Effects of Convection on Line Profiles and Abundances

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Abstract. The effects of convection on spectral line formation have been investigated by means of 3D, time-dependent, hydrodynamical simulations of stellar surface convection. One of main strengths of the approach is the parameter-free nature of the simulations and the spectral synthesis. In particular, there is no need to invoke any ad-hoc micro- and macroturbulent broadening as required in 1D analyses, since the Doppler shifts due to the self-consistently calculated convective motions provide the necessary broadening. The resulting spatially and temporally averaged solar Fe line profiles and asymmetries show excellent agreement with observations, which have enabled an accurate determination of the solar Fe abundance: $\log \epsilon_{\text{Fe}} = 7.47 \pm 0.05$. Convection simulations for low-metallicity stars show drastic differences compared with both solar-metallicity simulations and classical 1D model atmospheres. The optically thin layers have strongly sub-radiative equilibrium temperatures due to the dominance of adiabatic cooling over radiative heating. The very different temperature structures translate to significantly different emergent spectra and thus derived abundances. In particular, the primordial Li abundance may previously have been over-estimated by about 0.3 dex, although caution should be exercised since the steep temperature gradients in the low-metallicity simulations may be prone to departures from LTE.¹

1. Introduction

For late-type stars such as the Sun, convection is of particular interest as the convection zone extends to the surface layers and thereby directly influences the thermal structure and emergent spectrum. Since the use of stars as probes of stellar, galactic and cosmic evolution relies on a accurate understanding of the spectrum formation in the stellar photospheres, a proper treatment of convection in the model atmospheres is therefore crucial. Traditionally convection has been included in stellar evolution and atmosphere models by means of the mixing length theory (MLT) or some close relative thereof. Although simple such a procedure is uncertain due to the inherent assumptions of MLT: local, time-independence, 1D, ignoring radiative transfer effects etc. Furthermore, MLT

¹The www-version of this oral contribution can be found at http://www.astro.uu.se/~martin/talks/Tenerife99
contains several free parameters that need to be calibrated somehow. A more ambitious, albeit more CPU-demanding, approach is to compute 3D, hydrodynamical model atmospheres in which the convective motions and the thermal structure and inhomogeneities are self-consistently computed through a numerical solution of the hydrodynamical Navier-Stokes equations coupled to a simultaneous solution of the radiative transfer equation. This field was pioneered by Åke Nordlund and collaborators (e.g. Nordlund 1982; Stein & Nordlund 1989, 1998), and it has now reached such a sophistication that it is possible to make similar simulations for a variety of stars: main-sequence (A-K) stars, white dwarfs, red giants and even supergiants (Freytag, these proceedings). Recently the first simulations corresponding to metal-poor halo stars have been constructed (Asplund et al. 1999a). The solar simulations successfully reproduce the observed granulation topology and flow, intensity brightness contrast (Stein & Nordlund 1998), helioseismological constraints (Rosenthal et al. 1999) and spectral line shapes, shifts and asymmetries (Asplund et al. 1999b,c).

2. Simulations and spectral line calculations

The 3D model atmospheres of stellar granulation which form the basis for the spectral line calculations presented here have been obtained with a 3D, time-dependent, compressible, radiative-hydrodynamics code developed by Stein & Nordlund (1989, 1998). The hydrodynamical equations of mass, momentum and energy coupled to the 3D equation of radiative transfer are solved on a non-staggered Eulerian mesh with typically \(100^3 - 200^3\) gridpoints. The simulation box covers only a region of the surface convection zone and ignores effects due to rotation and magnetic fields. In order to obtain a realistic atmospheric structure, special consideration has been paid to include state-of-the-art input physics in terms of equation-of-state (Mihalas et al. 1988) and opacities, including line opacities (Gustafsson et al. 1975; Kurucz 1993). For the radiative transfer the simplifying assumption of LTE has been made together with the technique of opacity binning for the line-blanketing (Nordlund 1982). Further details on the simulations can be found in Stein & Nordlund (1998) and Asplund et al. (1999b).

