CP star atmospheres based on individual ODFs

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Abstract. We describe a new method for the computation of opacity distribution functions (ODFs) useful to calculate one-dimensional model atmospheres in local thermal equilibrium (LTE). The new method is fast enough to be applied on current workstations and allows the computation of model atmospheres which deviate significantly from (scaled) solar chemical composition. It has reproduced existing ODFs and model atmospheres for solar abundances. Depending on the type of chemical peculiarity the "individual" model atmosphere may have a structure and surface fluxes similar to atmospheres based on (scaled) solar abundances or deviate in a way that cannot be reproduced by any of the conventional models. Examples are given to illustrate this behavior. The availability of models with "individualized" abundances is crucial for abundance analyses and Doppler imaging of extreme CP stars.

Key words: Stars: atmospheres – Stars: atmosphere model – Line blanketing – Opacity distribution functions

1. Introduction

Opacity distribution functions are used to describe line opacities l_ν in LTE for a set of pairs of temperature T and gas pressure P assuming a fixed chemical composition and (in our case) a fixed value for the microturbulence ξ_t:

$$l_\nu = l_\nu(T, P, \text{chem. composition}, \xi_t). \qquad (1)$$

The frequency dependence of the l_ν is described by dividing the whole wavelength range relevant to the desired stellar atmosphere computations into 300 to 1200 channels. Each of these channels is devided into 10-12 subchannels which provide a statistical representation of line opacity (ranging from high to low values). The (radiative) flux integrated over a set of subchannels approximates the overall (radiative) flux for each particular channel. Thus, one can compute the total radiative flux throughout the model atmosphere, as well as surface fluxes and intensities. This technique was described in Strom and Kurucz (1966) and later used, for instance, by Gustafsson et al. (1975) and by Kurucz (1979).

2. Description of the new method

Muthsam (1979) was the first to compute model atmospheres for CP stars. In the mean time, the reliability of atomic data obtained from experiments has been improved. Similarly, available line lists have increased both in size and reliability by up to an order of magnitude. Hence, it is worthwhile to bring individual model atmospheres for CP stars to the standards for stars with solar elemental abundance (cf. Kurucz 1993).

For his work Muthsam (1979) used the opacity sampling (OS) technique which requires the computation of a crude synthetic spectrum. The latter has to be sufficiently accurate for both the calculation of the integral flux in a wavelength region similar in size to the channels used for the ODF technique as well as for the calculation of the total radiative flux in each model layer. The OS technique is more efficient for the computation of *single* models. As opposed to the ODF technique, opacity sampling allows the study of vertical stratification of elemental abundances. Moreover, the OS technique is also capable of representing the blanketing effect in cool stars where the wavelength distribution of the opacities may change dramatically with depth as new molecules are formed (cf. Ekberg et al. 1986). However, as we did not intend to study stratification or late type stars with our code, we rather decided to benefit from the main advantage of the ODF technique: the rapid computation of small *grids* of model atmospheres (as a function of T_{eff} and $\log g$). Such grids are very convenient for spectroscopic analyses, the computation of color and flux grids, the investigation of the flux distribution of pulsating stars, and Doppler imaging.

Speed and accuracy requirements for an ODF computation are determined by a) the number of T-P pairs in (1) used to represent the whole ODF, b) the number of spectral lines used for the opacity computation, and c) the size of the wavelength grid used for each channel "$l_{\overline{\nu}}$". Under the assumption that the structure of the model atmosphere does not change dramatically for a different chemical composition, we can adapt our computations according to each of these three quantities. First, the T-P pairs are selected from a model atmosphere that is closest in T_{eff} and $\log g$ as well as chemical composition to the "target" model atmosphere (or model grid within some limited T_{eff} and $\log g$ range). In a second step, we use the Vienna Atomic Line Data Base (VALD, Piskunov et al. 1995) together with its extraction tools PRESELECT and SELECT to choose between 70 000 and 600 000 lines (a range valid from λ Boo stars to extreme Si peculiar stars) out of 42 million lines. The lines are selected according to wavelength range, ionization stage, excitation potential, and the ratio of line vs. continuous opacity for the desired range of T-P pairs or a set of T-P pairs taken from the "closest" standard model atmosphere. Finally, the ODF as well as Rosseland and/or Planck mean opacities are computed in a two-stage process: an adaptive wavelength grid (similar to that one for SYNTH as described in Piskunov 1992) is used by the VOPDF code to compute line opacities for each T-P pair. These are processed by the OPDF code which uses an adaptive histogram

Table 1. Parameters used for ODF and model atmosphere computations.

Star name	T_{eff}[K]	$\log g$	ξ_t[km/s]	chem. composition as in
Vega	9550	3.95	2	Castelli & Kurucz (1994)
α Cir	7900	4.2	1.5	Kupka et al. (1996)
ET And	11500	3.6	2	Kuschnig et al. (1995)

and a running geometric mean to compute the desired opacity tables. Details will be given in Piskunov & Kupka (1998). Currently, the equation of state and the continuous opacities are taken from ATLAS9 as published by Kurucz (1993) to simplify the comparison with standard models. Without line extraction, a typical ODF computation takes between 2 and 24 hours on an Alpha workstation with a DEC-21164/A CPU running at 600 MHz (or between 6 and 72 hours for a DEC-21064/A at 266 MHz). The VOPDF/OPDF codes can immediately run in parallel as opacities for different T-P pairs do not depend on each other.

