

UV line profiles as a probe for atomic diffusion theory in stellar atmospheres

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Abstract In quiet stellar atmospheres that are stabilized, for example, by the presence of strong magnetic fields, a non-uniform distribution of chemical elements (abundance stratification) is predicted by the diffusion theory. Spectroscopic observations of magnetic Ap stars provide a strong support for the diffusion theory. Stratification predictions in the upper atmosphere, in particular, strongly depend on the magnetic field geometry. Optical lines used in stratification analysis of Ap stars do not probe the upper atmospheric layers and, hence, cannot provide reliable information on abundance gradients there. We show the expected effect of stratification on the profiles of strong lines in the UV region and how these lines may be used for constraining diffusion theory.

Keywords Chemically peculiar stars · Stellar atmosphere models · Diffusion · Element stratification · UV lines

1 Introduction

In stellar atmospheres with rather strong magnetic fields where convection and turbulence are believed to be suppressed (magnetic Ap stars, white dwarfs), diffusion of the elements due to different physical processes takes place. Radiative diffusion, proposed by Michaud (1970), is the most sophisticated theory of element separation. In this theory,

the diffusion of the elements is caused by the various forces acting on atoms such as the radiative force, gravity, electrical forces, etc. Recently, model atmospheres that take into account the stratification of the elements due to the diffusion process have been constructed (Hui-Bon-Hoa et al. 2000; LeBlanc 2003; LeBlanc and Monin 2003; LeBlanc et al. 2009). These models are based on the PHOENIX (Hauschildt et al. 1999) model atmospheres where the diffusion of 39 chemical elements from He to La was calculated simultaneously and self-consistently with the structure of the model atmosphere. Diffusion calculations predict the existence of strong abundance gradients in stellar atmospheres, that change the atmospheric structure and the intensity and shape of spectral lines observed in stellar spectra (Borsenberger et al. 1981; Babel 1992; LeBlanc and Monin 2003; LeBlanc et al. 2009). These models were successful in explaining several observational anomalies of blue horizontal-branch stars (Hui-Bon-Hoa et al. 2000; LeBlanc et al. 2010).

Alecian and Stift (2007, 2010) and LeBlanc et al. (2009) analyzed the effect of the horizontal magnetic field on element distribution due to the fact that ions' diffusion velocities are modified when they cross magnetic lines. Alecian and Stift (2007, 2010) also included the Zeeman effect in their calculations, but do not however, calculate the atmospheric structure self-consistently with the predicted elemental stratification.

In this paper, predicted changes in UV line profiles and line intensity caused by element stratification are used to search for observational manifestations of atomic diffusion in stellar atmospheres. Observational evidence for the stratification was discussed in detail by Ryabchikova et al. (2003). Calculations of the theoretical element distributions by Babel (1992) provided the step-like shape of abundance profiles which was employed in most of the subsequent empirical stratification studies.

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2 Empirical stratification analysis

All empirical results presented in our paper are based on the analysis of Ap star γ Equ (HD 201601).

2.1 Observations

High-resolution (resolving power $R = 115\,000$), high signal-to-noise-ratio ($S/N \approx 300\text{--}400$) spectrum of γ Equ was obtained with the UVES instrument (Dekker et al. 2000) at the ESO VLT in the context of program 076.D-0169(A) and was retrieved from the ESO archive (<http://archive.eso.org>). The UVES spectrum has been reduced with the automatic pipeline described in Ballester et al. (2000). It covers the 3050–9450 Å spectral region.

2.2 Model atmospheres

Model atmosphere parameters for γ Equ were calculated by T. Ryabchikova and D. Shulyak in iterative procedure similar to that described in Shulyak et al. (2009) for another Ap star HD 24712. Model calculations for stratified atmospheres use line-by-line opacity code LLmodels (Shulyak et al. 2004). After three iterations we obtain the following atmospheric parameters: $T_{\text{eff}} = 7550$ K, $\log g = 4.0$ for the star under consideration. Details of the modelling will be published in a separate paper.

