3D simulations of M star atmosphere velocities and their influence on molecular FeH lines

S. Wende\textsuperscript{1}, A. Reiners\textsuperscript{1}, and H.-G. Ludwig\textsuperscript{2}

\textsuperscript{1} Institut für Astrophysik, Georg-August-Universität Göttingen, Friedrich-Hund Platz 1, D-37077, Germany
e-mail: sewende@astro.physik.uni-goettingen.de
\textsuperscript{2} GEPI, CIfIST, Observatoire de Paris-Meudon, 5 place Jules Janssen, 92195 Meudon Cedex, France
e-mail: Hans.Ludwig@obspm.fr

Received 19 August 2009 / Accepted 13 October 2009

ABSTRACT

\textbf{Context.} The measurement of line broadening in cool stars is in general a difficult task. In order to detect slow rotation or weak magnetic fields, an accuracy of 1 km s\textsuperscript{-1} is needed. In this regime the broadening from convective motion become important. We present an investigation of the velocity fields in early to late M-type star hydrodynamic models, and we simulate their influence on FeH molecular line shapes. The M star model parameters range between $\log g$ of 3.0 - 5.0 and effective temperatures of 2500 K and 4000 K.

\textbf{Aims.} Our aim is to characterize the $T_{\text{eff}}$- and log $g$-dependence of the velocity fields and express them in terms of micro- and macro-turbulent velocities in the one dimensional sense. We present also a direct comparison between 3D hydrodynamical velocity fields and 1D turbulent velocities. The velocity fields strongly affect the line shapes of FeH, and it is our goal to give a rough estimate for the log $g$ and $T_{\text{eff}}$ parameter range in which 3D spectral synthesis is necessary and where 1D synthesis suffices. Eventually we want to distinguish between the velocity-broadening from convective motion and the rotational- or Zeeman-broadening in M-type stars which we are planning to measure. For the latter FeH lines are an important indicator.

\textbf{Methods.} In order to calculate M-star structure models we employ the 3D radiative-hydrodynamics (RHD) code CO\textsuperscript{5}BOLD. The spectral synthesis on these models is performed with the line synthesis code LINFOR3D. We describe the 3D velocity fields in terms of a Gaussian standard deviation and project them onto the line of sight to include geometrical and limb-darkening effects. The micro- and macro-turbulent velocities are determined with the “Curve of Growth” method and convolution with a Gaussian velocity profile, respectively. To characterize the log $g$ and $T_{\text{eff}}$ dependence of FeH lines, the equivalent width, line width, and line depth are regarded.

\textbf{Results.} The velocity fields in M-stars strongly depend on log $g$ and $T_{\text{eff}}$. They become stronger with decreasing log $g$ and increasing $T_{\text{eff}}$. The projected velocities from the 3D models agree within $\sim 100$ m s\textsuperscript{-1} with the 1D micro- and macro-turbulent velocities. The FeH line quantities systematically depend on log $g$ and $T_{\text{eff}}$.

\textbf{Conclusions.} The influence of hydrodynamical velocity fields on line shapes of M-type stars can well be reproduced with 1D broadening methods. FeH lines turn out to provide a mean to measure log $g$ and $T_{\text{eff}}$ in M-type stars. Since different FeH lines behave all in a similar manner, they provide an ideal measure for rotational and magnetic broadening.

\textbf{Key words.} line: profiles - stars: low-mass, brown dwarfs - Hydrodynamics - Turbulence

1. Introduction

Most of our knowledge about stars comes from spectroscopic investigation of atomic or molecular lines. In sun-like and hotter stars, the strength and shape of atomic spectral lines provides information on atmospheric structure, velocity fields, rotation, magnetic fields, etc. Measuring the effects of velocity fields on the shape of spectral lines requires a spectral resolving power between $R \sim 10,000$ ($\Delta \nu = 30$ km s\textsuperscript{-1}) for rapid stellar rotation, $R \geq 30,000$ ($\Delta \nu = 10$ km s\textsuperscript{-1}) for slower rotation and high turbulent velocities, and resolution on the order of $R \sim 100,000$ for the analysis of Zeeman splitting and line shape variations due to slow convective motion.

In slowly rotating sun-like stars, usually a large number of relatively isolated spectral lines are available for the investigation of Doppler broadened spectral lines. These lines are embedded in a clearly visible continuum allowing a detailed analysis of individual lines at high precision. At cooler temperature, first the number of atomic lines is increasing so that more and more lines become blended rendering the investigation of individual lines more difficult. At temperatures around 4000 K, molecular lines, predominantly VO and TiO, start to become important. At optical wavelengths, molecular bands in general consist of many lines that are blended so that the absorption mainly appears as an absorption band; individual molecular lines are difficult to identify. At temperatures in the M type stars regime (4000 K and less), atomic lines start to vanish because atoms are mainly neutral and higher ionization levels are weakly populated. Only alkali lines appear that are strongly affected by pressure broadening. Thus, the detailed spectroscopic investigation of velocity fields in M dwarfs is very difficult at optical wavelengths.

M-type stars emit the bulk of their flux at infrared wavelengths redward of 1 $\mu$m. This implies that observation of high SNR spectra in principle is easier in the infrared. Furthermore, M type stars exhibit a number of molecular absorption bands in the infrared, for example FeH. In these bands, the individual lines are relatively well separated and provide a good tracer of stellar velocity fields. The lines are intrinsically much narrower than atomic lines in sun-like stars because Doppler broadening due to the temperature related motion of the atoms and molecules is much reduced. Thus, the lines can be used for the whole arse-
nal of line profile analysis that has been applied successfully to sun-like stars over the last decades.

Examples of analyses using FeH lines are the investigation of the rotation activity connection in field M-dwarfs, which requires the measurement of rotation line broadening with an accuracy of 1 km s$^{-1}$ (Reiners 2007). Another example is the measurement of magnetic fields comparing Zeeman broadening in magnetically sensitive and insensitive absorption lines (see e.g. Reiners & Basri 2006). A precise analysis of FeH lines, however, is only possible if the underlying velocity fields of the M-dwarfs atmospheres are thoroughly understood. In this paper, we model the surface velocity fields of M type stars and their influence on the narrow spectral lines of FeH.

We calculate 3D-CO$^5$BOLD structure models (Ludwig et al. 2002) which serve as an input for the line formation program LINFOR3D (based on Baschek et al. 1966). Turbulences are included in a natural way using hydrodynamics, so that we are able to investigate the modeled spectral lines for effects from micro- and macro-turbulent velocities in the classical sense and their influence on the line shapes. The comparison with 1D-models gives a rough estimate of the necessity of using 3D-models in the spectral domain of cool stars. In the first part of this paper we investigate the velocity fields in the models and their dependence on log $g$ and $T_{\text{eff}}$. In the second part, we investigate the influence of velocity fields, log $g$, and $T_{\text{eff}}$ on the FeH molecular lines.

2. 3D model atmospheres

The three-dimensional time-dependent model atmospheres (hereafter “3D models”) are calculated with the radiation-hydrodynamics code CO$^5$BOLD (abbreviation for “COnservative COde for the Computation of COnpressible Convection in a BOX of L Dimensions with L=2,3”). It is designed to model solar and stellar surface convection. For solar-like stars like the M-type objects considered here, CO$^5$BOLD employs a local set-up in which the governing equations are solved in a small (relative to the stellar radius) Cartesian domain located at the stellar surface (“box in a star set-up”). The optically thin stellar photosphere and the upper-most part of the underlying convective envelope are embedded in the computational domain. CO$^5$BOLD solves the coupled non-linear equations of compressible hydrodynamics in an external gravitational field in three spatial dimensions (Freytag et al. 2002; Wedemeyer et al. 2004) together with non-local frequency-dependent radiative transfer in these 3D models convection is treated without any assumptions like in 1D mixing-length theory. The velocity fields and its related transport properties are a direct result of the solution of the hydrodynamic equations. Due to this, CO$^5$BOLD is a well-suited tool to investigate the influence of velocity fields on spectral line shapes. A CO$^5$BOLD model consists of a sequence of 3D flow fields (“snapshots”) representing the temporal evolution and spatial structure of the flow. To perform spectral synthesis calculations based on the 3D CO$^5$BOLD-models we use the 3D line formation code Linfor3D. It takes into account the full 3D thermal structure and velocity field in the calculation of the line profiles. It assumes strict Local Thermodynamic Equilibrium (LTE). In this paper we will call the spectral lines computed from three-dimensional atmosphere models “3D-lines”.

In order to analyze the influence of velocity fields in M-stars on FeH lines, we construct a set of CO$^5$BOLD-models with $T_{\text{eff}} = 2500$ K – 4000 K and log $g = 3.0 – 5.0$ [cgs]. Table I gives the model parameters. In the $T_{\text{eff}}$-sequence, we simulated main sequence stars and varied the surface gravity slightly with increasing effective temperature. For the log $g$-sequence, we computed models with different log $g$ values aiming at the same effective temperature of 3300 K but the models settle to slightly higher or lower $T_{\text{eff}}$ values. We decided not to adjust these resulting effective temperatures, because slight differences in $T_{\text{eff}}$ do not change the line profiles significantly. We accepted the $T_{\text{eff}}$ deviations to avoid the large computational effort which would be necessary to adjust the models to a common effective temperature. However, we apply corrections to the line shape related quantities such as equivalent width (see Section 4.3).

