D hydrostatic (gray line) model atmospheres for the extreme halo giant star HE0107−5240. The stellar parameters of the models and the details of the line formation calculations are described in Paper III. The 3D and 1D profiles were computed for the same iron abundance $\log \epsilon(\text{Fe}) \equiv \log N(\text{Fe})/N(\text{H}) + 12 = 2.01$. A micro-turbulence of $\xi = 2.0$ km s$^{-1}$ is adopted for the 1D calculations. The large differences between the temperature stratifications of the two models translate into differences in the predicted line strengths. Also, the velocity fields inherent to the 3D hydrodynamical model induce wavelength shifts and asymmetries in the emergent line profile. The black dashed line represents the line bisector, which is constructed connecting the midpoints of line segments running horizontally between the sides of the line profile; the curved shape of the bisector is an indicator of the asymmetry of the line. The 1D profile, on the contrary, is perfectly symmetric.
Iron plays a fundamental role in stellar physics as well as in cosmic chemical evolution. Because of the internal complexity of the iron atom, an enormous number of Fe spectral lines (literally millions) are present in the ultraviolet (UV), visible, and infrared (IR) regions of the spectrum. These lines contribute significantly to the total line opacity in stellar atmospheres and envelopes and can therefore have major effects on the structure and evolution of stars. Accurate determinations of Fe abundances in stars are fundamental for our understanding of cosmic and Galactic chemical evolution. Iron is produced and ejected into the interstellar medium in connection with supernovae type Ia and II. The trends of elemental abundance ratios (such as \([\text{C}/\text{Fe}],\) \([\text{O}/\text{Fe}],\) etc.) with respect to \([\text{Fe}/\text{H}]\) in stellar populations are therefore used for inferring the properties of the mechanisms of chemical enrichment and mixing in galaxies as a function of time (or number of exploded supernovae) and to test theoretical models of Galactic chemical evolution. For these and other reasons, the abundance of iron is generally adopted as an indicator of the overall metal content in stars.

In late-type stars, a large number of Fe I lines with well-determined parameters are accessible for stellar spectroscopic analyses. The derivation of Fe abundances from these lines, however, is not a straightforward task. The formation of Fe I spectral lines is, in these stars, subject to departures from LTE. In their pioneering work, Athay and Lites (1972) have identified over-ionization (Sec. 2.1) as the main non-LTE physical mechanism for iron. Most of the important photo-ionization transitions of Fe I, in fact, have their edges in the UV part of the spectrum. In the upper photospheric layers of late-type stars, the radiation field in the UV continuum typically exceeds the Planck function at the local temperature, thus favouring radiatively induced ionizations over recombinations. This mechanism can lead to significant underpopulation of all Fe I levels compared with the LTE predictions, ultimately affecting the strengths of Fe I lines and the Fe abundance determinations.

In recent years, various theoretical investigations have addressed the problem of quantifying the magnitude of non-LTE effects on Fe I line formation but with conflicting results. Particularly large divergences among the different studies are found in Fe abundance analyses of metal-poor stars. Some authors

\[ [\text{A}/\text{B}] = \log(n_\text{A}/n_\text{B}) - \log(N_\text{A}/N_\text{B})_{\odot}, \]

where \(N_\text{A}\) and \(N_\text{B}\) are the number densities of elements A and B, respectively, in the stellar atmosphere and subscript circled dot refers to the Sun.
Table 4.1: Adopted stellar parameters for the stars considered in Paper I.

<table>
<thead>
<tr>
<th>Star</th>
<th>$T_{\text{eff}}/\text{[K]}$</th>
<th>$\log g$ (cgs)</th>
<th>[Fe/H]$_{\text{LTE}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sun</td>
<td>5780</td>
<td>4.44</td>
<td>0.0</td>
</tr>
<tr>
<td>Procyon</td>
<td>6500</td>
<td>4.00</td>
<td>0.0</td>
</tr>
<tr>
<td>HD 140283</td>
<td>5700</td>
<td>3.70</td>
<td>$-2.5$</td>
</tr>
<tr>
<td>G64-12</td>
<td>6400</td>
<td>4.10</td>
<td>$-3.3$</td>
</tr>
</tbody>
</table>

(e.g. Thévenin and Idiart 1999) predict very large non-LTE abundance corrections ($> +0.3$ dex) while others (e.g. Korn et al. 2003) find altogether negligible effects ($< +0.1$ dex). Discrepancies between the various studies may be due to various reasons, such as differences in the adopted model atmospheres in the estimated efficiency of collisional processes, or in the input physics in general (e.g. photo-ionization cross-sections, background opacities, etc).

In particular, I and my collaborators have investigated, in Paper I, the effects of UV line-blocking on the non-LTE formation of Fe I lines. In late-type stars, a large number of atomic lines contribute to the total opacity in the UV. The presence of this line haze can produce significant line-blocking and reduce the mean intensities at these wavelength, making the over-ionization mechanism less efficient. The magnitude of the predicted non-LTE effects on Fe I depends, in general, on whether line-blocking is included or neglected in the analyses. The non-LTE calculations are performed with the statistical equilibrium code MULTI (Carlsson 1986) using 1D plane-parallel MARCS model atmospheres for a selection of four late-type stars (the Sun, Procyon, HD 140283, and G64−12), representative of the most relevant parameter space (see Table 4.1).

We have used an extensive up-to-date model Fe atom including about 3500 Fe I lines and over 300 Fe I bound-free transitions, with radiative data coming primarily from the iron project (Bautista 1997). All levels in the Fe model atom are coupled via collisional excitations and ionizations by electrons and neutral hydrogen. In particular, the rates for the inelastic H+Fe collisions are calculated using a Drawin-like approximation (Drawin 1968, 1969). According to quantum-mechanical calculations and experimental measurements for simple atoms, the Drawin-like, appears to over-estimate the rates of H+Fe collisions by factors of $10^{-10^6}$ (Lambert 1993; Barklem et al. 2003). With the lack of a more accurate and comprehensive description of H+Fe collisions, we choose to apply correction factors $S_H = 0.001$ and $S_H = 1$ to Drawin’s formula and compare the resulting non-LTE effects on Fe I lines for the two different collisional efficiencies.