To study qualitatively the possible effect of magnetic fields, two self-consistent diffusion models with the adopted parameters were calculated as described in LeBlanc et al. (2009). In the first model the magnetic effects are neglected while in the second model a 1 kG uniform horizontal magnetic field is assumed. Diffusion calculations start from a model atmosphere computed with homogeneous solar abundances. The abundances in every atmospheric layer are obtained under the assumption that all the possible forces acting on a given element are in balance and thus the resulting diffusion velocity is zero (i.e. so-called equilibrium abundances). The algorithm employed uses an iterative process where the atmospheric structure is adjusted as the abundances are modified due to diffusion. Therefore, abundance corrections are followed by temperature corrections. In turn, the changes in the physical structure lead to an imbalance of the forces acting on the chemical elements. The diffusion velocities become non-zero, and the abundances must then be corrected again in order to compensate for this imbalance. In order to avoid non-physical situations, maxima and minima for the abundances are imposed. In present models it is ± 3 dex from the initial solar abundances. More information about these models is found in LeBlanc et al. (2009).

For detailed spectrum and magnetic spectrum synthesis calculations we used the SYNTH3 and SYNTHMAG codes

(Kochukhov 2007). Atomic parameters of spectral lines for spectrum synthesis were extracted from atomic line database VALD (Kupka et al. 1999).

2.3 Empirical stratification

The observed evidence for the presence of non-uniform abundance distribution in stellar atmospheres was considered by Ryabchikova et al. (2003). In summary, arguments for the presence of stratification is made when one cannot fit the core and wings of the strong lines, weak and strong lines of the same element/ion with the same abundance, or when high-excitation lines of the ionized Fe-peak elements appear as relatively strong features in the stars with effective temperature less than 8000 K. In normal stars of the same temperatures high-excitation lines ($E_i > 10$ eV) are either very weak or not observed at all. This guides the procedure of line selection for our stratification study: lines in two ionization stages, in large range of excitation energies, in large range of the observed intensities for the same species, i.e. profiles of the chosen lines should be formed through a wide range of optical depths. Figure 1 (left panel) shows the chosen observed line profiles for Ca and their fit with the homogeneous and stratified Ca distribution (Fig. 1—right panel) in γ Equ atmosphere. Stratification calculations were performed using the step-function approximation for the abundance distribution (for details, see, e.g., Ryabchikova et al. 2005). This parameterized model of the vertical stratification is characterized by the upper and lower abundance values, as well as by the position and width of abundance jump. These parameters are constrained by simultaneous fit of the profiles of large number of atomic lines.

Calcium is a good candidate for stratification analysis, because the strongest resonance lines of Ca II $\lambda 3933.67$; strong lines of Ca II at $\lambda\lambda 3159, 3179, 3181$; IR triplet of Ca II at $\lambda\lambda 8498, 8542, 8662$ Å lie in spectral region covered by ground-based spectroscopy. These lines have strong extended wings blended with the lines of other elements. Moreover the wings of Ca II $\lambda 3933.67$ and IR triplet lines are overlapped with the wings of nearby Balmer H₈, He and Paschen P₁₆–P₁₃ hydrogen lines, producing obvious difficulties in establishing continuum. Our fitting procedure minimize standard deviation between the observed and calculated profile points, therefore all uncertainties in atomic parameters of blended lines as well as the uncertainty in continuum will strongly influence the solution. Except for the very cores of Ca II at $\lambda\lambda 3159, 3179, 3181$ Å, strong lines cannot be used directly in our procedure, but they allow us to verify the Ca distribution derived from other optical lines. Figure 2 shows that the Ca lines are better fitted when stratification is included in the atmosphere of γ Equ. Also, with the very small corrections in Ca distribution, shown by the dashed line in Fig. 1 we could fit the observed

