New Generations of Stellar Model Atmospheres

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Abstract.
Stellar model atmospheres form the basis for any element abundance determination and hence are crucial ingredients for studies of stellar, galactic and cosmic evolution. With recent observational progress with the advent of 8m-class telescopes and efficient spectrographs, the dominant source of uncertainty today originates with the assumptions and approximations in the analyses, emphasizing the great need for continuing efforts in improving the realism of stellar atmosphere modelling. In the present contribution I will describe recent progress in this regard by focussing on three complementary types of model atmospheres: line-blanketed non-LTE models of hot stars, 3D hydrodynamical models of cool stars and semi-empirical models for large-scale stellar abundance analyses.

1. Introduction
Determining stellar element abundances play an integral role in most endeavours to improve our understanding of stellar, galactic and cosmic evolution. The term observed abundances is somewhat of a misnomer, however, since the chemical composition of course can not be inferred directly from an observed spectrum. The obtained abundances are therefore never more trustworthy than the models employed to analyse the observations. The derivation of accurate abundances require realistic models of both the spectrum formation region and the spectrum formation process, an obvious fact which unfortunately is often overlooked in the analysis and in assessing the systematic errors. Costly new observational facilities like large telescopes and sophisticated instrumentation will only reach their full potential once combined with the appropriate analysis tools. Today, the uncertainties are no longer dominated by observational errors but by shortcomings in the modelling of stellar atmospheres and line formation. Nevertheless, much progress has been made lately in this respect and here I will highlight a few of these. Unfortunately due to page limitations I am unable to discuss many other impressive works for which I sincerely apologize. I will concentrate on one area each for hot and cool stars: line-blanketed non-LTE modelling and 3D hydrodynamical treatment of convection, respectively. I will conclude the review by making a call to arms to develop non-LTE inversion methods which are urgently needed to enable analysis of very large stellar samples.
2. Hot stars

2.1. Line-blanketed non-LTE model atmospheres

With the high temperatures encountered in hot star atmospheres, radiative rates mostly overwhelm collisional ones, rendering the assumption of local thermodynamic equilibrium (LTE) unacceptable. As a consequence the rate equations for all atomic level populations (assuming time-independence: statistical equilibrium) must be solved simultaneously with the radiative transfer equation, as well as the hydrodynamical equations of conservation of mass, momentum and energy (which in the absence of a wind simplify to hydrostatic and radiative equilibria), in a plane-parallel or spherical 1D geometry. Since the populations depend on the radiation field, which in turn is determined by the opacities and hence populations, this system of equations is extremely non-local and nonlinear with everything in principle depending on everything else, everywhere else. Complicating factors also arise from the fact that the intense radiation field often drive massive stellar winds, which among other things cause severe problems for the treatment of radiative transfer by shifting spectral lines in and out of the shadows of other lines formed in deeper layers.

The last couple of decades has seen very impressive progress in constructing non-LTE model atmospheres (e.g. Hillier & Miller 1999; Pauldrach et al. 2001; Werner 2003 and references therein). Much of this is due to the development of efficient numerical algorithms such as the approximate lambda iteration technique (e.g. Scharmer 1981). The mean intensity $J_\nu$ is obtained from the source function $S_\nu$ using an iterative procedure $J_\nu^n = \Lambda^* S_\nu^n + (\Lambda - \Lambda^*) S_\nu^{n-1}$ through an approximate (e.g. local) lambda operator $\Lambda^*$; $\Lambda S_\nu^{n-1}$ simply denotes a formal radiative transfer solution with the current estimate of $S_\nu$ (see e.g. Werner 2003 for a detailed description). Improved convergence properties can also be achieved through preconditioning of the equations. Equally important for the success has been the advent of appropriate atomic data and methods for the statistical representation of them. Data from Opacity Project, Iron Project and the like has allowed line-blanketing from millions of spectral lines involving thousands of atomic levels from different species to be taken into account with $\sim 10^8$ frequency points using the superlevel concept (Anderson 1989).