In our study, we have included the effects of line-blocking on the non-LTE Fe I calculations by sampling metal line opacities for about 9000 wavelength points in the spectral region between 1000 Å and 20000 Å and adding them to the standard background continuous opacities. For this purpose we have

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used the opacity package from the OS-MARCS code (Gustafsson et al. 2006, in preparation) taking into account the specific chemical composition of the given model stellar atmospheres. Level populations and ionization equilibria for the various metals are computed assuming LTE.

In Fig. 4.1, we compare the non-LTE Fe abundance corrections computed for the Sun and HD 140283 from Fe I lines including and excluding line-blocking in the background opacities, assuming fully efficient Drawin-like H+Fe collisions ($S_H = 1$). As a result of over-ionization, the opacities of Fe I lines are, in general, reduced (see also Fig. 4.2) shifting the whole line formation region inwards. In the layers where weak lines form, departures relative to LTE are approximately the same for most Fe I levels. For weak lines, therefore, the line source function remains close to the Planck function even in non-LTE; the lower line opacities in the non-LTE case compared with LTE directly result in weaker lines, and positive corrections have to be applied to the Fe abundances derived with LTE (for more details about Fe I line formation, see Saxner (1984) and Paper I). At metallicities near solar, line-blocking in late-type stellar atmospheres is very efficient and significantly reduces the effects of over-ionization, leading to smaller non-LTE corrections (about $-0.1$ dex). At very low metallicities, on the contrary, line-blocking is very weak and excluding it from the calculations causes only minor changes in the derivation of non-LTE Fe abundances (by less than 0.02 dex). It is clear that the large discrepancies among different studies of non-LTE Fe I line formation in metal-poor stars cannot be attributed to the treatment of line-blocking in the non-LTE calculations. At present, the main source of uncertainty in non-LTE Fe I line formation calculations is still represented by the poorly known rates of inelastic H+Fe collisions.
Figure 4.1: Non-LTE Fe abundance corrections for the Sun (top) and the metal-poor star HD 140283 (bottom) derived from Fe I lines in the visible and near UV (3000 ≤ λ ≤ 10000 Å) assuming fully efficient Drawin-like inelastic H+Fe collisions ($S_H = 1$). Open circles refer to calculations without background line opacities, filled circles to calculations with background line opacities. Crosses refer to non-LTE calculations for the Sun in which background line opacities are simulated by applying multiplication factors to continuous opacities as done by Bruls et al. (1992).
Figure 4.2: Departure of the total Fe I number density relatively to LTE as a function of standard optical depth at $\lambda = 5000$ for the Sun and HD 140283 computed for different treatments of line-blocking (for the explanation of the symbols, see also Fig. 4.1). Fully efficient Drawin-like H+Fe collisions ($S_H = 1$) are assumed.
5. Hydrodynamical simulations of giant stars (Paper II)

During the red giant phase of their evolution, stars undergo structural changes that ultimately lead to a rapid expansion of the stellar diameter and to a significant increase in absolute luminosity. Their intrinsically high brightnesses make red giant stars suitable observational targets for various investigations in stellar astronomy. Giant stars are, in fact, extensively used for spectroscopic abundance analyses of distant stellar systems in our Galaxy and its surroundings as well as in the Local Group. For instance, a significant number of stars targeted by large-scale spectroscopic analyses of the galactic halo and disk (e.g. McWilliam et al. 1995; Ryan et al. 1996; Fulbright 2000) are giants. Noteworthy is also the ESO “First Stars” observational campaign (e.g. Hill et al. 2002; François et al. 2003; Depagne et al. 2002; Sivarani et al. 2004; Cayrel et al. 2004; Spite et al. 2005) aiming towards a systematic and homogeneous abundance analysis of a large sample of extremely metal-poor halo giants ([Fe/H] \leq -2.5). The results of these and similar observational studies are of fundamental importance in astrophysics because they provide crucial information about stellar evolution and nucleosynthesis as well as the chemical enrichment of galaxies.

As for other late-type stars, nearly all abundance analyses of giant stars carried out today are still based on classical 1D LTE model stellar atmospheres, constructed under the assumptions of plane-parallel geometry or spherical symmetry, hydrostatic equilibrium, and flux constancy, and relying on simplified local models for convective energy transport (e.g. mixing length theory). In late-type stars the flows from the upper convective zone can overshoot into the photosphere and affect the regions where the emitted stellar flux originates. As explained in previous sections, classical 1D models cannot consistently reproduce in any way the complexity of the thermal structures and correlated velocity fields in the atmospheres of late type stars. Also, the predicted 1D thermal structures may deviate significantly from the actual average atmospheric stratifications, especially in the case of metal-poor stars. Because of these shortcomings, the use of 1D model stellar atmospheres of giant stars might lead to significant systematic errors, and be unsatisfactory for the purposes of high-precision abundance analyses. Realistic 3D hydrodynamical simulations of surface convection in red giant stars at different metallicities have been carried out in Paper II and used as time-dependent 3D hydrodynamical model stellar atmospheres in order to quantify the systematic
Table 5.1: Details of the 3D hydrodynamical simulations.