The opacities used in the CO$^5$BOLD model calculations originate from the PHOENIX stellar atmosphere package (Hauschildt & Baron 1999) assuming a solar chemical composition according to Asplund et al. (2005). The opacity tables were computed after Ferguson et al. (2005) and Freytag et al. (2009). These opacities are particularly well-suited for our investigation since they are adapted to very cool stellar atmospheres. The raw data consist of opacities sampled at 62,890 wavelength points for a grid of temperatures and gas pressures. For representing the wavelength dependence of the radiative field in the CO$^5$BOLD models the opacities are re-sampled into six wavelength groups using the opacity binning method (Nordlund 1982; Ludwig 1992; Ludwig et al. 1994). In this approach, the frequencies which reach monochromatic optical depth unity within a certain depth range of the model atmosphere, will be grouped into one frequency bin on the basis of their opacities. For each investigated atmospheric parameter combination the sorting of the wavelengths into groups is performed according the run of monochromatic optical depth in a corresponding PHOENIX 1D model atmosphere. The thresholds for the sorting are chosen in logarithmic Rosseland optical depth as $[+\infty, 0.0, -1.0, -2.0, -3.0, -4.5, -\infty]$. In each group a switching is done from a Rosseland average in the optically thick regime to a Planck average in the optically thin regime, except for the group representing the largest opacities, where the Rosseland average is used throughout. In this last bin, which describes the optically thick regions, only the Rosseland average is used because the radiative transfer is local and can be described as a diffusive process (Vo¨ gler et al. 2004).

The horizontal size of the models provide sufficient space to allow the development of a small number (10–20) of convective cells. Their number has to be large enough to avoid box-size dependent effects, but also small enough that there is a sufficient number of grid points available to resolve each individual cell. The size of the convective cells scales roughly inversely proportional to the surface gravity. Accordingly, the horizontal size of the computational box is set to larger sizes towards lower log $g$ values. The horizontal size of the model with $T_{\text{eff}} = 3275$ K is just large enough to fulfill the criteria of the minimal number of 10 convective cells (see Fig. 5), and we saw in test simulations that the results will not change with a larger model (in horizontal size). Therefore we will use this well evolved model as well. The vertical dimension is set to embed the optically thin photosphere, and a number of pressure scale heights of the subphotospheric layers below. We deliberately keep the depth of our models rather small to avoid problems due to numerical instabilities analogous to the ones encountered and discussed in our previous works on the hydrodynamics of M-type stellar atmospheres (Ludwig et al. 2002; 2006).

For the comparison with 1D models, we spatially average the 3D-model over surfaces of equal Rosseland optical depth at selected instants in time. We call the obtained sequence of 1D structures (3D-model). We follow the procedure of Steffen et al. (1995) and average the fourth moment of the temperature and
first moment of the gas pressure to preserve the radiative properties of the 3D-model as far as possible. The 3D velocity information is ignored in the (3D)-model and replaced by a micro- and macro-turbulent velocity. By construction, the (3D)-model has the same thermal profile as the 3D-model, but evidently without the horizontal inhomogeneities related to the convective granulation pattern. We will call the spectral lines synthesized from (3D)-models “(3D)-lines”.

### 2.1. Atmosphere structures

The temperature stratification shown in Fig.1 (top left) of the models with changing $T_{\text{eff}}$ appears very similar for all models in the region below $\log \tau > 1$. They reach their $T_{\text{eff}}$ around $\tau \sim 2/3$ and continue to decrease to higher atmospheric layers. Above $\log \tau \sim 1$ the temperature of the two hottest models increase more strongly than in the cooler cases. Since the models are almost adiabatic in the deeper layers (see below) the temperature gradient follows the adiabatic gradient, which is given by the equation of state and steeper in hotter models due to the inefficient $H_2$ molecule formation. This increase of temperature is also very similar to the lower $\log g$ models on the right side of Fig.1. These models also show a temperature gradient which becomes steeper to deeper atmospheric layers and with decreasing surface gravity again due to a steeper adiabatic gradient. All models reach an almost equal effective temperature at $\tau \sim 2/3$ and their temperature stratification does not differ strongly to smaller optical depth.

The entropy stratification for models with varying $T_{\text{eff}}$ (mid left in Fig.1) show a similar behavior for all models. It is adiabatic ($dS/d\tau = 0$) in layers below $\log \tau \sim 1$ and has a superadiabatic region ($dS/d\tau > 0$) between $\log \tau \sim 1$ and $\sim 1$ that moves slightly to smaller optical depth for hotter models. In these regions, with $dS/d\tau \geq 0$, the models are convectively unstable and become convectively stable in the outer parts of the atmosphere where $dS/d\tau < 0$. In the models with changing $\log g$ (mid right in Fig.1), we can see that the entropy behaves almost like in the $T_{\text{eff}}$ case. To lower surface gravities, the superadiabatic region is more significant. In higher layers, the models become convectively stable except the model with $\log g = 4.0$[cgs] which shows a second decrease of entropy to the outer part layers. To understand this behavior, we have to investigate the adiabatic gradient of this region which is very small and changes very little along the upper atmosphere. This is due to the equation of state used in the models and can be seen in Fig.16 of Ludwig et al. (2006) (model H4 in this figure equates to our $\log g = 4.0$ model). This figure shows that the upper atmosphere lies in a plane of small and constant adiabatic gradient. Due to this, the model becomes convectively unstable again in the upper layers. This is probably the reason for the, in comparison to other models, higher velocities in this model.

In the left bottom panel of Fig.1 the horizontal and vertical rms-velocities are plotted for models with different $T_{\text{eff}}$. Both velocity components increase with increasing $T_{\text{eff}}$. The maxima of the vertical velocity moves to slightly deeper layers with higher temperatures and the maxima of the horizontal velocity stays almost at the same optical depth. We can see a qualitatively similar dependence in the $\log g$ model sequence in the right bottom plot in Fig.1. Only the model with $\log g = 4.0$[cgs] shows peculiar behavior in the upper atmospheric layers, which is probably related to the entropy stratification in this model. We will describe the velocity fields in the models in more detail and with a slightly different method in the next section.

### 3. Velocity fields in the CO$^5$BOLD-models

Before we investigate the effect of velocity fields on spectral lines, we analyze the velocity fields in the models themselves and we will do this with respect to spectral lines. Spectral lines are broadened by velocity fields where the wavelength of absorption or emission of a particle is shifted due to its motion in the gas. Here we are mostly concerned with the macroscopic, hydrodynamic motions but have in mind that the thermal motions are also constituting an important contribution. If we envision each voxel in the RHD model cube to form its own spectral line, the whole line consists of a (weighted) sum of single lines. The velocity distribution might be represented by a histogram of the velocities of the voxels which gives us the velocity dispersion. We try to describe the velocity fields in that sense instead of using the rms-velocities shown in Fig.1. In the CO$^5$BOLD-models, a velocity vector is assigned to each voxel and consists of the velocities in x-, y-, and z-direction. We will investigate the vertical and horizontal component of the velocity dispersion in the models and the total velocity dispersion $\sigma_{\text{tot}} = \sqrt{\sigma_x^2 + \sigma_y^2 + \sigma_z^2}$. In order to describe the height dependent velocity dispersion we applied a binning method, i.e. we plot all velocity components of a certain horizontal plane of equal optical depth $\tau$ in the CO$^5$BOLD cube in a histogram with a bin size of 25 m s$^{-1}$. We fit the histogram velocity distribution with a Gaussian normal distribution function $G = \exp(-(z^2)/2)$ and take the standard deviation $\sigma$ as a measure for the velocity dispersion $\sigma$ in the models (see Fig.2). (The relation between the Gaussian standard deviation $\sigma$ and the standard deviation $\sigma_{\text{rms}}$ of the mean velocity is $\sigma = \sqrt{2 \cdot \sigma_{\text{rms}}^2}$). This is done for the $\sigma_x$, $\sigma_y$, and $\sigma_z$ component of the velocity vector for each horizontal plane from $\tau_{\text{min}}$ to $\tau_{\text{max}}$, which are the highest

### Table 1. Overview of different model quantities for models at constant $T_{\text{eff}}$ and different $\log g$ (upper part) and at constant $\log g$ and different $T_{\text{eff}}$ (lower part).