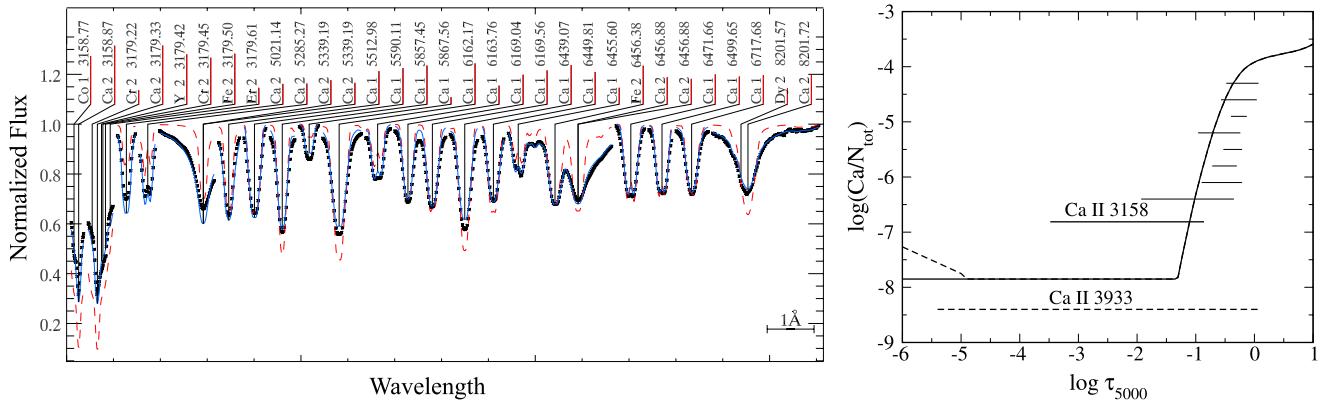
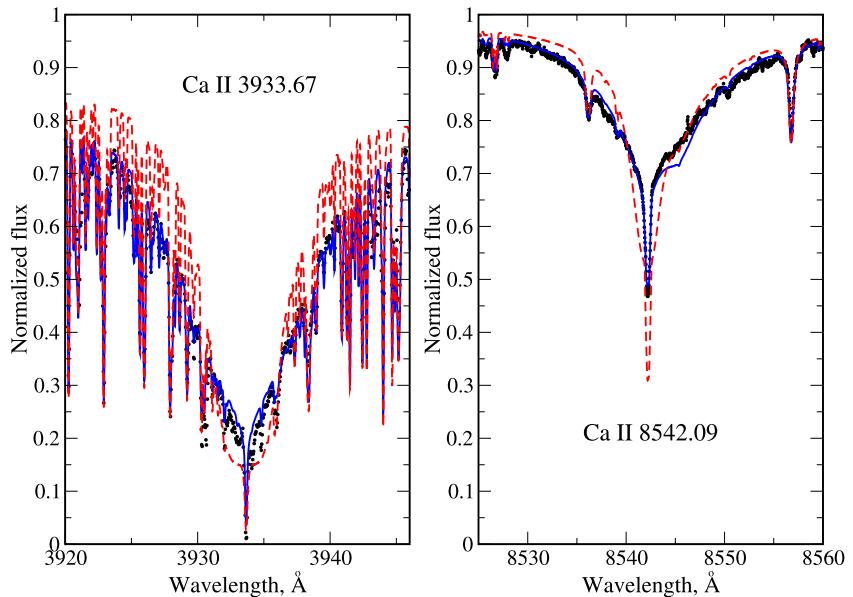


Fig. 1 *Left panel:* comparison between the observed Ca line profiles (black dots) of γ Equ and theoretical spectra calculated with the best-fitting stratified Ca abundance distribution (blue solid line) and with the homogeneous Ca abundance $\log(\text{Ca}/N_{\text{tot}}) = -5.40$ (red dashed line). The plotted spectral windows show segments of the γ Equ spectra used for the determination of Ca stratification; black dots show actual observed points. *Right panel:* empirical vertical Ca distribution

in the atmosphere of γ Equ. Horizontal solid lines show a range of depth formation for a few optical lines including a core of Ca II $\lambda 3158$ line; horizontal dashed line shows a range a depth formation of Ca II $\lambda 3933$ line. The small increase of Ca abundance needed at small optical depths to fit line cores of Ca II $\lambda\lambda 3933, 8542$ lines is represented by the dashed line

Fig. 2 Comparison between the observed line profiles (black dots) of γ Equ and theoretical spectra calculated with the Ca abundance distribution shown in Fig. 1 (blue solid line) and with the homogeneous Ca abundance $\log(\text{Ca}/N_{\text{tot}}) = -5.40$ (red dashed line) for the strong Ca II $\lambda\lambda 3933, 8542$ lines



line profiles of Ca II $\lambda 3933.67$ and $\lambda 8542.09$ reasonably well.