<table>
<thead>
<tr>
<th>⟨T_{eff}⟩ a</th>
<th>log g [cgs]</th>
<th>[Fe/H]</th>
<th>x,y,z-dimensions [Mm]</th>
<th>time b [min]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4697 ± 18</td>
<td>2.2</td>
<td>+0.0</td>
<td>1250 × 1250 × 610</td>
<td>13 000</td>
</tr>
<tr>
<td>4717 ± 12</td>
<td>2.2</td>
<td>−1.0</td>
<td>1125 × 1125 × 415</td>
<td>6 000</td>
</tr>
<tr>
<td>4732 ± 8</td>
<td>2.2</td>
<td>−2.0</td>
<td>1065 × 1065 × 360</td>
<td>8 000</td>
</tr>
<tr>
<td>4858 ± 10</td>
<td>2.2</td>
<td>−3.0</td>
<td>1065 × 1065 × 360</td>
<td>13 500</td>
</tr>
<tr>
<td>4983 ± 36</td>
<td>2.2</td>
<td>+0.0</td>
<td>1290 × 1290 × 960</td>
<td>15 000</td>
</tr>
<tr>
<td>5131 ± 19</td>
<td>2.2</td>
<td>−1.0</td>
<td>1250 × 1250 × 540</td>
<td>11 000</td>
</tr>
<tr>
<td>5035 ± 13</td>
<td>2.2</td>
<td>−2.0</td>
<td>1150 × 1150 × 430</td>
<td>10 500</td>
</tr>
<tr>
<td>5128 ± 10</td>
<td>2.2</td>
<td>−3.0</td>
<td>1150 × 1150 × 430</td>
<td>8 000</td>
</tr>
</tbody>
</table>

aTemporal average and standard deviation of the emergent effective temperatures.
bTime span of the parts of simulations used for spectral line formation purposes.

Differences between classical 1D and state-of-the-art 3D analyses. The numerical simulations have been performed using the code by Stein and Nordlund (1998); details about the construction of the simulations and the methods and techniques adopted for the 3D spectral line formation have been discussed in chapter 3.

Two series of surface convection simulations of red giant stars have been generated for this work. The first suite consists of simulations of giant stars with T_{eff} ≈ 4750 K, surface gravity log g = 2.2 (cgs) and metallicities [Fe/H] = 0, −1, −2, and −3; the second suite corresponds to giants computed for the same surface gravity and metallicities but somewhat higher effective temperatures (T_{eff} ≈ 5050 K). Table 5.1 lists some of the physical parameters and characteristic quantities of the convection simulations presented here. It is important to note that, in the simulations, the entropy of the inflowing gas at the lower boundary replaces the effective temperature as an independent input parameter (Stein and Nordlund 1998). As a result of that, the effective temperature of the simulations is not constant, but actually varies with time because the emergent radiative flux is susceptible to the evolution of the surface granulation pattern. The effective temperatures given in Table 5.1 are therefore averages over the whole time-sequences of the simulations.

The values of the average effective temperatures for the various simulations in the two series are not all identical. Constructing a new simulation with a specific effective temperature requires careful fine-tuning of the entropy of the inflowing gas at the lower boundary. As the main purpose of this study is to perform a differential comparison between 3D and 1D model stellar atmospheres computed for the same stellar parameters, it is acceptable to settle for values reasonably close to the targeted effective temperatures.
5.1 Scaling and initiating the simulations

Much of the work required to construct 3D hydrodynamical model atmospheres with given stellar parameters consists in generating proper initial snapshots which can evolve into reasonably stable and numerically well-behaved convection simulations. One possibility is to start from a quasi-homogeneous radiative equilibrium stratification, perturb it, and follow the evolution with time of the perturbations, to directly study the on-set of convection. However, with this approach, achieving thermal and dynamical relaxation for the convection simulations is in practice a very time consuming task; several adjustments might also be required before obtaining a well-behaved simulation at the targeted effective temperature. The other possibility, adopted here, is to appropriately scale a previous convection simulation to the targeted set of stellar parameters. This approach produces a reasonable guess for the initial snapshot as long as the characteristics of the surface convection for the original stellar parameters and the targeted ones are qualitatively the same. In the present work, the initial snapshots for the convection simulations of giant stars are generated by scaling previous hydrodynamical simulations of turn-off stars computed by Asplund and García Pérez (2001) for different metallicities. The vertical depth scale and the mean temperature-pressure stratification of the original convection simulation are scaled to the targeted stellar parameters by comparing the corresponding structures from classical 1D model stellar envelopes. Temperature and density inhomogeneities of the original 3D structure relative to the mean stratification are preserved in the scaled simulation. Concerning the scaling of the horizontal dimensions, we use the fact that, in late-type stars and at a given metallicity, the sizes of the granules are to first order inversely proportional to the surface gravity of the star (e.g. Stein and Nordlund 1998).

Using the scaled structures as initial snapshots, the simulations are first carried out at low numerical resolution \((50 \times 50 \times 125\) grid-points) in order to achieve thermal and dynamical relaxation more rapidly. Re-adjustments of the structures are needed in some cases when the effective temperatures end up being too different from the intended value. For the final simulation runs, the resolution of the mesh is increased to \(100 \times 100 \times 125\) allowing for a better representation of velocity fields and inhomogeneities.

5.2 Structure of the simulations

The atmospheric structures and the dynamics of the gas flows resulting from the surface convection simulations of red giants are qualitatively very similar to the ones previously computed by Asplund et al. (1999) and Asplund and García Pérez (2001) for dwarfs and turn-off stars. The morphology and evolution of the granulation patterns (Fig. 5.1), with large, warm upflows in the
midst of narrow, cool downflows are also essentially the same as in simulations of solar-type stars.

Figure 5.2 shows the resulting thermal structures from the four convection simulations with $T_{\text{eff}} \simeq 4750$ K. The 3D structures are compared with the temperature-density stratifications from plane-parallel MARCS model atmospheres (Gustafsson et al. 1975; Asplund et al. 1997) computed for the same stellar parameters. The temperatures in the upper photospheric layers of the convection simulations are regulated mainly by the competition between radiative heating/cooling and adiabatic cooling following the expansion of the ascending gas. At metallicities near solar ([Fe/H] $\simeq -1$), line-blanketing is sufficiently strong to provide sufficient radiative heating to balance adiabatic cooling in the upper photospheric layers; as a consequence, the mean 3D temperature-density stratification there closely resembles the corresponding 1D MARCS structure in which radiative equilibrium is enforced. Vice versa, at lower metallicities ([Fe/H] $\lesssim -2$), the mean 3D temperature stratifications remain significantly cooler than in the corresponding 1D model atmospheres. This is interpreted as an effect due to adiabatic cooling dominating over radiative heating as fewer and weaker lines become available in the upper photospheres of very metal-poor stars to reabsorb radiation from deeper layers (Asplund et al. 1999). This explanation, however, requires further testing; it cannot be excluded a priori that the balance between radiative heating and adiabatic cooling might be affected by the approximations involved in the solution of the radiative transfer equation (see also Sec. 5.4).