| Model code         | Size(x,y,z) [km] | Grid points (nx,ny,nz) | $H_e$ [km]$^\dagger$ | z-size [H$_e$] | $T_{\text{eff}}$ [K] | $\log g$ [cgs] |
|--------------------|------------------|------------------------|-----------------------|-----------------|----------------------|----------------|
| d333g30mm00w01     | 85000 x 85000 x 58350 | 180 x 180 x 150       | 282                   | 20.7            | 3240                 | 3.0            |
| d333g55mm00w01     | 28000 x 28000 x 11500 | 180 x 180 x 150       | 826                   | 13.9            | 3270                 | 3.5            |
| d333g40mm00w01     | 7750 x 7750 x 1850  | 150 x 150 x 150       | 250                   | 7.4             | 3315                 | 4.0            |
| d333g50mm00w01     | 300 x 300 x 260    | 180 x 180 x 150       | 18                    | 14.5            | 3275                 | 5.0            |
| d340g45mm00w01     | 4700 x 4700 x 1150  | 140 x 140 x 141       | 109                   | 10.6            | 4000                 | 4.5            |
| d338g49mm00w01     | 1900 x 1900 x 420   | 140 x 140 x 150       | 36                    | 11.7            | 3820                 | 4.9            |
| d335g50mm00w01     | 1070 x 1070 x 290   | 180 x 180 x 150       | 20                    | 14.5            | 3380                 | 5.0            |
| d328g50mm00w01     | 370 x 370 x 270    | 250 x 250 x 140       | 13                    | 20.8            | 2800                 | 5.0            |
| d325g50mm00w01     | 240 x 240 x 170    | 250 x 250 x 120       | 12                    | 14.2            | 2575                 | 5.0            |

$^\dagger$ at $\tau = 1$
Fig. 3. Upper panel: Radial ($\sigma_z$) and horizontal ($\sigma_H$) components of the velocity dispersion are plotted against the optical depth on a logarithmic scale. Bottom panel: Each bottom panel shows the contribution functions (CF) of an FeH-line at a wavelength of 9956.72 Å. Equivalent width $W_\lambda$ (solid) and the depression at the line center (dashed) of the line are plotted as a function of optical depth on a logarithmic scale. The models (from left to right) are located at $T_{\text{eff}}$ of 2800 K, 3380 K, 3820 K and 4000 K and a log $g$ value of 5.0, except the one with $T_{\text{eff}} = 3820$ K (log $g = 4.9$), and the one with $T_{\text{eff}} = 4000$ K (log $g = 4.5$) [cgs].

Fig. 4. Upper panel: Radial ($\sigma_z$) and horizontal ($\sigma_H$) components of the velocity dispersion are plotted against the optical depth on a logarithmic scale. Bottom panel: Each bottom panel shows the contribution functions (CF) of an FeH-line at a wavelength of 9956.72 Å. Equivalent width $W_\lambda$ (solid) and the depression at the line center (dashed) of the line are plotted as a function of optical depth on a logarithmic scale. The models are located at log $g$ values from left to right of 5.0 ($T_{\text{eff}} = 3275$ K), 4.0 ($T_{\text{eff}} = 3315$ K), 3.5 ($T_{\text{eff}} = 3270$ K) and 3.0 ($T_{\text{eff}} = 3240$ K) [cgs].

and the deepest points, in each model atmosphere. In this way we obtained the height dependent velocity dispersion $\sigma_{z,y,z}(\tau)$. We average over five model snapshots for a better statistical significance. In Figs. 3 and 4 the velocity dispersions for the horizontal components $\sigma_H = \sqrt{\sigma_x^2 + \sigma_y^2}$ and vertical component $\sigma_z$ are plotted against optical depth (black solid and dotted lines).

In the latter figures, we identify the maxima around log $\tau = -1$ of the velocity dispersions as the region where the up-flowing motion spreads out in horizontal direction and starts to fall back to deeper layers. We will call this point, the “convective turn-over point”. In a horizontal 2D cross-section of the vertical velocities, somewhat below this area, the up-flowing granulation patterns are clearly visible (see Fig. 5 for models with different log $g$ or Ludwig et al. (2006)). In a vertical 2D cross-section one can see the behavior of the up-streaming material (Fig. 6 shows an example for a model with $T_{\text{eff}} = 2800$ K). The material starts moving upwards almost coherently and before reaching higher layers (around $z = 200$ km in Fig. 6) of the atmosphere the vertical velocity dispersion $\sigma_z$ becomes maximal. After that point, the material spreads out in horizontal directions and starts falling down again. At this point, the dispersion of horizontal velocities $\sigma_H$ becomes maximal (convective turn-over point).

In Fig. 4 we can see at lower surface gravities that the maxima of the horizontal velocity dispersion are not centered around a specified optical depth anymore; it spreads out in vertical direction and span the widest range at log $g = 3.0$ [cgs]. The pressure
Fig. 1. From top to bottom, the temperature, entropy, vertical, and horizontal velocity are plotted as a function of optical depth. The column on the left side shows models with different $T_{\text{eff}}$ and constant $\log g$, on the right side the models are at a constant $T_{\text{eff}}$ with varying $\log g$. The rise of horizontal velocity in the $\log g = 4.0$ [cgs] model in the deeper atmospheric layers is due to interpolation from $z$- to $\tau$-scale.

Fig. 2. Histogram of the velocity distribution in vertical direction. The normalized number of points is plotted against the vertical velocity in m/s (solid line). The Gaussian (dashed line) fits the velocity distribution and determined an FWHM value $FWHM = 2\sqrt{\ln 2} \cdot \sigma$. The underlying model is located at $T_{\text{eff}} = 2800$ K and $\log g = 5$ [cgs].

Fig. 5. Horizontal cross-section around $\tau \sim 1$ of vertical velocity components. The models are located at $\log g$ values of 3.0, 3.5, 4.0, and 5.0 [cgs] (from upper left corner to lower right, respectively).

Fig. 6. 2D cross-section in x-z direction of the x-z velocity in a model with $\log g = 5.0$ [cgs] and $T_{\text{eff}} = 2800$ K. Overplotted are x-z velocity vectors. The direction of the material flow is indicated by the velocity vectors.

stratification changes, and the convective turn-over point moves to lower gas-pressure (not shown here) but stays at almost constant optical depth between $\log \tau = 0$ and $\log \tau = -2$. With varying temperature, the position of the convective turn-over point stays at almost constant optical depth.

3.1. Reduction of the 3D velocity fields

Commonly, micro- and macro-turbulence derived from spectroscopy are interpreted as being associated with actual veloc-
species present in the stellar atmosphere. In our simulations no oscillations are induced externally but small oscillations are generated in the simulations themselves. The velocity amplitudes of these oscillations reach maximal 10% of the convective velocities and have no significant influence on the macro-turbulent velocity. We would also not expect global oscillations for these objects, except for young stars with solar masses smaller than 0.1 $M_\odot$ induced by D-burning (Palla & Baraffe 2003). In the following, we try to make the connection between micro- and macro-turbulence and actual hydrodynamical velocity fields manifest by considering the velocity dispersion determined directly from the hydrodynamical model data, and compare it with the micro- and macro-turbulence derived from synthesized spectral lines (see Sec. 3.2). This connection is algebraically not immediate, and we only apply a simple model for translating the hydrodynamical velocities into turbulent velocities relevant to spectroscopy (see appendix). When interpreting comparisons shown below the very approximate nature of our model should be kept in mind. In this model, we include the geometrical projection of the components of $\sigma_{x,y,z}$ to the line of sight of the observer. We also have to consider the effect of limb-darkening of the stellar disk. For each velocity dispersion component we calculate a projection factor which includes both, geometrical projection and limb-darkening effects (more described in the appendix).

3.1.1. Weighted velocities

To investigate the influence of broadening from the projected and unprojected velocity dispersion on spectral lines, we use contribution functions for the equivalent width $W_j$ and the depression at the line center of an FeH line at 9956.7 Å (Magain 1986). The line gains its $W_j$ and depression in the region between $\log \tau = 1.0$ and $\log \tau = -4.0$, i.e. that is the region of main continuum absorption caused by FeH molecules. The maximum is roughly centered around $\log \tau = -1.0$ and moves to slightly lower optical depth with lower temperatures (at the lowest $T_{\text{eff}}$ of 2575 K, the maximum is centered around $\log \tau = -2.0$) or higher surface gravities. The contribution function of $W_j$ range over the region of the convection zone and reflects its influence on the line shape. Due to the latter fact, FeH lines are a good mean to explore the convective regions in M-dwarfs. In order to measure the velocities in the region where the lines originate, we compute the mean of the (projected) velocities weighted with the contribution function of $W_j$.

$$\sigma_{\text{weighted}} = \frac{\sum_{\tau=2}^{5} \sigma_{\tau} \cdot CF_{\tau}}{\sum_{\tau=2}^{5} CF_{\tau}}$$

The horizontal and vertical components of these weighted velocity dispersions are plotted in Figs. 7 and 8. We can see an increase of $\sigma_{H,z}$ with increasing effective temperature or decreasing surface gravity. We can see again that the projected horizontal velocity dispersions are significantly smaller than the unprojected ones due to the reasons mentioned above. The difference in the vertical component is much smaller. The velocity dispersions for the vertical component range from a few hundred m/s for cool, high gravity models to ~ 1 km/s for hot or low gravity models. The horizontal component range from a ~ 500 m/s for cool, high gravity models to ~ 2 km/s for hot or low gravity models. We compare the total projected velocity dispersion

$$\sigma_{\text{tot}} = \sqrt{\sigma_{H}^2 + \sigma_{z}^2}$$

in Sec. 3.2 with micro- and macro-turbulent velocities in the classical sense.

