

Model atmospheres: bridging models and observations

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Abstract. There has been extensive development in the generation of 1D, LTE model atmospheres and detailed spectra over the past 10 years. In addition, there have been promising advances in 3D, hydrodynamic and non-LTE modelling for several typical stars, especially the sun. Extensive accurate spectrophotometric observations of many hundreds of stars across the HR-diagram are also now available enabling a critical comparison of models and observations.

Key words. Stars: abundances – Stars: atmospheres – Stars: Spectroscopy – Catalogs

1. Introduction

There has been extensive development in the generation of 1D, LTE model atmospheres and detailed spectra over the past 10 years. ATLAS: Castelli, Munari et al.; MARCS: Gustafsson, Edvardsson, Eriksson et al.; PHOENIX- NEXTGEN: Hauschildt, Allard et al.; Burrows and Tsuji have also explored the coolest regime of M, L, T dwarfs. All these are 1D, LTE, plane-parallel (some spherical) models in hydrostatic equilibrium that have been very successful in describing the overall flux spectrum, colors and temperatures of stars. But they are unable to replicate some of the details of the line spectra, in particular, 1D models computed with convection handled through mixing-length-theory cannot reproduce the solar T-t relation. With the advent of better computational facilities, 3D modelling with realistic hydrodynamics has been pursued, principally by Stein, Nordlund and Asplund et al. for the sun together with ex-

tensive theoretical non-LTE calculations for particular atomic species. The last few years have also seen the publication of new atlases of intermediate resolution stellar spectra, one ground based (MILES) the other from space (STIS) providing precise spectrophotometry for a wide variety of stars with a range of metallicity. These new spectra are ideal for comparison with the detailed model atmosphere synthetic spectra.

2. Model atmosphere grids

The MARCS models (Gustafsson et al. 2003) covers the temperature range 2500K-8000K. The website¹ provides models and spectra between 4000K-8000K. The models for M giants and supergiants are described by Plez, Brett & Nordlund (1992) and Plez (1992); M dwarfs between 2000K-4000K by Brett & Plez (1993) The models are computed using opacity sampling for lines and the line lists comprise

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¹ <http://www.marcs.astro.uu.se>

atomic lines from VALD and many molecular lines.

The Kurucz-Castelli ATLAS models ² cover the temperature range 3500K - 47500K. They incorporate the line opacity using using Opacity Distribution Functions but the synthetic spectra (Munari et al. 2005) are generated using line-by-line computations. Some molecules, such as CaH, are missing, and that affects the appearance of M dwarf spectra but not the models. The initial grids have been extended to include additional C-rich models and lower Z models.

Cool star grids (2000K - 10000K) has also been computed by Hauschildt, Allard & Baron (1999)³.

Very cool models down to the brown dwarf regime have been made by Allard et al. (2001) (100K-5000K) ⁴; Tsuji (2005) made unified cloud models for L and T dwarfs; Burrows, Sudarsky & Hubeny (2006) and Ackerman & Marley (2001) modelled L, T dwarfs and exoplanets.

A major complication with the coolest models is the fact that for $T_{eff} < 3000\text{K}$ dust formation takes place. The Phoenix code considers different scenarios depending whether the dust condenses out and settles below the photosphere (COND) or whether it remains in the atmosphere and contributes to the opacity (DUSTY). Tsuji's unified cloudy models on the other hand attempt to model the M-L-T transitions as due to the formation of dust clouds with lowering temperature and additionally by varying the thickness of the cloud at fixed effective temperature. The M-L transition is essentially a function of effective temperature but the L-T transition reflects more the thickness of the dust cloud. Burrows, Sudarsky & Hubeny (2006) similarly model the spectra and colors of the L-T stars in terms of the growth in size of the dust particles.

² <http://wwwuser.oat.ts.astro.it/castelli/grids.html>

³ NEXTEGEN models, available from <http://www.hs.uni-hamburg.de/EN/For/ThA/phoenix/index.html>

⁴ <http://www.hs.uni-hamburg.de/EN/For/ThA/phoenix/index.html>

3. New spectral atlases

The MILES Atlas ⁵ (Sanchez-Blazquez et al 2006; Cenarro et al. 2007) comprises 985 stars spanning a large range in atmospheric parameters. The O - M star spectra cover the wavelength range 3525-7500 Å at 2.3 Å (FWHM) spectral resolution.