5.3 Spectral line formation calculations

Once they have run for a sufficiently long times, the convection simulations can then be used as time-dependent 3D model stellar atmospheres for spectral line formation calculations (see Sec. 3.8). Curves-of-growth of spectral lines can be computed with 3D model atmospheres and compared with the ones predicted with the use of classical 1D MARCS models, to estimate the impact of granulation on the derivation of stellar abundances. Systematic differences between the 1D and mean 3D stratifications, and the presence, in the 3D model atmospheres, of temperature and density inhomogeneities as well as velocity gradients can significantly affect the predicted strengths of spectral lines and therefore the derived elemental abundances.

In Paper II, the effects of granulation on spectral line formation calculations are investigated for a number of atomic (Li I, O I, Na I, Mg I, Ca I, Fe I, and Fe II) and molecular (CH, NH, and OH) lines, under the assumption of LTE. The value of the differences between 3D LTE and 1D LTE abundance determinations based on the analysis of a given line depends in general on the species of absorbers under consideration (e.g. atom, ion, or molecule), the physical parameters of the spectral line (lower level excitation potential, log $g_f$
Figure 5.1: Spatially resolved outgoing intensity in the continuum bin for four snapshots of 3D hydrodynamical simulations of red giants at different metallicities; the surface granulation pattern is clearly visible. In order to facilitate the comparison of the four cases, the patterns have been partially repeated periodically so that the physical dimensions of the four images are the same as for the \([\text{Fe/H}] = 0\) simulation. In particular, it is seen that the size of granules decreases with metallicity (see discussion in Collet et al. 2006b).
Figure 5.2: Thermal structures of four snapshots of 3D hydrodynamical simulations of red giants at different metallicities. Thin solid line: extreme temperatures at a given density in the 3D convection simulation. Thin dashed line: Mean temperature-density stratification of the 3D simulations (averaged over surfaces of equal optical depth at $\lambda = 5000$ Å). Thick solid line: Temperature-density stratification of 1D hydrostatic MARCS model atmospheres computed for the same stellar parameters.
value, wavelength), as well as on the parameters of the model atmosphere. To illustrate some characteristic effects of granulation on spectral line formation, I briefly discuss here the results of a differential $3D-1D$ LTE Fe abundance analysis based on fictitious Fe I lines. I refer to Paper II for more details about $3D-1D$ LTE abundance corrections based on spectral lines of other ions and molecules.

Figure 5.3 shows the differential $3D-1D$ LTE Fe abundances derived from Fe I lines at $\lambda = 5000 \, \text{Å}$ with varying strengths and excitation potentials for two red giants at solar and very low metallicity. At a given Fe abundance, weak Fe I lines appear stronger with 3D models than they do in 1D, leading to negative $3D-1D$ LTE abundance corrections. In particular, corrections are more pronounced at low metallicities and for low-excitation lines: the differential $3D-1D$ LTE Fe abundances derived from weak Fe I lines for the model at $[\text{Fe}/\text{H}] = 0$ are $\lesssim -0.1$ dex, while they can be as considerable as $-0.8$ dex at $[\text{Fe}/\text{H}] = -3$. As line strength increases, the differences between 3D and 1D Fe abundances typically remain large and negative in the very metal-poor case while they eventually grow positive for sufficiently strong lines at solar metallicity.

The behaviour of the differential $3D-1D$ Fe abundance corrections can be qualitatively interpreted by comparing the variations of the number density of Fe I particles with depth in 1D and 3D model photospheres (Fig. 5.4). At solar metallicity, the variations of temperature and density with optical depth are very similar in the 1D and mean 3D stratifications and so are the Fe I fractions. Consequently, the $3D-1D$ abundance corrections at solar metallicity cannot be ascribed to differences in the 1D and mean 3D stratifications but rather to the temperature and density inhomogeneities and possibly to the velocity gradients. The situation is radically different at very low metallicities. In the 1D MARCS stratification iron is mostly ionized throughout the stellar atmosphere; on the contrary, in the upper photospheric layers of the metal-poor 3D model atmosphere, a significant fraction of the total iron is in neutral form because of the much lower surface temperatures encountered there. The systematically cooler temperature structure and the higher Fe I fractions in the line formation layers compared with the 1D case explain why, for a given Fe abundance, Fe I lines are generally much stronger in 3D than in 1D, resulting in large negative $3D-1D$ LTE corrections to the Fe abundance.

From a qualitative point of view, the behaviour of the $3D-1D$ LTE abundance corrections as a function of line strength and metallicity for neutral lines of other elements is similar to the one predicted for Fe I lines. The actual magnitudes of the $3D-1D$ LTE effects depend on the details of the ionization equilibrium. The extreme sensitivity of molecule formation to temperature in the upper photospheres of late-type stars also leads to large and negative

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1The term “fictitious” refers here to indicate test lines whose parameters can be varied to study the characteristic behaviour of spectral lines in 1D and 3D models and in LTE solely as a function of lower-level excitation potential, wavelength, and log $gf$ value (Paper II).
Figure 5.3: 3D—1D LTE Fe abundance corrections derived from Fe I fictitious lines at $\lambda = 5000$ Å as a function of equivalent width $W_{\lambda}$ for two giant stars at solar (upper panel) and very low metallicity ([Fe/H] = −3; lower panel). Corrections are shown for Fe I lines with different lower level excitation potentials and for two different choices of 1D micro-turbulence.
Figure 5.4: Number density of neutral Fe atoms relative to number total number density of Fe particles ($N_{\text{FeI}}/N_{\text{Fe}}$) as a function of optical depth at $\lambda = 5000$ Å in the atmospheres of two giant stars at solar (upper panel) and very low metallicity ([Fe/H] = −3; lower panel). The gray shaded areas represent the distributions of the values of $N_{\text{FeI}}/N_{\text{Fe}}$ with optical depth in 3D hydrodynamical model atmospheres; darker areas correspond to values with higher probability. Overplotted are the curves for the 1D MARCS models corresponding to the same stellar parameters (solid line) and for the mean 3D stratification averaged over surfaces of constant optical depth (dashed line).
3D−1D LTE corrections for abundance analyses based on the molecular lines at very low metallicities.