The strong increase of the velocity dispersions in the atmospheres to higher layers (Figs. 3 and 4), which some models show, is related to convective overshoot into formally stable lay-
ers. These velocities are originated by waves excited by stochas-
tical fluid motions and by advective motions (Ludwig et al.
2002, and references therein). However, it will not affect the
spectral lines, because the lines are generated in the region be-
tween an optical depth of $\log \tau = 1.0$ and $\log \tau = -4.0$. The
lines on the model with $T_{\text{eff}} = 2575 \text{ K}$ are an exception, they are
formed in the outermost layers of the model and it is not possible
to compute the full range of formation of these lines, because the
atmosphere is not extended enough. One has to keep this in mind
when regarding the line dependent results of this model later in
this chapter.

3.2. Radial velocity shifts

Due to the fact that in a convective motion the up-flowing area is
larger, because it is hotter and less dense, than the down-flowing
one, one expect a net shift of the velocity distribution to positive
velocities. That means, the net amount of up-flowing area with
hotter temperature, i.e. more flux in comparison to the down-
flowing area, results in a blue shift in the rest wavelength posi-
tion of a spectral line (see e.g. Dravins 1982).

To see how the area of up-flowing material affects the rest
wavelength position of a spectral line, we computed ten FeH
spectral lines (more described in Sect. 4) on 3D models to mea-
ure the displacement of the line positions. In order to deter-
mine the center of the line, we used the weighted mean $C = \frac{\sum F \tau}{\sum \tau}$ which account for the asymmetric line shape. (To use the
weighted mean is appropriate here, since we have no noise in the
computed data.) The line shifts of the flux and the intensity are
given in Tab. 2. A negative value stands for a blue shift,
and a positive for a red shift. The values for each model are the
mean of five temporal snapshots. The absolute displacement of
the flux and intensity in the log $g$ series reflects the dependence
of the velocity fields on surface gravity, but for the $T_{\text{eff}}$ series a
connection is barely visible (see Figs. 7 and 8). This could be
due to the small geometrical size of the atmospheres in the $T_{\text{eff}}$
series (see Tab. 1). Only the the one with $T_{\text{eff}} = 4000 \text{ K}$ shows a
significant line shift and in this model the atmosphere is 1150 km
high due to the slightly smaller log $g$ value of 4.5 [cgs]. At this
point we will not go in deeper analysis of this topic.

Since we only use five snapshots, we are dealing with statist-
tics of small numbers and hence a big scatter in the results. This
scatter $\sigma_{\text{shift}}$ is in general one order lower than the shift of the
line and the integrated jitter of the line, which is important for
radial-velocity measurements, goes with $\sigma_{\text{jitter}} = \frac{\sigma_{\text{shift}}}{\sqrt{N}}$, where $N$
is the number of snapshots. Since in a star N is of the order of
$10^5$, the jitter will be of the order of mm $\text{s}^{-1}$.

We did not further investigate the effect of granulation
patterns on the line profiles but, as we will see below, the lines
are almost Gaussian and show no direct evidence for significant
granulation effects.

3.3. Micro- and macro-turbulent velocities

Due to the large amount of CPU-time required to compute 3D
RHD models and spectral lines on these models, we want study
the necessity of 3D models in the range of M-stars. Our goal is
to compare the broadening effects of the 3D velocity fields
on the shape of spectral lines with the broadening in terms of
the classical micro- and macro-turbulence profiles (see e.g. Gray
1977, 2008). The latter description is commonly used in 1D at-
mosphere models like ATLAS9 (Kurucz 1970) or PHOENIX and
related line formation codes. If the difference between 1D and
3D velocity broadening is small, the usage of fast 1D atmosphere
codes to simulate M-stars for comparisons with observations,
e.g. to determine rotational- or Zeeman-broadening, would be an
advantage.

If the size of a turbulent element is small compared to unit
optical depth, we are in the regime of the micro-turbulence. The
micro-turbulent velocities might differ strongly from one posi-
tion to another and have a statistical nature. The broadening ef-
fect on spectral lines can be described with a Gaussian which en-
ters the line absorption coefficient (Gray 2008). It can be treated
similar to the thermal Doppler broadening. The effect on the
shapes of saturated lines is an enhancement of line wings due
to the fact that at higher velocities the absorption cross section
increases and as a consequence the equivalent width ($W_{\lambda}$) of
the line is increased.

If the size of a turbulent element is large compared to unit opti-
cal depth (maybe better of the same size as unit optical depth),
we are in the regime of the macro-turbulence. It can be treated
similiar to rotational broadening as a global broadening of spec-
tral lines. The effect is an increase of the line width but the equiv-
alent width remains constant.

As we saw before, the velocity fields in the M-stars are not
very strong in comparison to the sound speed (see Tab. 2) and one
could expect that their influence on line shapes do not deviate
strongly from Gaussian broadening.

We compared line broadening with the radial-tangential profile
from Gray (1975) and a simple Gaussian profile and found that the latter is a good approximation with an accu-
rcy high enough for possible determination of rotational-
or Zeeman-broadening. Hence, in this investigation we will assume
Gaussian broadening profiles. That means, we can assume a
height independent isotropic velocity distribution for micro- and
macro-turbulent velocities. This is a very convenient way to sim-
ulate the velocity fields. One would expect that the anisotropic
nature and the height dependence of the hydrodynamical veloc-
ity fields have a significant influence on line shapes, so it is re-
markable that their influence on spectral lines can be described to
a high accuracy in this way. (At least in the investigated M-type
stars.) In Fig. 9 a few examples of (3D)-FeH spectral lines were
plotted, which were computed with a given micro-turbulent velo-
city (determined below) and then convolved with a Gaussian
broadening profile with a given macro-turbulent velocity. The
broadened (3D)-FeH lines fit the 3D-FeH lines very well. The
difference of the 1D and 3D centroid ($C = \frac{\sum \tau F}{\sum \tau}$) range in the
order of m/s for small velocity fields to 30 – 40 m $\text{s}^{-1}$ for strong
velocity fields in hot M star models or with low log $g$. The error
in flux is lower than 1% (see Fig. 9), this corresponds to an un-
certainty in velocity, for example rotational velocity, of less than
150 m $\text{s}^{-1}$ depending on the position in the line. It is also visible
in the latter figures that at low effective temperature effects from
velocity broadening are not visible in comparison with an un-
broadened (3D)-line in which the v.d.Waals broadening is
inaccurate. At higher effective temperatures, the difference be-
tween broadened and unbroadened (3D)-lines is clearly visible. We
found that in the range of M-type stars, 1D spectral synthesis
of FeH-lines using micro- and macro-turbulent velocities in the
classical description is absolutely sufficient to include the effects
of the velocity fields. In the following we will determine the ve-
locities needed.
Table 2. Displacement \( \Delta v_{\text{Flux}} \) and \( \Delta v_{\text{Intensity}} \) in m/s of the position of an FeH line from the rest wavelength on models with different \( T_{\text{eff}} \) (left side) and different log g (right side).

| \( T_{\text{eff}} \) (K) | \( \Delta v_{\text{Flux}} \) (m/s) | \( \Delta v_{\text{Intensity}} \) (m/s) | \( v_{\text{rad}} \) (m/s) | log g | \( \Delta v_{\text{Flux}} \) (m/s) | \( \Delta v_{\text{Intensity}} \) (m/s) | \( v_{\text{rad}} \) (m/s) |
|-----------------|-----------------|-----------------|-----------------|-----|-----------------|-----------------|-----------------|
| 2800            | 0               | 2               | 3750            | 3.0 | −56             | −25             | 6100            |
| 3275            | −1              | 3               | 4000            | 3.5 | −47             | −36             | 5500            |
| 3380            | −2              | 2               | 4850            | 4.0 | −16             | −7              | 5400            |
| 3820            | −1              | −5              | 6000            | 5.0 | −1              | 3               | 4500            |
| 4000            | −44             | −28             | 7000            |      |                 |                 |                 |

3.3.1. Determination of micro- and macro-turbulent velocities

The investigation of the micro-turbulent velocities was done with the curve of growth (CoG) method (e.g., Gray 2008). We artificially increase the line strength of an absorption-line (increase the log \( gf \) value) which in turn increase the saturation of the line and its influence of the micro-turbulent velocity, which results in an enhancement of \( W_{\lambda} \). In order to determine micro-turbulent-velocities, we use Fe I- and FeH-lines produced on (3D)-models with different micro-turbulent velocities (there are no differences in micro-turbulent velocities between both types of lines), i.e. for each log \( gf \)-value we compute a (3D)-line with micro-turbulent velocities between 0 km s\(^{-1}\) and 1 km s\(^{-1}\) in 0.125 km s\(^{-1}\) steps. In this way we obtained CoGs for 9 different micro-turbulent velocities. We compare the equivalent widths in the CoGs with the ones which was computed on the 3D-models and selected the velocity of the CoG which fits the 3D CoG best in the sense of \( \chi^2 \)-residuals. The macro-turbulent velocities are determined by computing a (3D)-model FeH line \((\lambda = 9956.7 \text{ Å})\) including the micro-turbulent velocities. This line is then broadened with a Gaussian profile and different velocities until it matches the 3D-model line.

