

3D hydrodynamical CO⁵BOLD model atmospheres of late-type giants: chemical abundances from molecular lines

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We investigate the influence of convection on the formation of molecular spectral lines in the atmospheres of late-type giants. For this purpose we use the 3D hydrodynamical CO⁵BOLD and classical 1D LHD stellar atmosphere codes and synthesize a number of fictitious lines belonging to a number of astrophysically relevant molecules, C₂, CH, CN, NH, OH. We find that differences between the abundances obtained from molecular lines using the 3D and 1D model atmospheres are generally small at [M/H]=0.0, but they quickly increase at sub-solar metallicities and may reach ~ -0.9 dex at [M/H]=-3.0. The 3D-1D abundance corrections show a significant dependence on the spectral line parameters, such as wavelength and excitation potential. Our comparison, therefore, points to a complex interplay between the spectral line formation and convection that should be properly addressed in stellar abundance analysis.

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1. Introduction

Late-type giant stars are important tracers of intermediate and old (>1 Gyr) stellar populations. They are luminous and can be detected in distant stellar systems of the Milky Way and Local Group galaxies and may thus provide important clues about the origins of different chemical species in the Universe. The latter can be achieved using accurate chemical abundances determined with realistic stellar model atmospheres and spectral synthesis calculations. However, suitability of the currently used 1D model atmospheres for achieving this goal has been seriously questioned with the advent of the new generation 3D hydrodynamical model atmospheres. Doubts are raised by the fact that convection influences strongly the average temperature stratification and produces horizontal temperature and density fluctuations that are absent in the 1D models, which may thus influence the physical conditions in the line forming regions (e.g., [3]).

2. Aim and tools

In this work we investigate the influence of convection on the formation properties of molecular lines in the atmospheres of late-type giants. We used 3D and 1D stellar model atmospheres to perform the analysis of artificial spectral lines corresponding to a number of astrophysically important molecules. The goal of this study was to derive quantitative constraints on the abundance estimates obtained from molecular lines using the 3D and 1D stellar model atmospheres. We will further call the difference between the abundances obtained using the two kinds of atmosphere models a 3D–1D abundance correction (e.g., [4], [2]).

Our analysis was based on the 3D and 1D model atmospheres calculated using the CO⁵BOLD and LHD stellar atmosphere codes, respectively. Both stellar atmosphere codes share the same micro-physics (opacities, equation of state) and atmospheric parameters (Table 1). Using the 3D and 1D model atmospheres we synthesized a set of fictitious spectral lines corresponding to several molecules: C₂, CH, CN, NH, OH. Spectral line synthesis was performed with the Linfor3D code under the assumption of LTE (for the description of all three codes see, e.g., [1], [5]). The wavelengths and excitation potentials of the fictitious spectral lines were 4000, 8500, 16000 Å and 0, 2 eV, respectively. The bluest wavelength was chosen as representative of molecular lines observed in this spectral region (e.g., CH G band at ~ 4300 Å). The 8500 Å and 16000 Å wavelengths coincide with the maximum and minimum of the H⁻ ion bound-free opacity, respectively.

The 3D–1D abundance corrections obtained for a given spectral line with the 3D and 1D model atmospheres were derived using the curves of growth. Only weak spectral lines ($\sim <5$ mÅ) were used in the analysis in order to eliminate the influence of the microturbulent velocity in the 1D models.

3. Results and discussion

3.1 3D–1D abundance corrections

The 3D–1D abundance corrections derived at four different metallicities from various molecular lines with different wavelength, λ , excitation potential of the lower level χ are shown in Fig. 1. The influence of convection is generally largest at lowest metallicity ($[M/H] = -3.0$). At a given

Model	Size(x,y,z) [Mm ³]	Grid points (n_x, n_y, n_z)	T_{eff} [K]	$\log g$ [cgs]	[M/H]
d3t50g25mm00	573 x 573 x 243	160 x 160 x 200	4970	2.5	0.0
d3t50g25mm10	573 x 573 x 245	160 x 160 x 200	4990	2.5	-1.0
d3t50g25mm20	584 x 584 x 245	160 x 160 x 200	5020	2.5	-2.0
d3t50g25mm30	573 x 573 x 245	160 x 160 x 200	5020	2.5	-3.0

Table 1: Parameters of the 3D CO⁵BOLD models of late-type giants used in the present study.