An extremely useful, wider wavelength range grid of high precision spectra are available in the HST/STIS Next Generation Spectral Library (NGSL) ⁶. This comprises 378 (when complete 600) high S/N spectra of Hipparcos stars covering a wide range in abundance, effective temperature, and luminosity distributed over four metallicity groups: very low $[\text{Fe}/\text{H}] < -1.5$; low $-1.5 < [\text{Fe}/\text{H}] < -0.5$; near-solar $-0.3 < [\text{Fe}/\text{H}] < +0.1$; super-solar $+0.2 < [\text{Fe}/\text{H}]$. The wavelength range is 2000 - 10200Å with $R \sim 1000$ resolution. Problems with 1-7% residual systematic errors in the red due to object centering in the slit are being addressed by Gregg and Lindler. These STIS NGSL stars make excellent spectrophotometric standards.

Finally, spectra for L and T dwarfs between 6300 - 10100 Å are available from Kirkpatrick (2003) ⁷.

Edvardsson (2007; private communication) compared 129 stars in common to MILES and NGSL. He found, on average, excellent agreement between 3532Å (the shortest wavelength of the MILES spectra) and 6400Å. Redward of 6400Å the NGSL spectra were systematically too bright in the mean by about 5% and the comparison showed a larger scatter. This is the problem with the original NGSL spectra mentioned above. Heap & Lindler (2007 private communication) have successfully removed this effect to better than 2%.

⁵ <http://www.ucm.es/info/Astrof/miles/miles.html>

⁶ <http://lifshitz.ucdavis.edu/~mgregg/gregg/ngsl/ngsl.html>

⁷ <http://spider.ipac.caltech.edu/staff/davy/ARCHIVE/>

4. Comparison with synthetic spectra

Bertone et al (2004) compared the ATLAS and NextGen synthetic spectra with empirical spectra and with each other. They found that the fitting accuracy of both theoretical libraries drastically degrades at low effective temperature where both ATLAS and NextGen models fail to properly account for the contribution of molecular features in the observed spectra of K-M stars. Compared to empirical calibrations, both ATLAS and NextGen fits tend, on the average, to predict slightly warmer (by 4- 8%) temperatures for both giant and dwarf stars of fixed spectral type, but ATLAS provides in general a sensibly better fit than NextGen.

I think that part of the problem is that the lines are being computed too strong for a given temperature, rather than the temperature being systematically wrong.

I also note that the Plez-MARCS spectra of M dwarfs better fit the observations, because they have more molecules (than ATLAS) and they compute the molecular opacity more realistically (than NextGen). We look forward to the updated MARCS cool models to enable a more critical comparison of M dwarf spectra.

Heap & Lindler (2007) have compared some NGS spectra with Munari et al. synthetic spectra. They found that the model fit below 3000Å was poor, presumably due to incomplete atomic data in the UV. The comparison for wavelengths between 3000 and 4000Å was also poorer than at longer wavelengths. Edvardsson (2007 private communication) has compared some MARCS model spectra of A stars and K giants with STIS spectra and find good agreement, although again the agreement is poorer below 4000Å.

5. Effective temperature calibrations

The IR flux method has been used very successfully to determine effective temperatures of FGK stars by Alonso, Arribas & Martinez-Rodgers (1999a,b). Ramirez & Melendez (2005a,b) have most recently used the IR flux method to determine the effective temperature scale of FGK stars. They find excellent agreement with direct measurements for the

mostly near-solar composition stars and excellent agreement with 1D model atmosphere red colors for solar composition stars given by Bessell, Castelli & Plez (1998) and Houdashelt et al. (2000a,b). They reiterate that the IR flux method is the least model-dependent method of estimating effective temperatures.

5.1. Uncertainties in the temperature scale for metal-poor stars

Ramirez & Melendez (2005) state that although comparison of their temperature scale with with other scales, both empirical and theoretical, are in reasonable agreement, both Kurucz and MARCS synthetic colors fail to predict the detailed metallicity dependence of V-I and V-K. Indeed, if the IRFM T_{eff} scale accurately reproduces the temperatures of very metal-poor stars, systematic errors of the order of 200 K are introduced by the assumption of (V-K) being completely metallicity independent.