The dependence of the micro- (\( \xi \)) and macro- (\( \zeta \)) turbulent velocities on surface gravity and effective temperature is plotted in Figs. 10 and 11. The macro-turbulent velocities in both cases show a quadratic dependence, and we can fit them with a second order polynomial. The micro-turbulent velocities could be fitted
by a linear function or a second order polynomial. We decided to use the second order polynomial, too.

Micro- and macro-turbulence velocities both show a similar dependence on surface gravity and effective temperature, which implies that there is a direct connection between both. A comparison of the macro (ζ)- and micro (ξ)-turbulent velocities with the sum of both (√ζ^2 + ξ^2) and the total projected weighted velocity dispersion σ_{proj} (see Sec. 3) is also shown in Figs. 10 and 11. The total projected weighted velocity dispersion is very similar to the macro-turbulent velocities and in most cases smaller than the sum of micro- and macro-turbulent velocity. It is remarkably, that it is possible, with this simple description of the total projected weighted velocity, to describe the broadening influence of the hydrodynamical velocity fields on spectral lines in comparison with the classical micro- and macro-turbulent description.

In order to obtain a good estimate of the line profile in 1D spectral line synthesis, knowledge of the micro- and macro-turbulent velocities is very important. Otherwise one could underestimate the equivalent width or the line width and hence obtain a wrong line depth.

We compare our micro- and macro-turbulent velocities to observational results from (see Bean et al. 2006a,b, Bean 2007). Our value of the macro-turbulent velocities are roughly of the same order. The higher macro-turbulent velocities from Bean et al. possibly contain rotational broadening, but the Bean et al. micro-turbulent velocities are roughly a factor two or three higher than ours. These velocities are obtained from observed spectra by the authors of the afore-mentioned papers using spectral fitting procedures. In detail, they used PHOENIX atmosphere models and the stellar analysis code MOOG (Sneden 1973). One has to keep in mind that the empirical determination of micro-turbulence is also endangered to suffer from systematic errors. For most of the lines that Bean and collaborators employ (line data from Barklem et al. 2000), the v.d. Waals damping constant is available. However, in some cases not, then usually Unsöld’s hydrogenic approximation is applied to calculate the value, and different authors use significantly different enhancement factors changing its value. This illustrates the level of uncertainty inherent to this approach. For instance, Schweitzer et al. (1996) use an enhance factor of 5.3 (for the resulting γ_f values) for their Fe I lines, while Bean et al. prefer 2.5 for Ti I lines (Bean 2007). To investigate the detailed influence of v.d. Waals broadening on determination of micro-turbulence velocities is very interesting, but goes beyond the scope of this paper. We want to point out, that it is perceivable that uncertainties in the damping constant can introduce significant systematic biases in the resulting value of spectroscopically micro- and macro-turbulence and they could easily be overestimated.

As mentioned above and illustrated Fig. 10 our prediction of the micro-turbulence grossly underestimates the micro-turbulence values measured by Bean et al.. This might hint at deficits in the hydrodynamical modeling and we cannot exclude the possibility that a process is missing in our 3D models leading to a substantially higher micro-turbulence. But due to the argumentation above and a comparison with the solar micro- and macro-turbulence, we argue that the Bean et al. values for the micro-turbulence are too high. However, before being able to draw definite conclusions the observational basis has to be enlarged.

### 4. T_{eff} \text{ and } \log g\text{-dependence of FeH molecular lines}

In this section we study the dependence of FeH molecular lines on T_{eff} and log g in our 3D- and (3D)-models. Again, the intention is to identify multi-D effects which might hamper the use of the FeH line diagnostics in standard 1D analyses. For this purpose we compute the (3D)-lines with no micro- and macro-turbulence velocity. With this method we can study the FeH lines without any velocity effects and can through direct comparison between 3D- and (3D)-lines clearly identify velocity induced effects.

#### 4.1. FeH line data

Wing & Ford (1969) were the first to detect a broad molecular absorption band around 991 nm in late M dwarfs. This band was later found in S stars (Wing 1972) and in sun spots (Nordh et al. 1977) identified the Wing-Ford band as the 0−0 band of a FeH electronic transition. The FeH molecule is well suited for the measurements mentioned in the introduction because of its intrinsically narrow and well isolated spectral lines. These lines are also an ideal tracer of line broadening in M-stars due to convection or very slow rotation (Reiners 2007). Since FeH lines were not very commonly used for the interpretation of stellar spectra in the past, only little data is recorded in the literature. With the work of Dulick et al. (2003), it is possible to determine the log gf value and the transition energies. For the partition function, a combination of the tabulated function in Dulick et al. (2003) and an analytically determined one from the Eq.1 in Sauval & Tatum (1984) is used.

Due to the high atmospheric pressures, v.d. Waals broadening is often significant in cool M-type dwarfs. No detailed calculations exist for the v.d. Waals broadening of FeH molecular lines. Lacking a more accurate treatment, we follow the approximate approach of Schweitzer et al. (1996) and apply Unsöld’s hydrogenic approximation, albeit – different from Schweitzer and co-workers – we do not apply an enhancement factor to the calculated broadening constant C_b.
The ionization energy of the FeH molecule enters the calculation of $C_6$, which, unfortunately, is not known. Only the dissociation energy is published of 1.59 ± 0.08 eV at 0 K (e.g. Dulick et al. 2003). To derive an estimate of the ionization energy, we heuristically compare the ionization and dissociation energies of a large number of hydrides taking data from Wilkinson (1963). We find an approximately linear relationship between the ionization and the dissociation energies of hydrides. For FeH we obtain an ionization energy of 6 eV for the known dissociation energy from a linear fit. Computation of this value from the ionization-potential of Fe and the dissociation energies of FeH and FeH$^+$ yields 7.3 eV (Bernath 2008, private communication), which is compatible with our value considering our rather crude procedure. The difference in FWHM of synthesized FeH-lines in the range between 6 and 7.3 eV amounts to ≈ 25 m/s. This uncertainty is quite acceptable in comparison to the total broadening of typically several 100 m s$^{-1}$ in this investigation.

### 4.2. An ensemble of 3D- and (3D)-FeH lines

We investigate ten FeH lines between 9950 Å and 9990 Å chosen from Reiners & Basri (2006) (see Tab. 3). We choose lines from different branches (Br), orbital angular momentum $\omega$, and rotational quantum number $J$. The wavelengths in Tab. 3 are given in vacuum and $E_\text{f}$ is the lower transition energy. While not directly relevant in the present context, because we do not study the effects of magnetic fields, we note that five lines are magnetically sensitive and five insensitive. We performed the line synthesis for fixed abundances on the $\text{CO}^0\text{BOLD}$ atmosphere models listed in Tab. 1. The spectral resolution is $R = 2 \times 10^6 \,(= 5 \times 10^{-3}\text{ Å})$ corresponding to a Doppler velocity of $v ≈ 150 \text{ m s}^{-1}$ at the wavelength of the considered lines (~ 9950 Å). Figures 12 and 13 illustrate the strong influence of surface gravity and effective temperature on the line shape for the 3D-models. In Fig. 12 one can see that for both, (3D)- and 3D-lines, the line depth, line width and equivalent width $W_\lambda$ decrease strongly with increasing effective temperature. The decrease of $W_\lambda$ is due to stronger dissociation of the FeH molecules at higher temperatures, i.e the number of FeH molecule absorber decreases. Differences in the line shape between 3D- and (3D)-lines with changing temperature are hardly visible. To higher $T_\text{eff}$ values, the influence of broadening on the 3D lines due to velocity fields is slightly visible and not covered by thermal and v.d.Waals broadening anymore. To cooler temperatures, the velocity fields decrease and the differences between the (3D)- and 3D-line shapes vanishes. The v.d.Waals broadening is larger then the thermal broadening or that from the small velocity fields in the RHD models. In the model with $T_\text{eff} = 2800 \text{ K}$, the lines start to become saturated. The FeH lines in the z-band at effective temperatures below ~ 2600 K become too saturated and too broad for investigations of quantities like magnetic field strength or rotational broadening below 10 km s$^{-1}$

The differences between 3D- and (3D)-line shapes of the log g-series in Fig. 13 is more obvious than in the $T_\text{eff}$ case. The differences in line depth and line width become significant with decreasing log g. The lines in the 3D-models are significantly broadened due to the velocity fields in the RHD models, hence the line width is larger and the line depth lower. As we saw in Chapter 3, these velocity fields increase with decreasing log g and could be described in the 1D case in terms of macro- and micro-turbulent velocities.