However, other elements, in particular, those of Fe-group, which have millions of spectral lines affecting the atmospheric structure through line blanketing, possess no strong lines similar to Ca II $\lambda\lambda 3933, 8542$ lying in the spectral region of ground-based observations. Regardless, we performed stratification analysis of these important elements as well (see Fig. 3), but more uncertainty exists for the size of abundance gradient. Optical lines provide realistic Fe distribution in the atmosphere from the photospheric layers to $\log \tau_{5000} \approx -2$. High-resolution, high S/N spectra in UV region are needed to obtain more precise Fe abundance distribution in the upper atmospheric layers.

3 Fe II lines in the UV region

Future space mission WSO-UV (Shustov et al. 2009) will be equipped with high-resolution ($R = 50\,000$) UV echelle spectrograph which provides spectral observations in the 1740–3100 Å range. This region contains plenty of Fe II lines. About 100 lines in the range 2249–3100 Å have accurate, experimentally measured atomic parameters. Most of them are strong transitions from the low-lying levels, therefore they may be used for testing the results of stratification analysis based on optical lines as well as for verifying the predictions of the diffusion theory.

An example of expected line profile changes in the atmosphere of γ Equ with different Fe distributions is shown

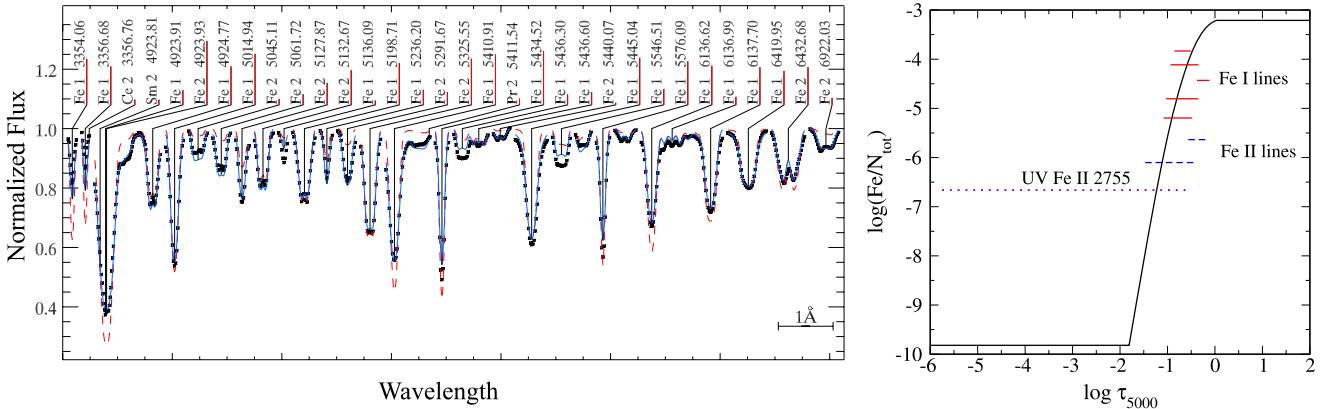


Fig. 3 Left panel: comparison between the observed Fe line profiles (black dots) of γ Equ and theoretical spectra calculated with the best-fitting stratified Fe abundance distribution (blue solid line) and with the homogeneous Fe abundance $\log(\text{Fe}/\text{N}_{\text{tot}}) = -4.50$ (red dashed line). The plotted spectral windows show segments of the γ Equ spectra used

for the determination of Fe stratification; black dots show actual observed points. Right panel: empirical vertical Fe distribution in the atmosphere of γ Equ. Horizontal solid and dashed lines show a range of depth formation for a few optical Fe I and Fe II lines, while horizontal dotted line shows a range of depth formation for UV Fe II line