5.4 Discussion

The use of 3D hydrodynamical model atmospheres of giant stars in spectral line formation calculations has, in general, a significant impact on abundance determinations. Differences between 3D and 1D abundance analyses can be especially large for the very metal-poor stars, with consequences on our theoretical understanding of stellar and Galactic chemical evolution. It should be noted that the corrections are significantly larger than the systematic errors generally quoted in standard abundance analyses (for a discussion, see, e.g. Gustafsson 2004b). It is thus deemed necessary to investigate how the assumptions made when solving the radiative transfer equation in the convection simulations or in the line formation calculations affect the derived 3D−1D abundance corrections. An important issue here is the treatment of scattering as true absorption. This approximation can in principle lead to systematic errors in the predicted temperature structure of the upper photosphere and therefore indirectly affect ionization and molecular equilibria in line formation regions. According to some preliminary tests, 1D MARCS model atmospheres of giant stars computed including scattering as true absorption are typically hotter in the upper photospheric layers compared with models where scattering is properly taken into account. In very metal-poor giant stars with the same stellar parameters as the stars considered in the present study, temperature differences at a given optical depth can reach 300 K or more in the optically thin layers. These results suggest that radiative heating rates might actually be over-estimated in the upper photospheric layers of the present 3D hydrodynamical simulations of very metal-poor giant stars.

The treatment of scattering as true absorption can be a matter of concern for the accuracy of line formation calculations. Rayleigh scattering by H i can in fact contribute significantly to the total continuous extinction in the UV and blue part of the spectrum. At these wavelengths, implementing scattering as true absorption leads to underestimated flux in the continuum and therefore also too weak spectral lines (Cayrel et al. 2004). The effect is expected to be more pronounced in very metal-poor stars, due to the weak line-blocking there, particularly in metal-poor 3D model atmospheres whose lower surface temperatures result in higher densities of scatterers (H i particles). Test calculations using the mean 3D stratifications as model atmospheres indicate that treating scattering as true absorption in the calculations has a relatively little effect on the predicted line strengths, at least for the type of giants considered in our study. However, the effect of the above assumption might, in practice, be larger in full 3D line formation calculations because of temperature and density inhomogeneities. The differential 3D−1D approach abundance anal-
ysis ensuring that the uncertainties in the treatment of scattering are at least reduced.

Another issue is the assumption of LTE for the solution of the radiative transfer problem. As explained in chapter 2, the energy partitioning of matter in the upper photosphere depends in general not only on the local gas temperature but also on radiation originating from deeper layers.

For instance, in the case of iron, strong over-ionization by radiation in the UV can lead to significantly weaker Fe I lines in metal-poor stars compared with the cases where LTE is enforced (Paper I). In other words, the effects of over-ionization on the strengths of Fe I lines are opposite to the ones of granulation; therefore, departures from LTE should be taken into account in the 3D line formation calculations in order to accurately determine 3D–1D corrections to the Fe abundances.
6. 3D abundance analysis of extreme halo stars (Paper III)

Three-dimensional hydrodynamical model atmospheres of very metal-poor stars can be used to investigate the impact of stellar granulation on the abundance analyses of the two extreme halo stars HE 0107–5240 and HE 1327–2326, recently discovered by Christlieb et al. (2002) and Frebel et al. (2005). These two objects are particularly interesting as their abundances in terms of iron peak elements are the lowest ever observed in stars.\(^1\) At the same time, HE 0107–5240 and HE 1327–2326 also show very large over-abundances of carbon, nitrogen, and oxygen relative to iron. Various hypotheses have been advanced to explain the origin and chemical compositions of these two stars. In particular, it has been suggested that they were born from the ashes of a previous generation of metal-free (Population III) stars. Their abundance patterns, therefore, would directly reflect the yields from the very first generation of metal-free stars to form in the early universe, and provide crucial information about the physical properties of Population III stars and chemical evolution in the early Galaxy. Umeda and Nomoto (2003) have proposed that the two stars might have formed out of material polluted by a single \(\sim 25 \, \text{M}_\odot\) Population III star exploding as supernova and experiencing mixing after the explosive nucleosynthesis, followed by fallback on the compact remnant. Iwamoto et al. (2005) have used the above scenario to show that small variations in the explosion energy of the supernova could in fact reproduce the chemical abundance patterns of both stars. Meynet et al. (2006) instead have suggested that the yields from the winds of rotating massive primordial stars could explain the C, N, and O excesses and possibly also Na and Al enhancements in HE 0107–5240 and HE 1327–2326 and other extremely metal-poor stars.

In order to identify the most plausible scenario for the formation of these stars, it is necessary to accurately determine the chemical compositions of HE 0107–5240 and HE 1327–2326. In Paper III, I and my collaborators present the results of the first abundance analysis of HE 0107–5240 and HE 1327–2326 based on 3D model atmospheres.