The (3D)-lines become slightly shallower and narrower towards smaller log g. The equivalent width of the lines decreases with decreasing log g due to decreasing pressure and hence decreasing concentration of of FeH molecules. Also the v.d.Waals broadening looses its influence to lower pressures and the line width decreases. We point out, that we use in all models the same solar like chemical compositions, hence the concentration of Fe and H stays the same. The creation of FeH also depends on the number of H$_2$-molecules, which become larger towards lower temperatures and will be important in cool models.

The slightly different effective temperatures in the models with different log g (see Tab. 1) affect the line depths as well. If the effective temperatures would be the same in the log g-models, one could expect a monotonic behavior in decreasing line strength for decreasing surface gravity in the (3D)-lines. However, because the model with log g $\approx 3.0$ is cooler, the line depth is deeper than that of the one with log g $\approx 3.5$. In the following analysis we will correct the FWHM, $W_\lambda$, and the line depth of the lines on models with different log g for their slightly different effective temperatures.

The ten FeH lines behave all in the same way as the presented ones. We do not see any effect of different excitation potentials or log $gf$ values in the line shapes that cannot be explained by their different height of formation. Thus, we expect that we can exclude an extraordinary interaction between these quantities and effective temperature or surface gravity. We will quantify this preliminary result in the next section.

### Table 3. Several of the investigated FeH lines (Reiners & Basri 2006).

| $\lambda_{\text{obs}}$ [Å] | log $gf$ | $E_\text{f}$ [eV] | Br. | $J$ | $Q$ | magn. sen. |
|---------------------------|---------|-----------------|-----|-----|----|-----------|
| 9953.08                   | -0.809  | 0.156           | R   | 10.5| 1.5| weak      |
| 9954.00                   | -2.046  | 0.199           | P   | 16.5| 2.5| strong    |
| 9956.72                   | -0.484  | 0.375           | R   | 22.5| 3.5| strong    |
| 9957.32                   | -0.731  | 0.194           | R   | 12.5| 1.5| weak      |
| 9973.80                   | -0.730  | 0.196           | R   | 12.5| 1.5| weak      |
| 9974.46                   | -1.164  | 0.108           | R   | 4.5 | 0.5| weak      |
| 9978.22                   | -1.190  | 0.030           | Q   | 2.5 | 2.5| strong    |
| 9979.14                   | -1.411  | 0.093           | R   | 2.5 | 0.5| strong    |
| 9981.46                   | -1.006  | 0.130           | R   | 6.5 | 0.5| weak      |
| 9982.60                   | -1.322  | 0.035           | Q   | 3.5 | 2.5| strong    |

### 4.3. FeH Line shapes

To quantify the visual results of Fig. 12 and Fig. 13 we measured $W_\lambda$, the FWHM, and the line depth of the ten investigated FeH-lines (see Tab. 3). We compare 3D- and (3D)-lines with each other to study the effects of the velocity fields in the 3D models and to explore the behavior of the FeH without broadening effects from the hydrodynamical motions. A run of these quantities is plotted in Fig. 14 and Fig. 15.

As we mentioned above, we have to correct the line quantities from models with changing log g for their slightly different $T_\text{eff}$. In Figs. 12 and 13 one can see how the investigated quantities depend on $T_\text{eff}$. We determined spline fits $\phi$ for the three quantities of each line. For these fitting functions $\phi$ we took into account all five different effective temperatures. In order to correct the line quantities to a reference temperature of $T_\text{eff}^{\text{Ref}} = 3275 \text{ K}$, we use a correction factor $\gamma = \frac{\text{sh}_{\text{min}}(T_\text{eff}^{\text{Ref}})}{\text{sh}_{\text{max}}(T_\text{eff}^{\text{Ref}})}$ and multiply the quantity for the log g-model with $\gamma$. This gives us...
Fig. 12. FeH lines with constant log g and varying $T_{\text{eff}}$. Plotted are pairs of 3D- and ⟨3D⟩-lines shifted by a constant for better visibility. The models are located at $T_{\text{eff}}$ values of 2800 K, 3275 K, 3380 K, 3820 K and 4000 K and a log g value of 5.0, except the one with $T_{\text{eff}} = 3820$ K (log g = 4.9), and the one with $T_{\text{eff}} = 4000$ K (log g = 4.5) [cgs].

Fig. 13. FeH lines with constant $T_{\text{eff}}$ and varying log g. Plotted are pairs of 3D- and ⟨3D⟩-lines shifted by a constant for better visibility. The models are located at a $T_{\text{eff}}$ around 3300 K and different log g values of 3.0 ($T_{\text{eff}} = 3240$ K), 3.5 ($T_{\text{eff}} = 3270$ K), 4.0 ($T_{\text{eff}} = 3315$ K) and 5.0 ($T_{\text{eff}} = 3275$ K) [cgs]. The large differences between 3D- and ⟨3D⟩-lines stem from the hydrodynamical velocity fields in the 3D models.

4.3.1. Equivalent Width $W_{\lambda}$

In the $T_{\text{eff}}$-series, $W_{\lambda}$ (see Fig. 14 upper panel) decreases with increasing $T_{\text{eff}}$. At higher $T_{\text{eff}}$ the number of FeH molecules decrease due to dissociation and hence $W_{\lambda}$. This can be seen in the 3D lines as well as in the ⟨3D⟩-lines. At $T_{\text{eff}} = 2800$ K, the influence of v.d.Waals broadening in the 3D- and ⟨3D⟩-lines becomes clearly visible in the line profile due to saturation of the FeH lines. The ten different FeH lines all behave in a similar manner. The only difference is the absolute value of $W_{\lambda}$, which depends on the log g f-value and excitation potential $E_l$ of each line.

Fig. 14. Run of $W_{\lambda}$ (top), FWHM (middle) and the line depth (bottom) of ten FeH-lines (see Tab. 3) on models with different $T_{\text{eff}}$. Squares are the data points for the ⟨3D⟩-models and diamonds for the 3D-models. $W_{\lambda}$ and FWHM are on a logarithmic ordinate for better visibility. We connect the data points of each line with fitting functions (see text) to guide the eye. Plotted are the quantities of the 3D-models (black solid lines) and the ⟨3D⟩-models (gray dotted lines). The models are located at $T_{\text{eff}}$ values of 2800 K, 3275 K, 3380 K, 3820 K and 4000 K and a log g value of 5.0, except the one with $T_{\text{eff}} = 3820$ K (log g = 4.9), and the one with $T_{\text{eff}} = 4000$ K (log g = 4.5) [cgs].

In the log g-series, the $W_{\lambda}$ (see Fig. 15 upper panel) increases with increasing log g. The change in concentration of FeH with lower log g, which results in smaller $W_{\lambda}$, depends on the changing pressure and density stratification. The difference between

Fig. 15. Run of $W_{\lambda}$ (top), FWHM (middle) and line depth (bottom) of ten FeH-lines (see Tab. 3) on models with different log g. Squares are the data points for the (3D)-models and diamonds for the 3D-models. We connect the data points of each line with fitting functions (see text) to guide the eye. Plotted are the quantities of the 3D-models (black solid lines) and the ⟨3D⟩-models (gray dotted lines). All quantities are corrected to a $T_{\text{eff}}$ of 3275 K.
The models are located at a different log$g$ values see Tab. 3. Upper panel: The models are located at a $T_{\text{eff}}$ around 3300K and different log$g$ values of $3.0 \ (T_{\text{eff}} = 3240 \text{K}), \ 3.5 \ (T_{\text{eff}} = 3270 \text{K}), \ 4.0 \ (T_{\text{eff}} = 3315 \text{K})$ and $5.0 \ (T_{\text{eff}} = 3275 \text{K})$ [cgs]. Lower panel: The models are located at $T_{\text{eff}}$ values of 2800 K, 3275 K, 3380 K, 3820 K and 4000 K and a log $g$ value of 5.0, except the one with $T_{\text{eff}} = 3820 \text{K} \ (\log g = 4.9)$, and the one with $T_{\text{eff}} = 4000 \text{K} \ (\log g = 4.5)$ [cgs].

3D- and (3D)-lines at small log$g$-values stems from the broadening by micro-turbulent velocities and vanishes to higher log$g$ values. This time the FeH lines are only mildly saturated, but the velocity fields in the RHD models (see Sec.3) are strong enough to affect the $W_4$ as well. Like in the $T_{\text{eff}}$-series, the ten different lines show no significant variations in their behavior. They only vary in the amount of $W_4$ due to different log$g$-values.

Since the differences in $W_4$ are very small, one can expect that the 3D correction to the FeH abundance is very small too. We derive abundance corrections from comparison between 3D and (3D) curve of growths for each set of lines on the different model atmospheres. The results are plotted in Fig. 15. In this case the correction to the different $T_{\text{eff}}$ of the log$g$ models is not applied. The 3D/(3D) abundance correction is between −0.001 dex for the coolest high log$g$ model and −0.07 dex for the log$g$ = 3.0 model. In all cases the abundance correction is negative which mean that the 3D lines appear stronger due to the enhanced opacity which becomes larger due to the micro-turbulent velocity.