Some work in this arena still remains however. Often the radiatively-driven wind is not self-consistently calculated from the theoretical radiative acceleration (the so-called wind-momentum problem of WR and similar stars) and instead a parametrized mass loss rate and velocity law are prescribed (e.g. Castor et al. 1975). Alternatively the calculations are restricted to either the quasi-hydrostatic photosphere or the supersonic wind parts. Observationally there is increasing evidence for both time-dependence and spatial inhomogeneities in the winds of hot stars in the form of shocks and clumps being accelerated outwards (e.g. Eversberg et al. 1998). Needless to say, time-dependent 3D non-LTE calculations is a very daunting task indeed but given the enormous progress achieved lately it is not inconceivable that also these issues will be addressed with the next generation of models in the coming years.
2.2. Implications for CNO abundances

The introduction of massive line-blanketing in the new generation of model atmospheres of hot stars directly affects the atmospheric structure, the ionization balance and the predicted emergent flux distribution. Indirectly it also modifies the estimated stellar parameters, in particular the effective temperature $T_{\text{eff}}$ and the mass loss rate. For main sequence O stars the inclusion of line-blanketing can lead to a substantial decrease in $T_{\text{eff}}$ of 1000-4000 K (Martins et al. 2002) at solar metallicity, which obviously also has an impact on the derived element abundances. Even larger differences are expected for giants and supergiants.

C, N and O are among the relatively few elements for which abundances can be determined in OB stars. With the improved atmospheric and ionization structures, the overall agreement between observations and predictions is in general quite impressive, with the exception of some lines formed in the extended wind (Pauldrach et al. 2001; Crowther et al. 2002). A common denominator in most analyses of Galactic and SMC/LMC O supergiants is the existence of non-solar CNO abundance ratios with a large N enrichment and weak C and O depletion. This indicates mixing of unprocessed and CNO-processed material, possibly related to rotational mixing (Meynet & Maeder 2000). Recently the first results for other external galaxies have appeared based on 8-10m telescopes, again suggesting He and N enrichments (Bresolin et al. 2002).

3. Cool stars

3.1. 3D time-dependent hydrodynamical model atmospheres

For late-type stars such as the Sun, the most pressing uncertainty stems from our poor understanding of convection. The visible surface from which the stellar spectrum originates represents the transition from convective to radiative energy transport. Traditionally convection has been treated by the mixing length theory (MLT) or some close relative thereof. In addition to being a very rudimentary description, MLT is a local theory, which ignores convective overshoot and radiative transfer effects. A far more realistic approach is to solve the hydrodynamical equations coupled to the equation of radiative transfer. Recently much progress has been made in performing 3D radiative-hydrodynamical simulations of stellar surface convection (e.g. Nordlund & Dravins 1990; Freytag et al. 1996, 2002; Stein & Nordlund 1998; Asplund et al. 1999, 2000a; Asplund & García Pérez 2001; Ludwig et al. 2002), which subsequently can be applied to studies of spectral line formation. These investigations have clearly shown that in many cases standard 1D analyses are very misleading in terms of derived element abundances.

The 3D model atmospheres developed by our group have been computed with a 3D, time-dependent, compressible, explicit, radiative-hydrodynamics code (Stein & Nordlund 1998). The hydrodynamical equations for conservation of mass, momentum and energy are solved on a Eulerian mesh with gridsizes of $\approx 10^3$. The physical dimensions of the grids are sufficiently large to cover many granules simultaneously and extended enough in the vertical direction to reach almost adiabatic conditions in the bottom. In terms of continuum optical depth the simulations extend at least up to $\log \tau_{\text{Ross}} \approx -5$, which for most purposes are
Figure 1. A snapshot from a 3D hydrodynamical model atmosphere of the Sun depicting the emergent continuous intensity on the top layer and the entropy structure on sides and the displaced bottom layer. The maximum temperature contrast occurs close to the visible surface, revealing the granulation pattern of warm upflows and cool downdrafts.