The LTE spectral line calculations presented here have been performed using the convection simulations as 3D, inhomogeneous model atmospheres (interpolated to a more restricted depth-scale in order to improve the numerical accuracy in the radiative transfer). For each snapshot the line formation is computed using typically 30 different angles. Both spatially resolved and spatially and temporally (typically some 60 snapshots covering about an hour of stellar time) averaged profiles have been considered. It is noteworthy that no micro- and macroturbulence enter the spectral synthesis. However, for flux profiles additional broadening due to rotation has been taken into account in the disk-integration, which therefore is the only free parameter in the procedure besides the abundance of the element in consideration, although rotation does not of course influence the derived elemental abundances.
Figure 1. A selection of the spatially resolved profiles of the Fe\textsc{i} 608.2 nm line from a specific instant in the solar simulation. Upflowing regions typically have stronger, blue-shifted lines with higher continuum intensities than the downflows. The temperature reversal in the upper atmosphere, i.e. upflows become cooler than the downflows due to adiabatic cooling, is clearly seen in the line cores.

3. Solar line formation

Spatially resolved profiles show an astonishing variety of shapes, strengths and shifts, as illustrated in Fig. 1. It is clear that the spatially averaged profile will be sensitively dependent on the details of the 3D photospheric granulation structure. The strength of a line is mainly determined by the overall temperature structure, which therefore is biased towards upflowing regions (granules). The width of a line reflects the total velocity amplitude between up- and downflows, while the line shift (which in the case of the Sun amounts to between 0 and 600 m s\(^{-1}\)) depends on the temperature-velocity correlations in the line forming region. The intrinsic asymmetry of the line (as measured by e.g. the bisector) is due to the details of the convective overshoot. Therefore, obtaining a good agreement between observed and predicted profiles and bisectors lend strong support to the realism of the simulations.

To emphasize the importance of the convective motions in the line formation, Fig. 2 shows the predicted spatially averaged profile of the same Fe\textsc{i} line as in Fig. 1 but with all convective velocities in the simulations artificially removed. Clearly the shape, shift and asymmetry show a very poor resemblance to observations. Incidentally, this profile is very similar to those predicted by classical
Figure 2. The predicted spatially averaged profile (red diamonds) of the Fe I 608.2 nm line when artificially removing all convective velocities in the convection simulation. In comparison with the solar intensity atlas (blue solid line, Brautl & Neckel 1987) the predicted line is much too narrow and has the wrong line shift and asymmetry. This theoretical profile is very similar to those calculated with classical 1D model atmospheres without micro- and macroturbulence.

1D model atmospheres without invoking additional ad-hoc broadening due to micro- and macroturbulence. This should be contrasted to the real predicted profile when including the self-consistent velocity field, which is shown in Fig. 3. The agreement is essentially perfect. Therefore both micro- and macroturbulence have the same origin: the Doppler shifts introduced by the convective motions. Intermediate strong lines tend to show slightly poorer agreement in the line cores, which may be due to departures from LTE or a slightly erroneous temperature structure in those high atmospheric layers.

Line asymmetries and shifts provide an even more sensitive test of the realism of the simulations. The main advantages of working with solar Fe lines are the existence of very accurate atomic data (wavelengths, gf-values, etc.) and observed high-resolution spectra on an absolute velocity scale. Fig. 4 shows a few examples of observed and predicted bisectors; since both types of profiles are on an absolute wavelength scale no shifts in the bisectors have been allowed. Again, the agreement is quite satisfactory. In fact the agreement is better than expected for the lines shown, since the uncertainties in the laboratory wavelengths and wavelength calibration of the solar atlas are typically 30–50 m s⁻¹.

The excellent correspondance in line shapes for the Fe lines allows an accurate determination of the solar Fe abundance (Asplund et al. 1999c), which has
Figure 3. The spatially and temporally averaged Fe I 608.2 nm line (red diamonds) from the solar simulation compared with the solar intensity atlas (blue solid line, Brault & Neckel 1987). The agreement is essentially perfect, even without any ad-hoc broadening due to micro- and macroturbulence.

recently been a matter of debate (Blackwell et al. 1995; Holweger et al. 1995). The main advantages are that we do not need to use any equivalent widths, microturbulence or Unsöld enhancement factors for the damping (Anstee & O'Mara 1995). The procedure therefore eliminates three of the four blamed factors for the discrepancies between the Oxford and Kiel groups, leaving the gf-values as the sole major uncertainty. The 3D convection simulation should also be a more realistic description of the solar photosphere than the Holweger-Müller (1974) model. With the Oxford Fe I lines we derive \( \log \epsilon_{\text{FeI}} = 7.47 \pm 0.05 \) while the Kiel lines give \( \log \epsilon_{\text{FeI}} = 7.43 \pm 0.06 \). The difference basically reflects the difference in the two gf-scales. A similar abundance is found with Fe II lines: \( \log \epsilon_{\text{FeII}} = 7.47 \pm 0.09 \). The photospheric Fe abundance is therefore consistent with the meteoritic value (Asplund 1999), which would appear to finally settle the dispute regarding the solar Fe abundance.