4.3.2. FWHM

The dependence of the line width (measured as the width of the line at their half maximum (FWHM)) on $T_{\text{eff}}$ is shown in the middle panel of Fig. 14. At low $T_{\text{eff}}$, one can see that the FWHM of the 3D- and (3D)-FeH lines decreases with increasing $T_{\text{eff}}$. The v.d.Waals broadening loses influence and also the dissociation of FeH molecules leads to smaller and narrower lines. After $T_{\text{eff}}$ around 3380 K, the FWHM of the 3D lines reaches a flat minimum and starts to become larger again to higher $T_{\text{eff}}$. This rise in the line width is probably related to the rising velocity fields in the RHD models, since thermal broadening takes place in both, 3D- and (3D)-lines and the latter still decrease. The rise of the velocity in the models with a $T_{\text{eff}}$ of 3380 K and 4000 K could also be due to the slightly lower surface gravity in these models, but we think that the main influence stems from the higher temperatures. The (3D)-lines decrease monotonically with increasing $T_{\text{eff}}$ and reflects the behavior of $W_4$. The difference in FWHM between 3D- and (3D)-lines is very small at $T_{\text{eff}} = 2800 \text{K}$ and increases with increasing $T_{\text{eff}}$ to $\sim 0.8 \text{km s}^{-1}$ at the highest $T_{\text{eff}}$. We have seen in Sec.3.2 that this can be explained with the micro- and macro-turbulence description. The offset between the FWHM of the ten lines is due to their different log$g$-values i.e. large log$g$-values results in large FWHM. But since we are interested in broadening from the velocity fields, we have to take into account that lines with small log$g$-values, i.e. weak lines, formed deeper in the atmosphere where the convective motions are stronger. These lines are more broadened from the hydrodynamical velocity fields and hence more widened.

In the log$g$-series, the dependence of FWHM (Fig. 15 middle panel) is very different for 3D- and (3D)-lines. In the 3D case the FWHM stays almost constant with decreasing surface gravity between log$g$ of 5.0 and 4.0 for most lines. This is due to the smaller amount of v.d.Waals broadening, which loses its influence due to lower pressure in models with smaller surface gravity. This is compared from the broadening due to the rising velocity fields. With log$g$ smaller than 4.0, the width starts to increase for all lines. This increase of line width in the 3D case is a consequence of the hydrodynamic velocity fields which increase strongly with decreasing log$g$. In the (3D) case, without the velocity fields, the FWHM decreases with decreasing surface gravity and reflects the behavior of the $W_4$. The difference between 3D- and (3D)-lines reach its maximal value at log$g = 3.0$ [cgs] and is around 1.3 km s$^{-1}$. This is on the order of the velocity fields in the RHD models (see Fig. 8). One could fit 1D spectral synthesis FeH lines to observed ones (with known $T_{\text{eff}}$) with the micro- and macro-turbulence description (see Sec. 3.2) and it will be possible with the obtained velocities to determine a surface gravity with the help of Fig. 11.

We did not see any significant different behavior between the ten FeH lines. Neither in the $T_{\text{eff}}$-series nor in the log$g$-series.

4.3.3. Line Depth

In the bottom panel of Fig. 14 one can see the dependence of the line depth on $T_{\text{eff}}$. The line depth increases with decreasing $T_{\text{eff}}$, and almost all FeH lines, except the one with the lowest log$g$-values are saturated at $T_{\text{eff}} = 2800 \text{K}$. The difference in line depth between 3D- and (3D)-lines is changing in the $T_{\text{eff}}$-interval. At high $T_{\text{eff}}$, the line depth of the (3D)-lines is deeper than that of the 3D lines. At $T_{\text{eff}} = 2800 \text{K}$, this difference almost vanishes. This behavior is due to the saturation of the FeH lines at low $T_{\text{eff}}$ because both, the 3D- and (3D)-lines reach their maximal depth. The decrease of the line depth with increasing $T_{\text{eff}}$ is due to the dissociation of the FeH molecules at higher temperatures.

The line depth of the log$g$-series is shown in the bottom panel of Fig. 15. At low log$g$, the line depths of the 3D and (3D)-lines increase almost linearly with increasing log$g$. The 3D lines increase with a strong slope and the (3D)-lines with a weaker slope. The difference in line depth between 3D- and (3D)-models is maximal at log$g = 3.0$ [cgs] and vanishes almost at log$g = 5.0$ [cgs]. It is consistent with the velocity fields present in the atmospheres of the RHD models broadening the lines and lower the line strength of the 3D lines. The (3D)-lines
reflect the decreasing number of FeH molecules with decreasing log g due to the lower pressures.

5. Summary and Conclusion

We investigated a set of M-star models with $T_{\text{eff}} = 2500\,K - 4000\,K$ and log g = 3.0 – 5.0 [cgs]. For these models, the 3D hydrodynamic radiative transfer code COBOLD was used. The horizontal and vertical velocity fields in the 3D models were described with a binning method. The convective turn-over point is clearly visible in the atmospheric velocity dispersion structure. To investigate the influence of these velocity fields on spectral line shapes, a description for geometrical projection and limb-darkening effects was applied. With the use of contribution functions, we took only these parts in the atmosphere into account where the lines were formed. The resulting velocity dispersions range from 400 – 1600 m s$^{-1}$ with decreasing log g and with increasing $T_{\text{eff}}$ from 200 – 1400 m s$^{-1}$. These values agree well with velocities deduced from line shapes. We expressed the hydrodynamical velocity fields of the 3D models in terms of the classical micro- and macro-turbulent velocities. With this description and the obtained micro- and macro-turbulent velocities, it is possible to reproduce 3D spectral lines on 1D atmosphere models very accurately, hence time consuming 3D treatment of FeH molecular lines in the regime of cool stars is not necessary for line profile analysis. A comparison of our velocities with a set of velocities determined from observations with spectral fitting methods showed that the macro-turbulent velocities agree, but the micro-turbulent velocities are a factor of two or three smaller than the ones determined from observations.

A line shift due to the larger up-flowing area in the convection zone was investigated too. It is on the order of a few m/s up to 50 m s$^{-1}$ for a very low gravity model. The time dependent jitter in line positions is only about m/s and would be reduced to mm s$^{-1}$ in a real star, due to high number of contributing elements.

In order to use FeH molecular lines for investigations of spectroscopic/physical properties in cool stars (e.g. Zeeman- or rotational broadening), we explored the behavior in a set of lines on log g and $T_{\text{eff}}$. We investigated ten FeH lines between 9950Å and 9990Å on our models with the spectral synthesis code LINFOR3D. FeH lines react on different effective temperatures as expected due to the change in chemical composition and pressure. The lines showed also a weak dependence on surface gravity due to changing densities and pressure. The broadening from velocity fields in the 3D models of the log g series is very strong, but for the $T_{\text{eff}}$ series the broadening from velocity fields is almost covered by v.d.Waals broadening. The difference in line width for hot models is up to 0.5 km s$^{-1}$ and for low gravity models around 1 km s$^{-1}$. That means for the 1D spectral synthesis, that one has to include correct micro- and macro-turbulent velocities for small surface gravities or hot $T_{\text{eff}}$. Due to the fact that the FWHM log g dependence of FeH lines goes in the opposite direction as the log g dependence of the velocity fields, the FeH lines become a great mean to measure surface gravities in cool stars. Because the velocity fields scale with log g and it should be easily possible to detect them.

FeH lines with different quantum numbers do not show significant differences for both, log g- and $T_{\text{eff}}$-series. That means the broadening of the lines does not depend on J, $\Omega$, or the branch. Furthermore, lines with weak magnetic sensitivity behave just like lines with strong magnetic sensitivity. All lines are broadened in the same way by thermal and hydrodynamical motions. Only the transition probability expressed in the log gf value influences the behavior of the lines. The line with the lowest gf-values did not saturate at low $T_{\text{eff}}$, but in general they are similar to the other FeH lines.

It is possible to treat the FeH molecular lines with different quantum numbers as homogenous in the absence of magnetic fields. That allows to use FeH lines to measure magnetic fields (Reiners & Basri 2006, 2007). Hence we conclude, that these lines also are an appropriate mean to measure magnetic field strength in M-type stars.