sufficient to avoid numerical artifacts of the open upper boundary on spectral line formation. Periodic horizontal boundary conditions are employed, allowing the simulations to describe a small and representative region of the stellar surface (Fig. 1). The temporal evolution of the simulations cover several convective turn-over time-scales to allow thermal relaxation to be established and to obtain statistically significant average atmospheric structures and spectral line profiles following disk-integration. The input parameters discriminating different models are the surface gravity $\log g$, metallicity $[\text{Fe}/\text{H}]$ and the entropy of the inflowing material at the bottom boundary. The effective temperature of the simulation is therefore a property which depends on the entropy structure and evolves with time following changes in the granulation pattern.

In order to obtain a realistic atmospheric structure, it is crucial to have the best possible input physics, and properly account for the energy exchange between the radiation field and the gas. The adopted equation-of-state is that of Mihalas et al. (1988), which includes the effects of ionization, excitation and dissociation. The continuous opacities come from the Uppsala package (Gustafsson et al. 1975 and subsequent updates) while the line opacities are from Kurucz (1993). The 3D radiative transfer is solved at each time-step under the assumptions of local thermodynamic equilibrium (LTE, $S_\lambda = B_\lambda$) and opacity binning. The opacity binning includes the effects of line-blanketing in a manner reminiscent of opacity distribution functions.

It should be stressed that the here described 3D hydrodynamical model atmospheres do not include any free parameters which are tuned to improve the agreement with observations. Yet the simulations are highly successful in repro-
ducing key observational constraints, such as helioseismology, detailed spectral line shapes, and granulation characteristics (e.g. Stein & Nordlund 1998; Asplund et al. 2000a,b). Thus the usual free parameters (mixing length parameters, micro- and macroturbulence) hampering classical 1D analyses have finally become obsolete with the advent of the new generation of 3D model atmospheres. The major drawbacks with such 3D modelling is their computationally demanding nature and that so far only a relatively limited stellar parameter space has been chartered. Through the continuous improvement in computer hardware and software the former problem will be steadily relaxed in the coming years, while already work is being undertaken to extend the modelling to other types of stars, most notably A stars (Freytag et al. 1996), M dwarfs (Ludwig et al. 2002), supergiants (Freytag et al. 2002) and red giants.

3.2. Implications for CNO abundances

Spectrum formation is a highly non-local and non-linear process. It is therefore not surprising that 3D analyses in general yield element abundances which are not the same as with traditional 1D investigations, given both the different photospheric mean structures and the presence of spatial inhomogeneities. In many cases the differences can be profound with far-reaching consequences. Here I will limit the discussion on the impact of 3D model atmospheres on C, N and O for the Sun and metal-poor stars.

**Sun:** The solar spectrum offers a multitude of atomic and molecular lines to determine the abundances of C, N and O. Primary diagnostics are: [C I] 872.7 nm, high-excitation C I lines, and CH vibration-rotation transitions in the IR for C; permitted N I lines and NH vibration-rotation lines in the IR for N; [O I] 630.0 nm, high-excitation O I lines, and OH vibration-rotation and rotation-rotation transitions in the IR for O. Secondary, supportive roles are offered by electronic CH, C2, CN and OH lines. Astonishingly, with 1D model atmospheres the discrepancies between different indicators amount to as much as 0.2-0.3 dex, casting doubts on the use of such models for stars where not all types of lines can be employed. In particular for O the dissonance is striking with the often preferred OH lines (e.g. Grevesse & Sauval 1998) indicating about 0.3 dex higher abundance than the O I 777 nm triplet with the [O I] line in between.