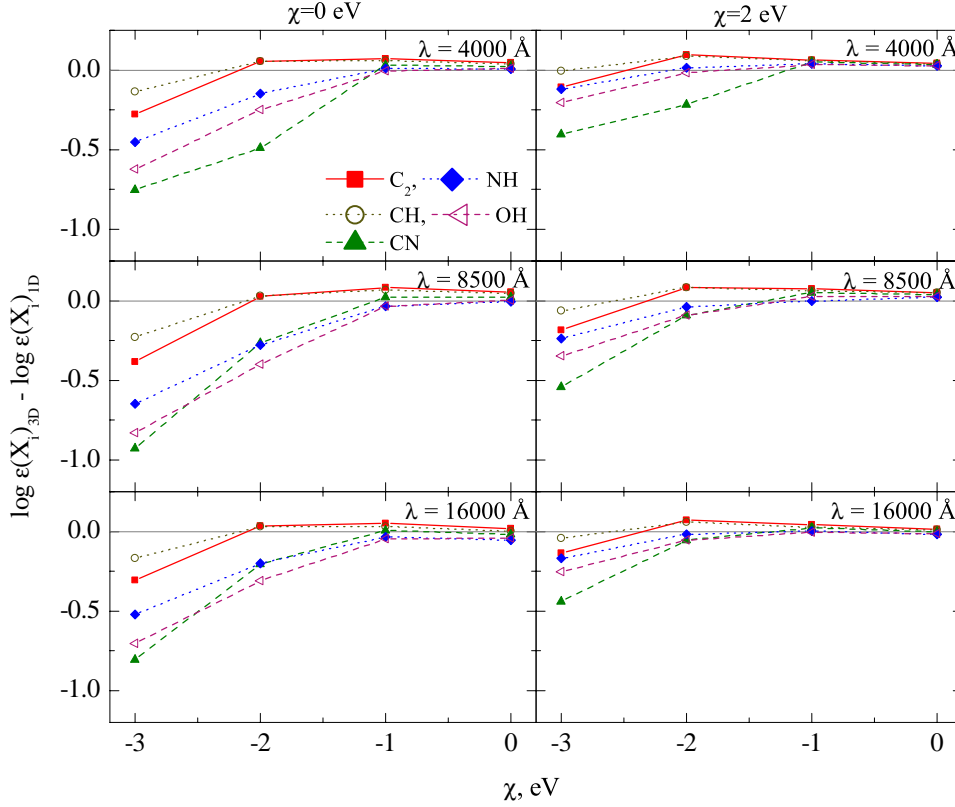


Figure 1: The 3D–1D abundance corrections for different molecular species derived using fictitious lines with excitation potentials $\chi = 0, 2$ eV, plotted versus metallicity at three different wavelengths, 4000, 8500, 16000 Å.

metallicity, the size of 3D–1D abundance corrections decreases with increasing excitation potential of a given spectral line, χ (Fig. 1). The 3D–1D abundance corrections at low metallicities differ significantly in their magnitude which ranges from ~ -0.1 dex in case of CH to ~ -0.9 dex in case of CN.

3.2 Thermal structures in the 3D models

The comparison of the temperature profiles of the 3D model with the corresponding temperature stratifications of the 1D LHD model and the temporarily and spatially averaged 3D hydrodynamical (hereafter, $\langle 3D \rangle$) model is shown in Fig. 2. At solar metallicity the 1D LHD model