Appendix

![Fig. 17. Projection factors (vertical solid line and horizontal dotted line) as a function of the limb darkening coefficient $\varepsilon$.](image)

To compare the hydrodynamical velocity dispersion in 3D-COBOLD models with the spectroscopic quantities micro- and macro-turbulent velocities, we assume a simple geometrical model and try to resample the broadening of absorption lines. An intensity beam “sees” the velocity field under a certain angle and the spectral line is broadened by the projection of these velocities. In this sense we project the geometrical velocity components on a line of sight under a certain angle and integrate over all angles in a half sphere. We also take a linear limb-darkening law into account. We assume a velocity function $f(v)$ in velocity space and an intensity line profile

$$I(v) = V(v) \cdot I_0 / L(\theta),$$

where $V(v)$ is a line profile function, $I_0$ the continuum intensity at the center of the disk and $L(\theta)$ a limb-darkening law. The integrated flux of the intensity line profile broadened by the velocity function is then given by their convolution and disk integration, i.e.

$$F = \int_{-\infty}^{\infty} f(v) \ast I(v) \cos \theta \, dv,$$

with $dv = \sin \theta \, d\theta \, d\phi$, $\phi \in [0, 2\pi]$, $\theta \in [0, \pi/2]$. If we assume that $V(v)$ does not vary with different positions on the disk, it can be factored out (Gray 2008) and

$$F = V(v) \ast I_0 / W(\varepsilon),$$

with

$$W(\varepsilon) = \int_{-\infty}^{\infty} f(v) \cdot L(\theta) \cos \theta \, dv.$$
With Eq. 5 we are left with a flux-like expression for the velocity function. The dispersion of the velocity function is given by

$$\sigma^2 = \langle (f(v)^2) - (f(v))^2 \rangle$$

and we can write for the projected velocity dispersion $\Sigma$:

$$\Sigma^2 = \frac{1}{N} \int_0^{2\pi} \int_0^{\alpha/2} \left( \langle (f(v)e)^2 \rangle - \langle (f(v)e)^2 \rangle \cdot L(\theta) \cos \theta \right) d\omega$$

where $f(v) = \left( \begin{array}{c} f_x(v) \\ f_y(v) \end{array} \right)$ is the velocity vector containing all velocities in a model cube, $e = \left( \begin{array}{c} \cos \phi \sin \theta \\ \sin \phi \sin \theta \\ \cos \theta \end{array} \right)$ is the basis vector in spherical coordinates, and $L(\theta) = 1 - \epsilon + \epsilon \cdot \cos \theta$ is a linear limb-darkening law with the limb-darkening coefficient $\epsilon$. $N$ is a normalization factor $N = \int_0^{2\pi} d\phi \int_0^{\pi/2} L(\theta) \cos \theta \sin \theta d\theta = \pi(1 - \frac{\epsilon}{2})$. We included the limb-darkening in the normalization because, in opposite to the flux, the velocity dispersion for an isotropic velocity field has to be conserved. The average is taken over the velocities and does not affect the angle dependent parts. Basically we have to integrate:

$$\langle (f_e)^2 \rangle - \langle f_e \rangle^2 = \langle (f_x^2 - f_y^2) \cos \phi^2 \sin^2 \theta \rangle + \langle (f_x^2 - f_y^2) \sin \phi^2 \sin^2 \theta \rangle + \langle (f_x^2 - f_y^2) \cos \phi \sin \phi \sin \theta \rangle + 2\langle (f_x f_y - f_y f_x) \cos \phi \sin \phi \sin \theta \rangle + 2\langle (f_x f_y - f_y f_x) \cos \phi \sin \phi \sin \theta \rangle + 2\langle (f_x f_y - f_y f_x) \cos \phi \sin \phi \sin \theta \rangle.$$

If we want to compute the average of this quantity, we need the mean and the squared mean of the quantities, but not the combinations of the velocity components, because these products vanish in the integration over the half sphere due to their angle dependent coefficients. After the integration of Eq. 7, $\Sigma^2$ becomes

$$\Sigma^2 = \frac{\langle (f_x^2 - f_y^2)^2 \rangle}{20(\epsilon - 3)} + \frac{\langle (f_x^2 - f_y^2)^2 \rangle}{20(\epsilon - 3)}.$$  

We can see, that for an isotropic velocity field $f_x(v) = f_y(v) = f(v)$ follows that $\sigma^2 = \langle (f(v)^2) - (f(v))^2 \rangle$ and does not depend on $\epsilon$ or the geometrical projection anymore. Setting $\epsilon = 0$, then follows from Eq. 8 that $\Sigma^2_{\phi} = \frac{1}{2} \sigma^2_{\phi}$ and $\Sigma^2_{\theta} = \frac{1}{2} \sigma^2_{\phi}$ due to geometrical effects.

The projection factors for the vertical $\left( \frac{6\epsilon - 30}{20(\epsilon - 3)} \right)$ and horizontal $\left( \frac{2\epsilon - 15}{20(\epsilon - 3)} \right)$ component are plotted as a function of the limb-darkening coefficient $\epsilon$ in Fig. 17. They vary only about 5% from no darkening to a full darkened disk. The reduction for the vertical velocity is about 30% and for the horizontal components 50%

For the sake of completeness, we obtain in a similar way the mean velocities in three spatial directions $\langle f_{x,y,z}(v) \rangle$ which are given by

$$\langle f_{x,y,z}(v) \rangle_{projected} = \frac{1}{N} \int_0^{2\pi} \int_0^{\alpha/2} \langle f_{x,y,z}(v)e \rangle \cdot L(\theta) \cos \theta d\omega.$$  

The horizontal velocities vanish due to projection but there is still a vertical component which is reduced to geometrical and limb-darkening effects.

$$\langle f_x(v) \rangle_{projected} = \langle f_x(v) \rangle_{projected} = 0,$$

$$\langle f_z(v) \rangle_{projected} = \frac{1}{2(\epsilon - 3)} \langle f_z(v) \rangle.$$  

Acknowledgements. SW would like to acknowledge the support from the DFG Research Training Group Grk - 1351 “Extrasolar Planets and their host stars”. AR acknowledges research funding from the DFG under an Emmy Noether Fellowship (RE 1664/4-1).

HGL acknowledges financial support from EU contract MEXT-CT-2004-014265 (CIFIST). We thank Derek Homeier for providing us with the opacity tables.

References.

Asplund, M., Grevesse, N., & Sauval, A. J. 2005, in Astronomical Society of the Pacific Conference Series, Vol. 336, Cosmic Abundances as Records of Stellar Evolution and Nucleosynthesis, ed. T. G. Barnes, III & F. N. Bash, 25-32

Barklem, P. S., Piskunov, N., & O’Mara, B. J. 2000, A&A, 142, 467

Bashchek, B., Holweger, H., & Traving, G. 1966, Astronomische Abhandlung der Hamburger Sternwarte, 8, 26

Bean, J. L. 2007, PhD thesis, The University of Texas at Austin

Bean, J. L., Benedict, G. F., & Endl, M. 2006a, ApJ, 653, L65

Bean, J. L., Sneden, C., Hauschildt, P. H., Johns-Krull, C. M., & Benedict, G. F. 2006b, ApJ, 652, 1604

Dravins, D. 1982, ARA&A, 20, 61

Dulick, M., Bauschlicher, Jr., C. W., Burrows, A., et al. 2003, ApJ, 594, 651

Ferguson, J. W., Alexander, D. R., Allard, F., et al. 2005, ApJ, 623, 585

Freytag, B., Allard, F., Ludwig, H., Homeier, D., & Steffen, M. 2009, A&A, in prep.

Freytag, B., Steffen, M., & Dorch, B. 2002, Astronomische Nachrichten, 323, 213

Gray, D. F. 1975, ApJ, 202, 148

Gray, D. F. 1977, ApJ, 218, 530

Gray, D. F. 2008, The Observation and Analysis of Stellar Photospheres (The Observation and Analysis of Stellar Photospheres, by D.F. Gray. Cambridge: Cambridge University Press, 2008.)

Hauschildt, P. H. & Baron, E. 1999, Journal of Computational and Applied Mathematics, 109, 41

Kurucz, R. L. 1970, SAO Special Report, 309

Ludwig, H. G. 1992, PhD thesis, University of Kiel

Ludwig, H.-G., Allard, F., & Hauschildt, P. H. 2002, A&A, 395, 99

Ludwig, H.-G., Allard, F., & Hauschildt, P. H. 2006, A&A, 459, 599

Ludwig, H.-G., Jordan, S., & Steffen, M. 1994, A&A, 284, 105

Magain, P. 1986, A&A, 163, 135

Nordh, H. L., Lindgren, B., & Wing, R. F. 1977, A&A, 56, 1

Nordlund, A. 1982, A&A, 138, 527

Palla, F. & Baraffe, I. 2005, A&A, 432, L57

Reiners, A. 2007, A&A, 467, 259

Reiners, A. & Basri, G. 2006, ApJ, 644, 497

Reiners, A. & Basri, G. 2007, ApJ, 656, 1121

Sauval, A. J. & Tatum, J. B. 1984, ApJS, 56, 193

Schweitzer, A., Hauschildt, P. H., Allard, F., & Basri, G. 1996, MNras, 283, 821

Sneden, C. A. 1973, PhD thesis, AA(THE UNIVERSITY OF TEXAS AT AUSTIN.)

Steffen, M., Ludwig, H.-G., & Freytag, B. 1995, A&A, 300, 473

Vogler, A., Bruls, J. H. M. J., & Schüssler, M. 2004, A&A, 421, 741

Wende et al.: 3D simulations of M star atmosphere velocities and their influence on molecular FeH lines

Wilkinson, P. G. 1963, ApJ, 138, 778

Wing, R. F. 1972, in Les Spectres des Astres dans l’Infrarouge et les Microondes, 123–140

Wing, R. F. & Ford, W. K. J. 1969, PASP, 81, 527