\(^1\)The iron abundances of HE 0107–5240 and HE 1327–2326 are \([\text{Fe/H}] = -5.3\) and \([\text{Fe/H}] = -5.4\), respectively, i.e. about 200,000 times lower than the solar one.
6.1 The 3D model atmospheres

We use one of the convection simulations of metal-poor red giant star from Paper II \( (T_{\text{eff}} = 5130 \, \text{K}, \log g = 2.2, [\text{Fe/H}] = -3) \) as a time-dependent, 3D, hydrodynamical model atmosphere of HE 0107−5240. The physical parameters of the convection simulation are the same as those estimated for HE 0107−5240, with the exception of the metallicity which is higher. However, the thermal stratifications of 1D MARCS model atmospheres computed for a metallicity \([\text{Fe/H}] = -3\) and for the specific chemical composition of HE 0107−5240 are very similar which reflects the fact that hydrogen is the dominating element, both determining the thermodynamical and optical properties of the gas (Christlieb et al. 2004). Also, at \([\text{Fe/H}] = -3\), the lower CNO abundances compensate in part for the higher abundances of iron-peak elements. A differential analysis based on 3D and 1D model red giant atmospheres with a metallicity \([\text{Fe/H}] = -3\) is therefore expected to provide a reasonable basis for estimating of 3D−1D abundance corrections for HE 0107−5240. For the analysis HE 1327−2326 we instead use a convection simulation of metal-poor turn-off star \( (T_{\text{eff}} \simeq 6200 \, \text{K}, \log g = 4.04 \, [\text{cgs}], \text{and } [\text{Fe/H}] = -3) \) from Asplund and García Pérez (2001). While this value of surface gravity is intermediate between the actual estimates for HE 1327−2326, \( \log g = 3.7 \) and \( \log g = 4.5 \), the derived abundances are only marginally sensitive to the choice of \( \log g \) (Aoki et al. 2006).

The 3D abundance analyses of HE 0107−5240 and HE 1327−2326 are carried out following a differential 3D−1D LTE procedure as described in Sec. 3.8. While all 3D and 1D MARCS model atmospheres have been constructed for a metallicity \([\text{Fe/H}] = -3\), the chemical compositions are assumed to be the same as those estimated for HE 0107−5240 and HE 1327−2326 when computing the ionization and molecular equilibria and the continuous opacities for the line formation calculations. This assumption is crucial for 3D−1D the analysis: adopting a composition with metallicity \([\text{Fe/H}] = -3\) would overestimate the abundance of elements with low ionization potentials (e.g. Na, Ca, Al) and therefore the electron density, affecting the ionization balance and line strengths.

6.2 Main results

The main effect of stellar granulation is to decrease, in the 3D LTE analysis of HE 0107−5240 and HE 1327−2326, elemental abundances derived in 1D from weak low-excitation lines of neutral atoms and molecules. In particular, the 3D LTE analysis of Fe i lines suggests about \(-0.2 \, \text{dex}\) lower Fe abundances for the two stars than the 1D analysis. The 3D LTE abundances of carbon, nitrogen, and oxygen derived from CH, NH, and OH molecular lines are found to be lower by about \(-0.8 \, \text{dex}\) or more than those estimated using
Figure 6.1: Comparison between the 1D LTE (thin lines) and 3D LTE (thick lines) elemental abundance ratios in HE 0107−5240 (squares) and HE 1327−2326 (crosses); arrows indicate upper limits. The solar abundances by Asplund et al. (2005) are assumed.

1D model atmospheres. The basic interpretation of these effects is the same as for the differential 3D−1D LTE analyses of very metal-poor stars considered in Paper II. More details on the 3D−1D LTE corrections for other elements are given in Paper III.

Figure 6.1 summarizes the results of the 3D−1D LTE analysis of HE 0107−5240 and HE 1327−2326, showing the elemental abundance ratios relative to iron corrected for 3D−1D effects. The significant downward revision of the CNO abundances indicates that the yields of first-generation stars might be systematically lower than what previously estimated by 1D analyses. The 3D LTE [C/Fe] ratio, however, appears in closer agreement with the predictions of the stochastic Galactic chemical evolution model of Karlsson (2006) relying on the yields by Meynet et al. (2006). It will be interesting to also investigate whether the revised abundance patterns can still be interpreted in the light of the proposed formation scenarios for extreme halo stars in general.

It is important to caution the reader that many of the lines considered in the abundance analysis of HE 0107−5240 and HE 1327−2326 may be subject to departures from LTE. In the present work, we attempt to estimate the magnitude of the non-LTE effects on Fe I lines by means of a 1D analysis, following the same differential approach as used in Paper I. We perform the non-LTE
Table 6.1: Non-LTE Fe abundances derived for HE 0107−5240 and HE 1327−2326 using 1D MARCS models and the mean 3D stratifications (⟨3D⟩). Three different efficiencies of the inelastic H+Fe collisions are considered (see main text for details).

<table>
<thead>
<tr>
<th>Star</th>
<th>Model</th>
<th>[Fe/H]_{LTE}</th>
<th>$S_H = 0.001$</th>
<th>$S_H = 1$</th>
<th>$S_H = 1$ (+ Therm.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HE 0107−5240</td>
<td>⟨3D⟩</td>
<td>−5.60</td>
<td>−4.50</td>
<td>−4.65</td>
<td>−4.75</td>
</tr>
<tr>
<td>HE 0107−5240</td>
<td>1D</td>
<td>−5.40</td>
<td>−4.40</td>
<td>−4.50</td>
<td>−4.65</td>
</tr>
<tr>
<td>HE 1327−2326</td>
<td>⟨3D⟩</td>
<td>−5.95</td>
<td>−4.70</td>
<td>−4.95</td>
<td>−5.05</td>
</tr>
<tr>
<td>HE 1327−2326</td>
<td>1D</td>
<td>−5.70</td>
<td>−4.60</td>
<td>−5.05</td>
<td>−5.15</td>
</tr>
</tbody>
</table>