4. Stellar line formation

The convection simulations and 3D spectral syntheses can naturally be applied also to stars other than the Sun (e.g. Dravins & Nordlund 1990; Allende Prieto et al. 1999; Allende Prieto et al, these proceedings). Such an approach allows an investigation of the nature of convection and granulation in different stellar environments and can serve as (hopefully) more reliable model atmospheres.
Figure 4. A few examples of observed (blue solid line with error bars) and predicted (red solid line) solar Fe I line bisectors. Both types of bisectors are shown on an absolute velocity scale and no velocity shifts have been applied. In contrast, predicted profiles with classical 1D model atmospheres are of course completely symmetric since they lack any velocity field.

for abundance analyses and asteroseismology. A vital ingredient is a detailed comparison between observed and predicted line bisectors to ensure that the simulations are sufficiently realistic in describing the stellar photospheres.

Recently the first 3D convection simulations of metal-poor halo stars have been performed (Asplund et al. 1999a). Though qualitatively similar to solar granulation there are notable and unexpected differences in the appearance of convection. For solar-metallicity stars the gas in the surface layers remains close to radiative equilibrium, since radiative heating from spectral lines balances the cooling from adiabatic expansion of the ascending material. For halo stars, however, the shortage of sufficiently strong spectral lines allows the adiabatic cooling to dominate more, which results in very low atmospheric temperatures. This effect is completely opposite to predictions from classical hydrostatic model atmospheres in which radiative equilibrium is enforced and shallower temperature gradients are expected for decreasing metallicities. In the optically thin layers the difference between the horizontal mean temperature in the simulations and the corresponding 1D model atmospheres can amount to more than 1000 K.

The drastically different thermal structure compared with the 1D prediction naturally translates to a different emergent spectrum and thus derived elemental abundances. Lines of neutral minority species, low excitation transitions and stronger lines are formed in the higher layers and are affected by the low temperatures encountered there, making the lines stronger for a given abun-
dance. Other lines, in particular high excitation transitions and lines of ionized species, which are formed in the deeper layers, are much less affected or even show the opposite trend compared with 1D model atmospheres. Of particular interest is the Li I 670.8 nm line in halo stars which is believed to reflect the primordial Li abundance produced in the Big Bang nucleosynthesis. According to the results from the 3D LTE predictions, the Li abundances may previously have been over-estimated by 0.2–0.35 dex. Furthermore, significant “3D effects” are present for e.g. B I (about 0.2 dex), Ca I (0.1–0.2 dex) and Fe I (0.3–0.4 dex). It is noteworthy that lines of Be II, O I and Fe II are only marginally affected. Although not yet investigated temperature-sensitive lines like the OH lines may be poor O diagnostics when used together with 1D model atmospheres.

We caution, however, that the results rely on several underlaying assumptions, which can alter the interpretations. The effective temperatures of the 3D models have been assumed to be identical to those estimated with the IR flux method using 1D model atmospheres, and may therefore be systematically in error. However, preliminary calculations reveal only minor differences (≤ 50 K) between the 3D simulations and 1D MARCS model atmospheres in terms of the IR flux method. The adopted $T_{\text{eff}}$ is therefore unlikely to be a significant source of worry. More seriously, the line transfer calculations have assumed LTE, which may be questioned for some species. The steep temperature gradients may be prone to significant departures from LTE in the form of e.g. over-ionization. Indeed there are observational evidence for this to be the case: with the adopted stellar parameters ionization balance of Fe I and Fe II is not fulfilled, which indicates that over-ionization is a significant factor. If Fe I is indeed over-ionized one may speculate that Li I should show a similar effect, in particular since even in the Sun, the Li line formation is far from in LTE (Kiselman & Asplund, these proceedings). Clearly, 3D NLTE calculations for Li in metal-poor stars have a very high priority.

5. Conclusions

3D, hydrodynamical simulations of solar and stellar surface granulation show a very high degree of realism in terms of spectral line formation. Without invoking any free parameters like mixing length parameters, micro- and macroturbulence, the predicted solar line profiles agree essentially perfectly with the observed profiles. Thus both micro- and macroturbulence can be explained by the action of the Doppler broadening due to the convective motions. Furthermore, both Fe line shifts and asymmetries are remarkably well predicted, which lends further support to the accuracy of the simulations in describing the solar photosphere.