3. Comparisons and Results

We present here some of the results of opacity calculations for three different CP stars. For the first case, Vega, we compared available *observations* of its flux distribution from the Lyman to the Paschen series with surface fluxes derived from our own, *individual model atmospheres* for Vega (see Table 1) as well as with fluxes derived from a set of *standard model atmospheres* assuming a scaled solar abundance (by -0.5 dex, using an ODF published on CDROM 3 of Kurucz). The stellar parameters and chemical compositions were taken from Castelli & Kurucz (1994). The model atmosphere computations were done with different variants of the ATLAS9 code of Kurucz. Details will be given in Piskunov & Kupka (1998). The overall agreement between observations, individual models, and standard models is quite good. The fluxes of individual and standard models are usually closer to each other than to the observations. Small differences between the "standard models" and "individual models" mainly originate from differences in the gf-values of the line lists used, a different treatment of hydrogen lines, and from the fact that we used the individual chemical composition determined for Vega. The latter does not change the model structure, but generates some specific flux features. This is supported by the result that the standard and the individual model atmospheres deviate by less than 30 K for all layers within the continuum as well as within the line formation region. Numerical experiments provide no evidence for a difference between individual models created from ODFs with 1% or 0.1% as a minimum ratio of line vs. continuum opacities. Hence, we used the larger minimum ratio for most of the other ODF computations to save CPU time.

As a second case, we compared model atmospheres based on Kurucz' ODFs for scaled solar abundances (by -0.2 dex, 0.0 dex, and +0.2 dex) with models based on an individual ODF with an abundance pattern as described in Kupka et al. (1996) for the mildly overabundant roAp star α Cir (cf. Table 1). Here, the T vs. optical depth and the T vs. P relations fall essentially between the scaled solar abundance patterns with 0.0 dex and +0.2 dex. Hence, the line profiles remain unaffected by the new model atmosphere. The behaviour of the flux distribution is more complicated and is shown in Figure 1. Though Fe appears to be slightly underabundant in α Cir, the individual model atmosphere of this star produces a flux distribution closer to the case of an overabundance of +0.2 dex, a slightly enhanced UV line blanketing after the Balmer jump, various features of Sr II (at 4077 Å and at 4215 Å) and a mild depression at 5200 Å.
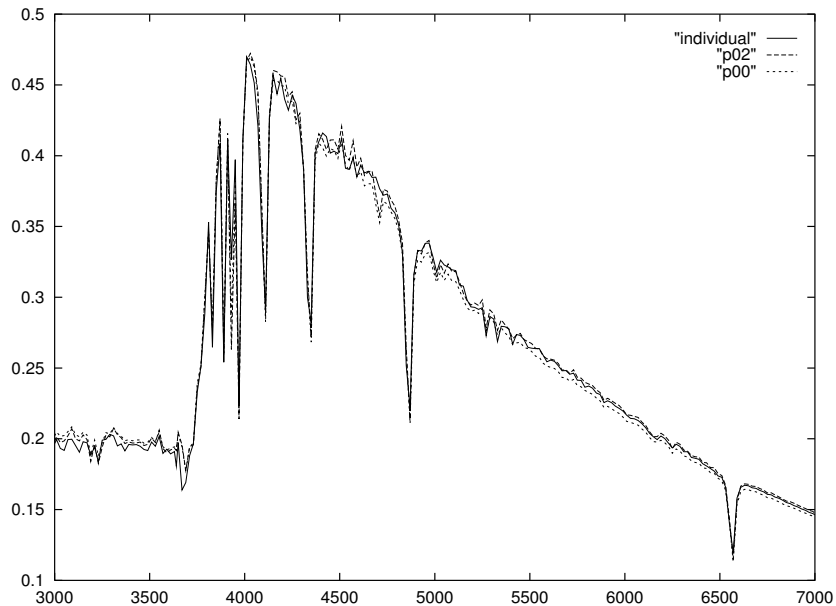

Figure 1. Flux distribution from model atmospheres for α Cir: individual (chemical composition as in Kupka et al. 1996), solar scaled by +0.2 dex, and solar. F_λ is plotted here as a function of wavelength in Å and scaled by a factor of 10^7.

Finally, we computed ODFs with different He, Si, and Fe abundances representing the mean composition and abundance spots of the strongly Si overabundant star ET And and compared the individual models with those computed under the assumption of a scaled solar abundance (+0.0 dex and +1.0 dex). Already for a mean overabundance of Si of +1.0 dex, deviations from the "standard models" occur that cannot be "simulated" by changing T_{eff}, log g, or by choosing a specific scaling factor for the abundance. Though a specific feature or a single layer may be "fitted" easily, one cannot match the height of the Balmer

discontinuity, or the relation of T vs. optical depth, or the flux distribution in the visual and the UV at the same time for this star, and abundance analyses based on scaled solar abundance patterns suffer from systematic errors.

4. Summary

We have presented a new method for the computation of model atmospheres for CP stars based on the ODF approach. The method was successfully compared with standard models. Application to various CP stars shows that model atmospheres for some abundance patterns (λ Boo stars or mildly peculiar roAp stars) can be computed using scaled solar abundances. For other patterns, systematic deviations occur which cannot be approximated by choosing a model atmosphere based on properly scaled solar abundances, making the computation of individual ODFs (or model atmospheres based on the OS technique) mandatory for applications such as abundance analyses and Doppler imaging. One prominent example are Si peculiar stars, essentially because Si is genuinely abundant and many of its absorption lines cluster in certain wavelength regions. More details on this work will be given in Piskunov & Kupka (1998).

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