We have recently re-analysed all of the above-mentioned solar diagnostics using our 3D hydrodynamical solar model atmosphere, the best possible atomic and molecular data, and high-quality solar atlases. Reassuringly, we find excellent agreement between different lines for C, N and O, in sharp contrast to the 1D case. In particular, the presence of cool pockets in the photosphere due to convection produces stronger molecular lines and hence lower derived abundances compared with standard 1D model atmospheres. Our preliminary results indicate log $\epsilon$(C) = 8.41 ± 0.03, log $\epsilon$(N) = 7.80 ± 0.04, and log $\epsilon$(C) = 8.66 ± 0.03, where the here quoted uncertainties are only the standard deviations between the different abundance indicators (Allende Prieto et al. 2001, 2002; Asplund et al., in preparation). It is noteworthy that this represents a substantial decrease from previously adopted values (e.g. Fig. 2) but is in good agreement with results for nearby B stars, local interstellar medium and solar corona/wind measurements. The resolution of these long-standing discrepancies gives further credibility to the new generation of 3D hydrodynamical model atmospheres.
Figure 2. The derived solar O abundances from the OH vibration-rotation lines in the IR using a 3D model atmosphere (filled circles) and the semi-empirical 1D Holweger-Müller model (open circles) as a function of excitation potential of the lower level.

Metal-poor stars: The differences between 1D and 3D model atmosphere predictions are perhaps most pronounced in metal-poor halo stars (Asplund et al. 1999). Due to the weak coupling through spectral lines between the radiation field and the gas at low metallicities, the temperatures in the optically thin photospheric layers can reach very low values with a proper treatment of convection, significantly below the radiative equilibrium temperatures enforced in standard 1D model atmospheres. For spectral lines sensitive to those atmospheric depths, the resulting differences can be profound. In particular, molecular features, minority ionization stages and low-excitation lines are very vulnerable and significant systematic errors can be expected in 1D analyses. This inadequate atmospheric modelling probably lies at the heart of the long-standing oxygen problem in metal-poor stars, i.e. that different diagnostics support either a flat plateau at $\text{[O/Fe]} \sim +0.4$ (not accounting for the new low solar O abundance mentioned above) or linear rising trend reaching $\text{[O/Fe]} \sim +1$ at $\text{[Fe/H]} = -3$. In particular, the application of 3D model atmospheres bring down the very high oxygen abundances from OH lines (Asplund & García Pérez 2001) but also those of the $[\text{O}~\text{I}]$ line (Nissen et al. 2002); 3D non-LTE calculations of $\text{O}~\text{I}$ yield similar results as in 1D non-LTE (Asplund et al., in preparation). The final verdict is not yet in, partly due other out-standing factors such as non-LTE effects on OH, but it appears that the truth, not surprisingly perhaps, lies in between the hotly contested plateau and linear trend (Nissen et al. 2002). Similarly, many conclusions about C and N abundances in metal-poors probably have to be revised. Normally such determinations are based on molecular lines such as CH,
NH and CN, and hence the abundances are likely significantly over-estimated in 1D. Naturally this would bring down the claimed [C/Fe] and [N/Fe] trends at low metallicity, as well as the incidence of very C-rich halo stars. Work is currently under way to address these issues.

4. Large-scale stellar abundance analyses

4.1. The need for semi-empirical model atmospheres

The new generations of stellar model atmospheres described above are both theoretical, as are almost all other models. However, the properties of the stellar atmospheres are encoded in the observed stellar spectra which at least in principle can be deciphered to yield the photospheric structure using inversion techniques. This method has often been employed among solar physicists with the Holweger-Müller (1974) and the VAL-3C (Vernazza et al. 1981) solar models being the most well-known examples. Surprisingly, such semi-empirical model atmospheres have rarely been used for stellar spectroscopy. I believe that the time is now ripe for pursuing such modelling, in fact crucial in order to make optimum use of future satellite and ground-based telescope facilities.