However, Nissen et al (2007) derived temperatures for metal-poor stars from fitting the H β line profile and came to a different conclusion. They state that when using the (V-K)₀ calibration of Ramirez & Melendez, stars with [Fe/H] > -2.0 have a mean deviation $T_{eff}(V-K)_0 - T_{eff}(H\beta)$ of about -50 K, whereas stars with [Fe/H] < -2.5 have a mean deviation of +124K. Hence, their H β -based effective temperatures do not confirm the hot T_{eff} scale of very metal-poor turnoff stars derived by Ramirez & Melendez (2005) from their application of the infrared flux method.

The reason for this discrepancy is not clear, but the V-K, V-I and H β temperature scale for metal-poor stars based on 1D model atmospheres are consistent with each other.

6. 3D and non-LTE modelling

Asplund (2005) provides an excellent review of 3D modelling and non-LTE analyses for stellar atmospheres. Stein & Nordlund (1998) pioneered the hydrodynamic modelling of the sun and more recent papers by Carlsson et al.(2004) and Freytag, Steffen & Dorch (2002)

have extended that work. Using the 3D hydrodynamical code for the Sun, Grevesse, Asplund & Sauval (2007) have been remarkably successful in obtaining consistent oxygen and carbon abundances from carrier species such as OH, [OI] and OI which yielded discrepant abundances with 1D MLT atmospheres. The lower oxygen abundance they derived for the Sun has significant ramifications especially for fitting the solar oscillations. Collett, Asplund & Trampedach (2007a,b) have used 3D modelling to explore the analysis of red giant spectra. Akerman et al. (2004) and Fabbian et al. (2006) calculated the non-LTE corrections to the OI and CI abundances derived from 1D LTE analysis in the sun and in cool metal-poor stars.

3D modelling has been successful in reproducing the solar granulation pattern of convective cells evident in images of the solar photosphere. The granulation is due to upflowing (hotter) and downflowing (cooler) material which results in temperature inhomogeneities in the surface layers. These temperature inhomogeneities as well as the velocity fields result in line profiles varying with time and position through the stellar layers in ways unaccounted for in 1D models.

6.1. Differences predicted between 3D and 1D analyses

Asplund (2005) and Collett, Asplund & Trampedach (2007b) have undertaken 3D and non-LTE analyses of several typical dwarf and giant stars of normal and low metal-abundance and as a result have made predictions of the corrections necessary to make to the results of 1D abundance analyses.

The mean temperatures in the upper layers of the 3D (and supposedly more realistic) models are predicted to be cooler than in 1D models, especially in very metal-poor stars. This will result in the molecular lines of CH, NH, OH being stronger in 3D than 1D because more molecules will form at the cooler temperatures. Too high atomic abundances will be therefore be derived from molecular lines using 1D temperature structures. The cooler upper layers will also lead to apparent over-ionization in

1D analysis compared to 3D and different behaviour of lines of different excitation potential. Low excitation forbidden lines are relatively unaffected but high excitation and resonance lines will need correction.

Collett, Asplund & Trampedach (2007b) have examined the corrections to the O and C abundances from OH and CH lines in red giants of a wide range of metallicity. Figure 1 shows some of these large differences predicted to be more than -1 dex for OH lines for metallicities below -3 dex. Large effects of apparent overionization of Fe are also predicted in very metal-poor stars. The FeII lines yield similar Fe abundances from 3D or 1D analysis but for FeI the predicted differences shown in Fig.2 are up to -1 dex for stars with metallicities below -3 dex solar.

Non-LTE predicts small effects for atomic lines in the sun, but larger effects for stars with higher T_{eff} , lower $\log g$ and lower [Fe/H]. Non-LTE fluxes are likely to be brighter in the UV and the blue.