Fe I line formation calculations for HE 0107−5240 and HE 1327−2326 using 1D MARCS model atmospheres of the two stars as well as the mean 3D temperature stratifications with optical depth deduced from the convection simulations. Inelastic H+Fe collisions are implemented following a Drawin-like recipe (Drawin 1968, 1969). Given the uncertainties in the Drawin-like description, we apply correction factors $S_H$ to the collisional cross-sections. In particular, we consider here three different cases: $S_H = 0.001$, $S_H = 1$, and $S_H = 1$ with enforced thermalization of the uppermost level of our Fe I model atom with the ground level of Fe II. The results of the non-LTE Fe I line formation calculations are presented in Table 6.1. Because of the steep temperature gradients with depth and the weak UV line-blocking, over-ionization effects are found to be very large, even when fully efficient H+Fe collisions are implemented. According to our calculations, the overall non-LTE corrections to Fe abundances based on Fe I lines clearly outweigh the corrections due to granulation. Christlieb et al. (2004) and Frebel et al. (2005), on the contrary, report significantly smaller non-LTE effects on the Fe abundance determinations for HE 0107−5240 and HE 1327−2326 (about 0.2 dex). The differences with respect to our results are primarily due to their use of much higher efficiencies for the H+Fe collisions. A more thorough analysis within the framework of 3D models is certainly necessary to accurately determine the magnitude of the combined effects of stellar granulation and non-LTE on Fe I line formation in these extreme halo stars.
7. Future prospects

The work presented in this thesis can be continued and improved in various directions. I intend to further analyse the physical properties of the present surface convection simulations of red giant stars and study, in particular, the details of the temperature and density structures, the dynamics of gas flows, and the granular energetics. In this respect, I would be also interested in extending the study of surface convection to red giant stars with somewhat lower gravities than the ones considered here and explore how the properties of hydrodynamical simulations vary as a function of stellar parameters. Such convection simulations, once available, will also be used for spectral line formation calculations and for elemental abundance determinations with 3D hydrodynamical model atmospheres.

It will also be important, especially for the purposes of 3D spectral line formation, to investigate how the adopted numerical resolution of the simulations and physical dimensions of the computational domains affect the predicted temperature and density structures and velocity fields in the present convection simulations of giant stars. Too coarse a numerical resolution would prevent velocity gradients in the simulations from being accurately resolved, resulting in insufficient Doppler broadening due to convective motions, and, therefore, in too narrow spectral lines. Such numerical effects can lead to systematic errors in abundance determinations based on 3D model atmospheres and must be tested for.

The approximations involved in the solution of the radiative transfer equation in both the modelling of surface stellar convection and the 3D spectral line formation calculations also deserve closer inspection. Concerning the modelling of convection, it is necessary to explore possible sources of uncertainty in the estimates of the radiative heating/cooling rates which can significantly affect the temperature structures of the convection simulations. In this respect, the opacity-binning technique used for the present simulations requires further testing, not the least at very low metallicities. Improvements are certainly also needed in the treatment of scattering for the solution of the radiative transfer. The current approach, including scattering as true absorption, is in general not satisfactory: the use of this approximation may significantly affect the balance between heating and cooling at the surface of convection simulations of metal-poor stars, as well as the predicted fluxes and line strengths in the UV. As such effects are expected to be even larger for red giants at lower gravities than the
ones considered here, it is probably necessary to relax this approximation in future calculations.

The results presented in this thesis indicate that departures from LTE for spectral lines might, in general, be large in metal-poor late-type stars and should not be neglected. In this work, the effects due to stellar granulation and departures from LTE have been investigated only separately. An investigation of non-LTE effects on spectral line formation calculations within the framework of 3D hydrodynamical model atmospheres of red giant stars is therefore of high priority. In particular, it would be interesting to study 3D non-LTE for lines of elements such as Fe, Mg, Ca, C, O, due to their important role in the understanding of the early phases of Galactic chemical evolution. Even with the assumption of statistical equilibrium, however, the computational burden of full non-LTE calculations with 3D model atmospheres is extremely large, especially when complex atoms such as Fe are considered. I am therefore planning to first use a “1.5D” approach (i.e. treating vertical columns in the 3D structure as a set of 1D model atmospheres) to study the combined effects of granulation and non-LTE. This method should provide a reasonable estimate of the actual effects.
8. My contribution to the included papers

• **Paper I.** I carried out all the non-LTE calculations for Fe with the statistical equilibrium code *MULTI* by Carlsson (1986). I introduced the modifications in the original code in order to include the background line opacities from metals and study the effects of line-blocking. The model Fe atom was initially assembled by Frédéric Thévenin (energy levels and radiative transitions data). I extensively tested it and optimized it for the spectral line formation calculations and included the relevant collisional data in it. I carried out the analysis of the results and wrote most of the paper.

• **Paper II.** I carried out the 3D hydrodynamical surface convection simulations of giant stars at different metallicities using the code by Stein and Nordlund (1998). Equation of state and opacities were implemented using the code developed by Regner Trampedach. I generated the initial snapshots of the simulations by scaling previous simulations of turn-off stars by Asplund and García Pérez (2001). I performed all 3D and 1D line formation calculations and all related tests, carried out the differential 3D—1D abundance analysis, and wrote the paper.

• **Paper III.** I carried out the 3D hydrodynamical convection simulation of the very metal-poor red giant. The 3D simulation for the turn-off star was adopted from Asplund and García Pérez (2001). I performed the 3D LTE line formation calculations, carried out the differential 3D—1D abundance analyses of the two extreme halo stars HE 0107−5240 and HE 1327−2326, and wrote the paper.
9. Summary in Swedish


Nästan alla spektroskopiska analyser av stjärnor av sen spektraltyp (kallare än cirka 7500 K i de atmosfärslager varifrån det mesta av ljuset kommer) som utförts är fortsatt baserade på klassiska modellatmosfärer, konstruerade med förenklande antaganden om stationära lager i hydrostatiskt jämvikt, en rudimentär behandling av konvektiva energitransporten, och förutsättningen om lokal termodynamiskt jämvikt (LTE) vid beräkningen av strålningstransport och spektrallinjer. Dessa stora förenklingar kan ofta leda till mycket stora systematiska fel i modeller och beräknade spektrallinjer, och därför i bestämningssting av grundämnesförekomster. I denna avhandling diskuteras jag några exempel på situationer där bättre bestämningar av förekomster kan
göras, med hjälp av aktuella förbättringar vad gäller behandlingen av strålningstransport och den teoretiska modelleringen av stjärnatmosfärer.