Perhaps the biggest problem with using the above-mentioned theoretical model atmospheres for stellar abundance analyses is their computationally intensive nature. Although less sophisticated model atmospheres are less CPU-demanding, also standard abundance analyses are time-consuming in terms of the work involved. Even today the largest studies of stellar abundances involve only a few hundred stars (e.g. Reddy et al. 2003). To fully disentangle the formation and evolution of for example our own Galaxy would require a far more ambitious approach with much larger stellar samples (Freeman & Bland-Hawthorn 2002). Fortunately this is now becoming feasible with new multi-object high-resolution spectrographs like FLAMES/VLT. Several other, even more ambitious instruments are currently in the design phase or being discussed in detail, such as the RAVE project (Steinmetz et al. 2002) and the GAIA satellite (Perryman et al. 2001). The wealth of information these facilities will provide is truly astonishing, as is the magnitude of data needed to be analysed. Without an efficient automatic procedure to derive the inherent information in the spectra, these projects will not come to an optimal execution. Semi-empirical model atmospheres represent one such promising possibility, provided the spectral resolving power is sufficient.

4.2. Ingredients and outlook for the future

Semi-empirical model atmospheres are obtained through an iterative procedure aimed at improving the overall agreement between the calculated and observed spectra. Since the temperature structure is modified in this way the model does not in general fulfill flux constancy as in standard theoretical model atmospheres, nor is there any need to invoke uncertain and questionable recipes for convective energy transport, such as the mixing length theory, which can lead to grossly misleading results (e.g. Asplund et al. 1999; Asplund & García Pérez 2001). In fact, this allows at least in principle a possibility to gain insight into convection and non-standard energy transport, such as acoustic and magnetic heating.
With the temperature determined from the observations, the gas pressure is normally fixed by the assumption of hydrostatic equilibrium while the electron pressure is the result of the ionization balance using the current estimate of the chemical composition. Thus knowledge of the surface gravity is necessary from for example parallaxes or photometry unless it can be obtained from satisfying the ionization balance of some key elements. Essentially all existing modelling is based on a 1D plane-parallel geometry but some attempts with multi-component atmospheres have been made, corresponding for example to convective up- and downflows (Frutiger et al. 2000). Naturally, inversions must rely on accurate atomic data to yield realistic results.

The main disadvantages with semi-empirical modelling comes with the numerical difficulties often associated with ill-posed inversion problems and the assumption of LTE normally made in the line formation calculations. The former can to a large extent be overcome by including a wide range of spectral lines with different line formation depths, ionization stages and excitation potentials. Of particular importance, at least for late-type stars, is to include elements with both neutral and ionized lines and strong lines with pressure-damped wings. Although not yet utilized, hydrogen lines as well as various molecular lines have a great potential in this respect. The second major shortcoming can only be resolved by relaxing the assumption of LTE, which automatically makes the inversion procedure much more challenging and cumbersome. Very little work with the exception of the pioneering contribution by Soccas-Navarro et al. (1998) has been done on non-LTE inversion. It is, however, of absolute pivotal importance to include such effects, given the fact that LTE is often a poor assumption for the line formation process, leading otherwise to erroneous atmospheric structures and inferred conclusions. It suffices here to mention the case of Fe I which offers the most useful lines for inversion modelling in late-type stars but suffers from over-ionization, in particular at low metallicities.

Recent endeavours like the Opacity Project and Iron Project have come a long way in addressing the great needs for atomic data for non-LTE calculations. Although it would be advantageous to treat all elements in non-LTE for the inversions, as a first step it may be sufficient to do so for the most important elements for determining the actual atmospheric structure, such as Fe, Mg and Ca, while the line formation of other significant species for late-type stars like H and various molecules (e.g. CO) can likely be well approximated by LTE. Other trace elements which are unimportant for setting the atmospheric structure but whose abundance may be of interest can then be handled either in LTE or non-LTE after the initial inversion has converged. This procedure should restrict the computing time to just a few times a normal non-LTE calculation with a fixed 1D atmosphere. Adopting the superlevel concept to reduce the number of atomic levels for complex atoms like Fe should speed up the computations further and bring the non-LTE inversion concept fully within the realms of possibility for the coming few years. This should enable truly grandiose studies of galaxy formation and evolution possible with current and future observational capabilities.

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to the conference celebrating André’s 70th birthday, which will hopefully take
place in a similarly wonderful environment and atmosphere. Even further into
the future I hope I am not too old to also participate in the conference held in
connection with André’s retirement.

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