6.2. Caveats concerning inhomogeneity corrections from 3D modelling

There are some indications that the current results of 3D modelling are not the final word. Ayres et al (2006) using thermal profiling of the solar atmosphere with 2.3-4.6 μ CO lines finds an oxygen abundance of 700 ppm rather than the 460 ppm derived by Asplund et al (2004). (Assuming C/O=0.50). They claim that the Asplund 3D model is too cool in the middle photosphere and too warm at high altitudes, that is, the temperature gradient is too steep in the visible continuum forming layers. They also note that the CO-rich zone occurs where the thermal fluctuations are mild ~40K.

Asplund has also commented that the 3D model of the Sun does not fit the solar limb-darkening perfectly and his group is continuing to explore this problem observationally and theoretically.

There is evidence that the abundance corrections predicted for the OH lines and the FeI lines at very low metallicity are overestimated. Bessell & Christlieb (2008 private communication) have carried out 1D analy-

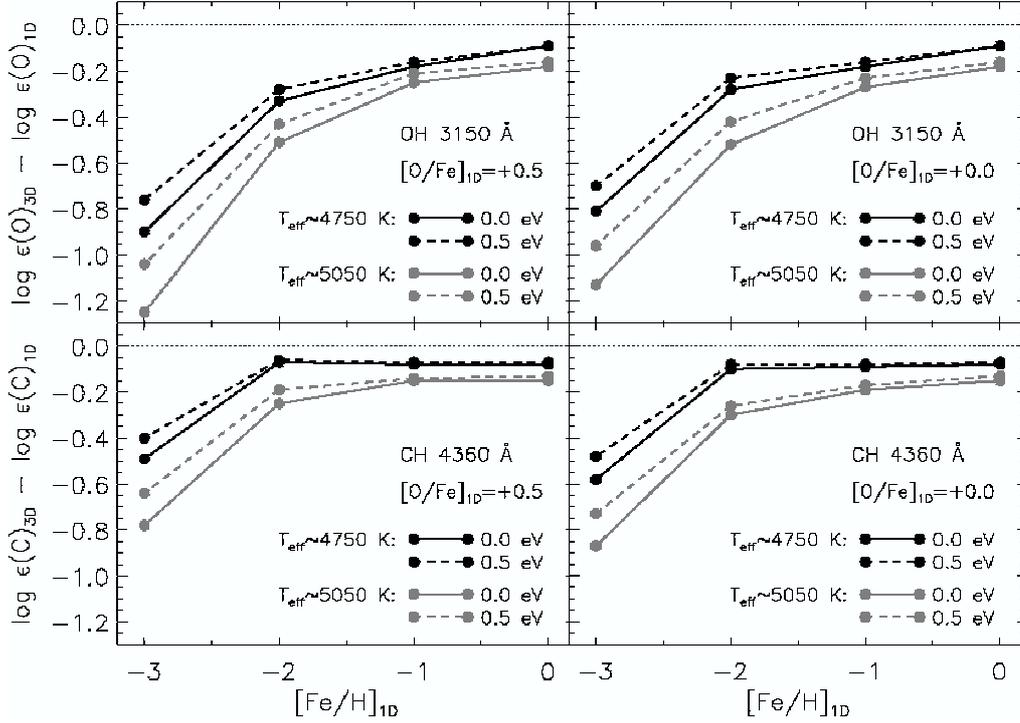


Fig. 1. Predicted differences in O and C abundances between 3D and 1D analysis of OH and CH lines.

ses for two extremely deficient stars deriving O abundance from OH lines and Fe abundances from both FeI and FeII. One star, CD -38°245 with $T_{\text{eff}}=4850\text{K}$ and $\log g=2.0$, has $[\text{Fe}/\text{H}]=-4.0$ and from many OH lines, an abundance of $[\text{O}/\text{H}]=0.9$ was derived. Stars with similar temperature and gravity but metallicity of $[\text{Fe}/\text{H}]\sim-2$ have $[\text{O}/\text{Fe}]=0.5$ implying at most a correction of -0.4 dex rather than the -1.2 dex predicted at only -3 dex. In CD -38°245, $[\text{FeII}/\text{FeI}]=0.2$ using the theoretical isochrone value for $\log g$, again much smaller than predicted by 3D modelling. Even more remarkable is the fact that we measured $[\text{FeII}/\text{FeI}]=0.2$ in HE0107-5240 which has $[\text{Fe}/\text{H}]=-5.4$.