Spectrallinjebildning utan förutsättningen om lokal termodynamisk jämvikt: effekterna av "linjeblocking" (Artikel I)


Hydrodynamiska simuleringar för jättestjärnor (Artikel II)

I denna artikel undersöker vi effekten av att använda realistiska tredimensionella (3D) hydrodynamiska modellatmosfärer för röda jättestjärnor med olika metallinnehåll vad gäller beräkningen av
spektrallinjer från atomer och molekyler. Vi utförrealistiska, ab initio, 3D-, hydrodynamiska simuleringar av ytkonvektion hos stjärnor med olika temperatur och metallinnehåll med hjälp av ett datorprogram skrivet av Stein och Nordlund (1998). Vi använder simuleringarna som tidsberoende hydrodynamiska modellatmosfärer för spektrallinjeberäkningar för linjer från flera olika atomer och joner (Li, O, Na, Mg, Ca, Fe och Feii) och fria radikaler (CH, NH och OH) under det förenklande antagandet om LTE. Därefter jämför vi differentiellt dessa linjestyrkor och dem från snarlikaslinjeberäkningar för klassiska endimensionella (1D) hydrostatiska planparallella MARCS-modellatmosfärer, i syfte att uppskatta effekten av 3D-modeller på härledningen av grundämnesförekomster. Skillnader mellan modellstrukturerna i 1D och 3D liksom inhomogeniteterna i temperatur och täthet och gradienterna i hastighetsfält i 3D-modellerna kan avsevärt påverka de beräknade linjestyrkorna och bestämningarna av förekomsterna av förekomsterna från spektrallinjer.

Effekterna av inhomogeniteterna, stjärngranulationen, är särskilt stora vid låga metallinnehåll. Temperaturerna i de övre lagren i hydrodynamiska 3D-modeller av atmosfärer för metallfattiga röda jättestjärnor är verkligensignifikantlägre än vad klassiska 1D-modeller med samma fundamentala stjärnparameterar ger. De kallare temperaturerna gör att svaga spektrallinjer från neutrala atomer och molekyler blir starkare med 3D-modellerna än med 1D-modellerna, om LTE förutsätts. Vi finner därför att 3D-1D-korrektionerna till grundämnesförekomster som härleds från dessa linjer är stora och negativa, åtminstone under förutsättningen LTE. I synnerhet är korrektionerna för förekomster från kol, kväve och syre, som härleds linjer från CH-, NH- och OH-radikaler) med låg excitation, typiskt en reduktion av storleksordningen en faktor 3 till 10 för jättar med mycket lågt metallinnehåll (kring 1/1000 av solens). Stora negativa korrektioner (ungefär en reduktion med en faktor 6) erhålls också i LTE för svaga lågt exciterade FeI-linjer. Emellertid förväntar vi oss avsevärd avvikelser från LTE för sådana linjer (Artikel I) och dessa skall tas med i beräkningen om man noggrant vill utvärdera effekten av stjärngranulationen på järnhalterna.

Förekomstanalys med 3D-modellatmosfärer för extrema halo-stjärnor (Artikel III)

Noggranna förekomstanalyser för extremt metallfattiga stjärnor är avgörande för vår förståelse av grundämnesuppbryggnaden i de första stjärnorna i universum och i de tidigaste faserna i Vintergatans utveckling. I Artikel III undersöker vi effekten av realistiska hydrodynamiska 3D-modellatmosfärer på bestämningen av grundämnesförekomster i de kolrika, unikt järnfattiga stjärnorna HE 0107−5240 och HE 1327−2326. Vi
10. Acknowledgments

I would like to express my deepest gratitude to my supervisors, Bengt Gustafsson and Martin Asplund, for their invaluable guidance during my PhD studies. Bengt, I am grateful for all the things I learnt from you, and for the curiosity, creativity, optimism, and enthusiasm with which you constantly look at astronomy and science in general: they have been and will always be a source of inspiration for my scientific work.

Martin, it has been a real pleasure for me to have the possibility to work and discuss astronomy with a scientist like you. I thank you for your patience, your professionalism, all the time you have dedicated to clarifying my doubts, and for always giving me the freedom to mature and pursue my scientific ideas independently.

I am also grateful to all the people at the Uppsala Astronomical Observatory who have contributed to create such a pleasant and stimulating scientific environment. In particular, I would like to thank Kjell Eriksson, for his warm-heartedness and for all the times I had the pleasure to interact with him on scientific matters; Bengt Edvardsson for his kindness and generosity; Nikolai Piskunov, for always taking time to answer in detail any of my questions about science, data reduction, or numerical problems. Björn Davidsson for all our stimulating discussions on science and not only; Marie Nordström, Nils Bergvall, Susanne Höfner, Erik Zackrisson, and all the artists of the “Rum och Rymd” project, for sharing with me their visions and thoughts on art and the cosmos. I would also like to thank all present and former members of the Stellar Atmosphere group, Ana, Andreas, Bernd, Bertil, Brigitta, Emma, Lars, Michelle, Nils, Norbert, Oleg, Paul, Rurik, Samuel, Torgny, Ulrike, Vladimir, and Wladimir: you all contributed to make my years at the department memorable.

I would like to thank Alessandro and Luca for our Italian moments, and my friends of the “Finska Nation” in Uppsala, in particular Enzo, Rico, Matthias and Anne, Mike and Hanna, for their positive attitude towards life, their creativeness and generosity, and for all the good time we have spent together.

I thank all my “Aussie” friends of Mount Stromlo Observatory, in particular Regner and Charlotte, Sebastian and Kate, Damian and Cristina, Christine, Marilena, and Mary for their hospitality and cordiality during my various visits Down Under.
I thank my friends and my family in Italy, for their support, and my parents for their continuous love and understanding and for always encouraging my interest in science.

I finally thank you, Mirva, for all the love and inestimable support you have been giving me during these years, and without which my work would have been much harder.
Bibliography


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