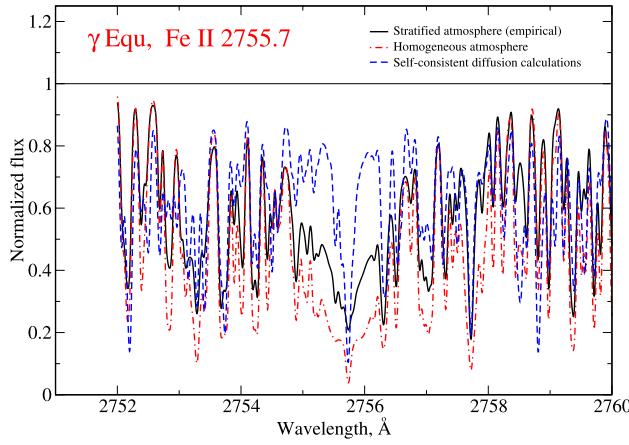


Fig. 4 Computed Fe II λ 2755.7 Å line profiles with different Fe abundance distribution in γ Equ atmosphere: homogeneous (red dashed-dotted line), empirical stratification from optical lines (black line) and diffusion calculations without magnetic field (blue dashed line)

in Fig. 4. Theoretical Fe distribution from self-consistent diffusion model without magnetic field is compared to the empirical one on Fig. 5. One can see very large difference between UV Fe II λ 2755.7 Å line profile synthesized with homogeneous and stratified Fe distributions. The wings of this strong line practically disappear when we employ Fe distribution predicted by the diffusion theory. A comparison of the empirical and theoretical Fe distributions presented in Fig. 5 shows a similarity between the slopes of two curves and therefore gives credence to the presence of diffusion in the atmospheres of Ap stars. Difference found in upper atmospheric abundances above $\log \tau_{5000} \approx -2$ is not important because of the limitations on supported abundances introduced in theoretical diffusion calculations (see Sect. 2.2).

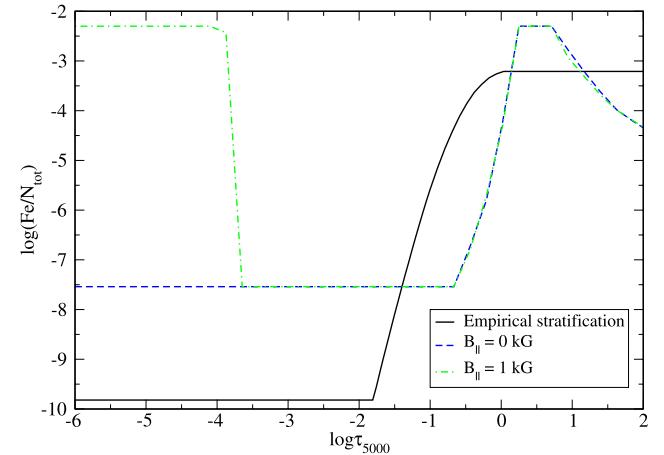
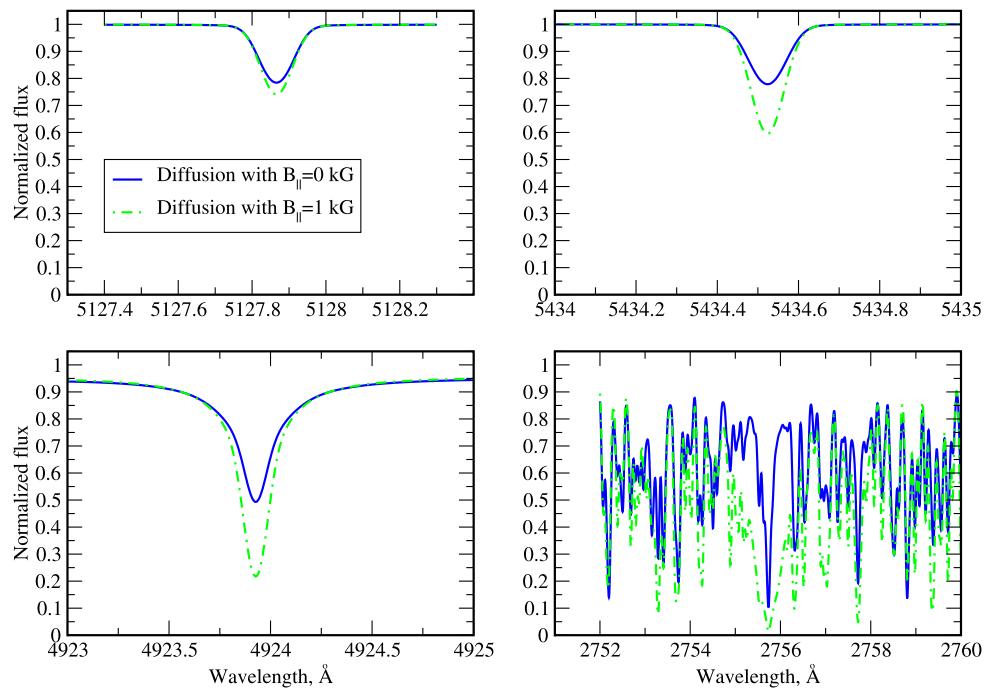