It seems that there is much less cooling of the upper layers than predicted by the current 3D models for very metal-poor giants.

7. Conclusions

1D LTE model atmospheres with convection handled by mixing-length-theory provide optical spectra and optical fluxes in good agreement with empirical temperature scales except for very low metal abundance stars. 3D hydrodynamic and non-LTE model atmospheres better fit the Sun than do 1D models and make predictions of much larger corrections for low metallicity stars. However, improvements need to be made in both 1D LTE modelling and 3D non-LTE modelling to better fit observations.

Better agreement between observations and 1D model atmospheres will come about through the inclusion of additional molecules in ATLAS models, and by improvement in the molecular line lists and treatment of the molecular line opacity by all model makers. Further fine tuning of atomic line lists, especially in the UV, is also required to produce better synthetic spectra. Better synthetic spectra will also re-

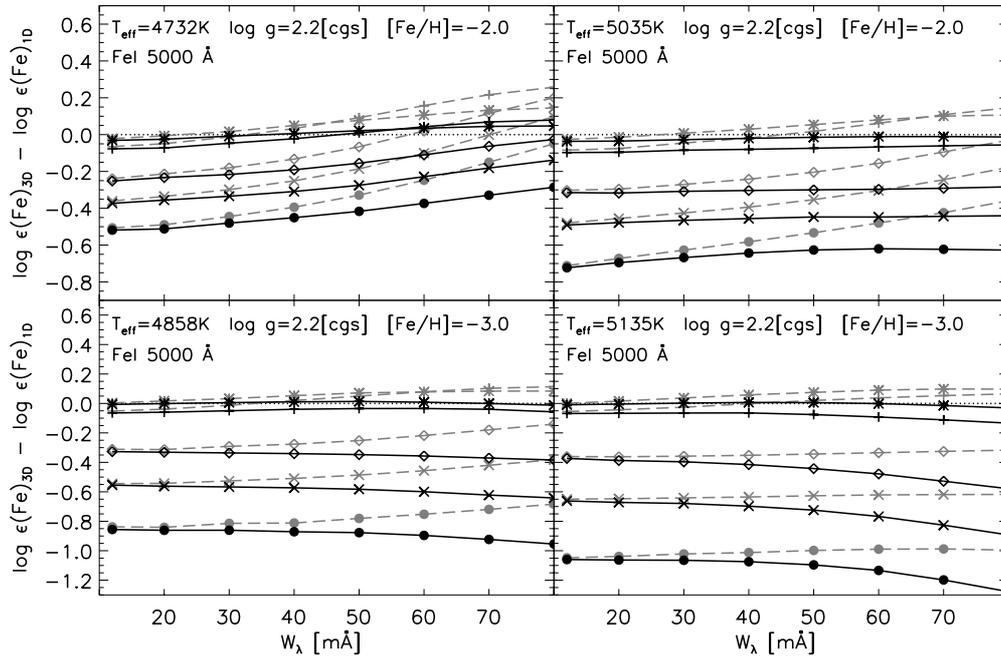


Fig. 2. Predicted differences in Fe abundance between 3D and 1D analysis of FeI lines.

sult from computation of full spectrum synthesis rather than opacity sampling. A definitive comparison of STIS spectra and MARCS and Munari et al synthetic spectra still needs to be done.

Significant improvements in modelling can be expected from better treatment of radiative transfer in 3D hydrodynamical model atmospheres, from an examination of the non-LTE 3D interplay for some elements and from better estimates for collisional cross-sections that are so important in non-LTE computations. Detailed comparison of line profiles in low metallicity stars and 3D models needs to be made and Infrared Flux Method effective temperatures need to be determined for many more metal-deficient stars.

Asplund's coworkers, Fabbian, Trampedach, Hayek, Pereira and Scott are tackling many of the outstanding theoretical and computational problems as well as obtaining better solar spectra at various solar-disk positions. A basic understanding of the nature of L and T dwarf spectra exists

but details of the condensation, growth and behaviour of dust in their atmospheres are vague and the effective temperature scale of T dwarfs is as a result very uncertain.

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