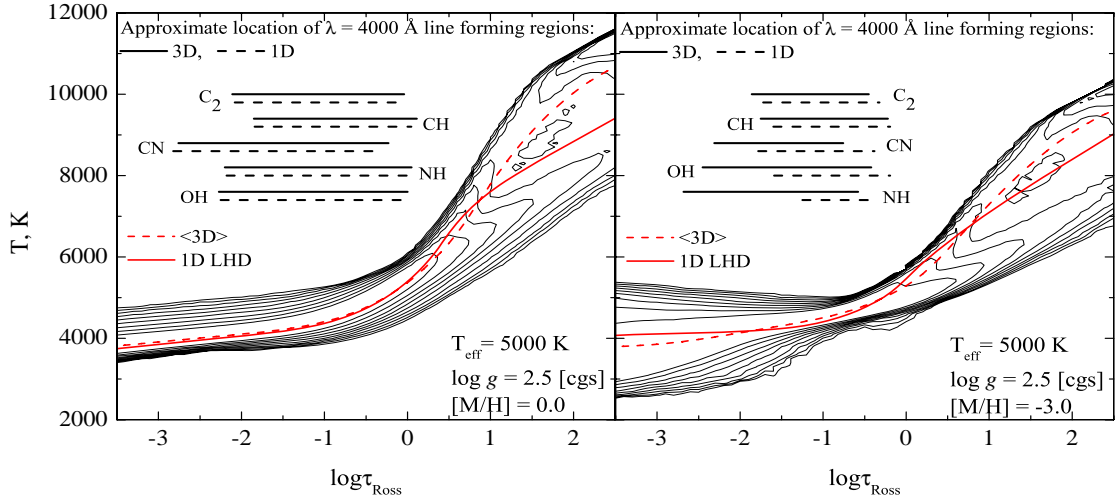


Figure 2: Temperature profiles of the 3D hydrodynamical and classical 1D models of the late type giant plotted versus Rosseland optical depth at two different metallicities, $[M/H] = 0.0$ (left) and $[M/H] = -3.0$ (right). The contour plot shows the density of the individual temperature profiles of the 3D model. The dashed line represents the temperature profile of the temporally and spatially averaged $\langle 3D \rangle$ model, while the solid line represents the corresponding 1D model. Horizontal black lines in the upper part of the plots show the approximate location where various molecular lines form in the 3D and 1D models (solid and dashed lines, respectively).

closely traces the most probable temperature profile of the 3D model. However, at $[M/H] = -3.0$ and beyond $\log \tau_{\text{Ross}} \sim -3.5$ the 3D model is cooler than the corresponding 1D model (Fig. 2).

The formation of different molecular lines occurs at different optical depths, both at solar and sub-solar metallicities (Fig. 2). However, since the differences between the temperature stratifications of the averaged 3D and 1D models are small at $[M/H]=0.0$ the corresponding 3D–1D abundance corrections are minor. The situation changes at lower metallicities where even small differences in the location of molecular line formation are associated with significant changes in the local temperatures, due to rapidly increasing differences between the temperature profiles of the averaged 3D and 1D models in the outer atmosphere. This may explain why, for example, the 3D–1D abundance corrections are smallest in the case of C_2 and CH , which form deepest in the 3D atmosphere and are least affected by differences in the temperature profiles.

3.3 Comparison with the work of other authors

The only similar study where the effects of convection on spectral line formation in late-type giant stars were analyzed was done by [5]. The results obtained in the two studies agree in a sense that largest 3D–1D abundance corrections are seen in case of the most metal-poor atmosphere models (Fig. 3). However, the magnitude of the abundance corrections obtained in our study is significantly smaller. The origin of these differences is not fully clear yet. In part, it might be related to the fact that the $\langle 3D \rangle$ –1D temperature differences are larger in [5], particularly at lowest metallicities, but one should keep in mind that gravities in the two sets of models are also slightly different.

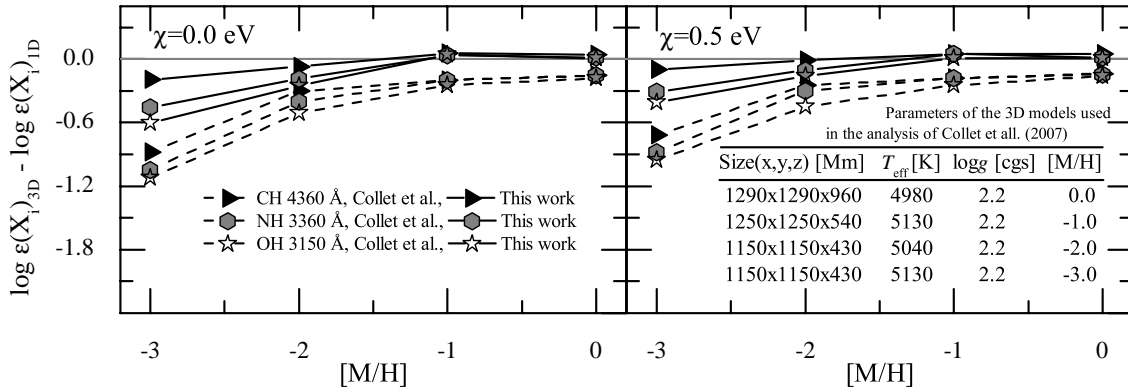


Figure 3: The 3D–1D abundance corrections for CH 4360 Å, NH 3360 Å, OH 3150 Å lines. Dashed lines are results of [3], solid lines represent calculations obtained in this study. Table inside the figure gives the parameters of the 3D models used by [3].

4. Conclusions

Convection alters significantly the thermodynamical structure of late-type giant atmospheres, especially in the outer layers, and its influence grows larger with decreasing metallicity. At lowest metallicities, the temperature in the outer layers of the averaged 3D model is significantly lower than in the corresponding 1D model atmosphere. This leads to significant differences between the molecular abundances derived using the 3D and 1D model atmospheres: for example, in case of CN they may be as large as -0.9 dex at $[M/H] = -3.0$. The 3D–1D corrections predicted for the individual molecules are also markedly different, with the largest spread at lowest metallicities. The strong dependence of the 3D–1D abundance corrections on oscillator strength, wavelength, and excitation potential of particular spectral line clearly exposes the limitations of the 1D models in stellar abundance work, especially when studying metal-poor stellar populations.

References

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