Another major advantage of applying 3D convection simulations to the problem of spectral synthesis is that the effects of temperature inhomogeneities are accounted for, which is lost with classical 1D model atmospheres. Since different lines show different sensitivity to the temperature structure, some lines may be well described by a 1D structure while others are very poorly predicted. The 3D simulations contain much more information than 1D models and should therefore be more realistic, in particular since several otherwise hampering free parameters can be eliminated in the analyses. Now when the necessary tools are available to construct 3D hydrodynamical model atmospheres and even 3D
NLTE calculations (e.g. Botnen 1997), it is crucial that the current observational progress with the advent of the new generation of 8m telescopes is accompanied by a simultaneous improved theoretical modelling, in order to ensure that the interpretation of stellar spectra is not limited by the modelling uncertainties and to avoid possible systematic errors.

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**Discussion**

*K. Strassmeier:* Wouldn't the effect from neglecting the surface B field plus the surface differential rotation (for the solar case) be enough to make the good fit to average line profiles go away?

*M. Asplund:* The solar line profile comparison was done using intensity observations at disk center of the quiet Sun and therefore rotational broadening does not enter. The Fe lines we have compared all have small Lande factors and should thus be minimally affected by the relatively low magnetic field strength in the quiet Sun.

*J. Linsky:* Many years ago Anderson and Athay computed a one-dimensional solar model with many iron lines included and they found significant departures from LTE and the thermal structure required ad-hoc heating. On the other hand your 3-D calculations fit the iron line profiles that are consistent with LTE. So, are their derived non-LTE effects an artifact of the one-dimensional nature of their calculations?

*M. Asplund:* It is difficult to tell whether this may be the case until 3D NLTE calculations for Fe have been performed. However, more recent NLTE calculations (e.g. Schukina & Trujillo Bueno, these proceedings) reveal only minor departures from LTE using a variety of different 1D model atmospheres. It is quite conceivable that minor departures from LTE only result in insignificant changes to our 3D LTE profiles since e.g. a small over-ionization can be basically compensated for by a slightly different derived Fe abundance when using our 3D convection simulations.

*G. Wuchterl:* 1) Concerning the free parameters: do you have a subgrid turbulence model and is it free of parameters? 2) Do you think it will be possible to replace the mixing length theory (MLT) in stellar evolution models? Because using direct hydro-simulations for stellar evolution would require proceeding at very high Courant numbers.

*M. Asplund:* 1) There is no subgrid turbulence model used neither in the actual convection simulations nor in the 3D spectral synthesis but we do apply a hyperviscosity diffusion scheme in the solution of the hydrodynamical equations for stability reasons. 2) For most of the convection zones, the convection is completely adiabatic and therefore recipes like MLT are perfectly acceptable (unless mixing due to overshoot etc is of interest). MLT is therefore suitable in stellar
evolution models provided the free parameters (like the mixing length) is calibrated using more detailed calculations like those presented in my talk. In these simulations the entropy jump between the surface and the interior can be accurately estimated. This has been done both by our group (by R. Trampedach) and by the Kiel group (by B. Freytag, H.-G. Ludwig and M. Steffen).

K. Chan: A comment: I guess that the “subgrid turbulence” mentioned by Dr. Wuchterl means the enhanced numerical viscosity that needs to be used in all numerical simulation of stellar convection. It is a free parameter. Whether this parameter affects the results depends on the resolution and the quantities of interest.

M. Asplund: This is correct. The numerical code has been stabilized using a hyper-viscosity diffusion scheme. The diffusion parameter has been determined from standard hydrodynamical test cases (e.g. shock tubes) and is thus not really a free parameter in our convection simulations. However, we have investigated the influence of the diffusion scheme on the resulting convection pattern and found insignificant differences, mainly because properties like the temperature structure (which is most important for the line formation) is basically determined by the total amount of radiative cooling at the stellar surface and mass conservation.

References

Asplund M., 1999, submitted to A&A
Asplund M., Nordlund Å., Trampedach R., Allende Prieto C., Stein R.F., 1999b, submitted to A&A
Asplund M., Nordlund Å., Trampedach R., Stein R.F., 1999c, submitted to A&A
Dravins D., Nordlund Å., 1990, A&A 228, 203
Nordlund Å., 1982, A&A 107, 1
R. Stern, R. Neuhäuser