Fig. 5 Vertical Fe distribution in the atmosphere of γ Equ derived empirically (solid black line), and calculated theoretically for zero magnetic field (dashed blue line) and for horizontal magnetic field $B = 1$ kG (dashed-dotted green line)

The most serious disagreement between the empirical and theoretical Fe distributions appears in the position of the abundance jump which differs by $\Delta \log \tau_{5000} \sim 1$ dex. It is this difference that defines the line wing behavior. The reason for deeper position of the abundance jump in theoretical diffusion calculations is not yet understood but might be due to the equilibrium approximation used in the models of LeBlanc et al. (2009). In real situations, diffusion is a time-dependent process that could lead to different solutions than those predicted by equilibrium configurations. The presence of a wind or the amount of a given element that can be brought up to the atmosphere by time-dependent diffusion could modify its stratification profile. For example, the amount of matter that can be brought up in the atmosphere might not be sufficient to attain the equilibrium

Fig. 6 Fe I and Fe II line profiles computed with Fe stratifications from self-consistent diffusion model without magnetic field shown by blue dashed line in Fig. 3 (blue line) and for a model with horizontal magnetic field $B = 1 \text{ kG}$ represented by a green dashed-dotted line in Fig. 3 (green dashed-dotted line)



solution. This difference might also be due to the limitations of the empirical fit in the presence of a magnetic field (see Sect. 3.1). We hope that high-resolution spectral observations of Ap stars in UV region will bring additional constraints for diffusion theory.

3.1 Magnetic field effects

As mentioned in Sect. 1, Alecian and Stift (2007, 2010) and LeBlanc et al. (2009) analyzed the effect of a horizontal magnetic field on element distribution. For better understanding magnetic effects, we computed self-consistent diffusion models with zero and 1 kG uniform horizontal magnetic field. γ Equ is a well-known magnetic star having an average surface magnetic field $\langle B_s \rangle = 4 \text{ kG}$ (Mathys and Lanz 1992), therefore a value of 1 kG for a horizontal component is a reasonable estimate. Profiles of a few Fe lines computed for models without and with magnetic field are displayed in Fig. 6. Corresponding Fe abundance distributions are shown in Fig. 5. According to our diffusion calculations, horizontal magnetic field significantly changes abundance distribution in the upper atmospheric layers above $\log \tau_{5000} \approx -4$, where Fe abundance shows a rapid increase up to maximum allowed concentration. This jump in the abundance influences most of the observed line profiles, but the largest effect is expected for UV lines. An increase of abundances in the upper layers predicted by the theoretical calculations in the presence of magnetic field cannot be resolved by empirical stratification analysis using step-function approximation. Rather it may cause a small shift of the abundance jump in the empirical model towards the upper layers, which is actually observed (see Fig. 5).

4 Conclusions

An analysis of line profiles with high resolution and high S/N ratio in the UV region provides a unique possibility for a detailed study of element distribution in the upper atmospheric layers (above $\log \tau_{5000} = -3$) of Ap stars. Such observations should allow to study the effect of the presence of a magnetic field on abundance stratification predicted by the diffusion calculations. UV observations could therefore impose constraints on future modelling of Ap atmospheres.

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