

## NEW METHODS IN MODELING OF HOT STELLAR ATMOSPHERES

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**Abstract.** In the present study we had three main aims. First to study the possibility of reducing the initial model atmosphere data to short analytical polynomials. The second was to use as the depth variable the logarithm of the local gas pressure instead the Rosseland mean. The third aim was to check the applicability of the derived formulae and proposed computation methods to obtain high precision self-consistent results in modeling hot plane-parallel stellar atmospheres. Introducing the dimensionless (reduced) local quantities  $\theta = T/T_{\text{eff}}$  and  $\beta = P/P(T_{\text{eff}})$  it has been shown that for hot convection-free stellar atmospheres the curves  $\log \theta$  versus  $\log \beta$  reduce an initial grid of models to simple polynomials and bring forth some general features of the model stellar atmospheres. Even for stellar atmospheres having the convective zones in the deeper atmospheric layers, the outer part of the atmosphere (up to  $T = T_{\text{eff}}$  and for  $T_{\text{eff}} > 5000$  K) can be described in the same manner by curves  $\log \theta$  versus  $\log \beta$  as for the hotter stars. Iterative modeling of any hot stellar atmosphere can be started from these formulae (obtained for solar abundances), using rational polynomial ratios for  $P(T_{\text{eff}})$ , obtaining from these data the needed  $T$  versus  $P$  dependence. To check suitability of the formulae, the iterative correction of the model stellar atmospheres has been carried out by the traditional Unsöld-Lucy method and by the novel least squares optimization based on Levenberg-Marquardt method, followed by Broyden correction loop. It has been shown that the flux constancy obtained by it is almost 2 dex higher than obtained by the Unsöld-Lucy method. The precision estimators as criteria of the modeling algorithms self-consistency and of the computational precision level have been proposed and used.

**Key words:** stars: atmospheres – stars: early-type – stars: fundamental parameters

### 1. GENERALLY ON PLANE-PARALLEL MODEL ATMOSPHERES

In order to use any method of iterative correction in computing model stellar atmospheres, starting models are needed. There are different methods to solve the problem. The most simple of them is to recalibrate the solar thermal profile and thereafter to correct it. As the optical depth, most often the Rosseland mean optical depth has been taken. However, also some monochromatic optical depth as the depth variable of model stellar atmosphere has been used. This wavelength has been usually chosen so that the emergent flux at the wavelength corresponds well to the black-body radiation at  $T_{\text{eff}}$ . For instance, both of the methods have

been illustrated by Gray (2005) in his monograph.

Nowadays there has been computed a tremendous number of the model stellar atmospheres, which use and generate large data-bases. The most sophisticated, and the most applicable to large varieties of input physics are the plane-parallel and spherical LTE and NLTE model computations made by PHOENIX software. A review of the temperature correction methods used in this software is given in a paper by Hauschildt et al. (2003). For plane-parallel LTE model stellar atmospheres probably most widely have been applied the software package ATLAS9 elaborated by Kurucz (1970, 1994), its updated variant ATLAS12 (Castelli 2005), and the software package MARCS, elaborated primarily for modeling of relatively cool stellar atmospheres (Gustafsson et al. 2008). In addition, there are different other softwares (cf., TLUSTY, TMAP, CO5BOLD) each of which has its special best elaborated features. During the last decade the emphasis in elaborating of model stellar atmosphere grids has been shifted to the analysis of the galactic synthetic spectra, formed by contributions of different stellar populations with different metallicities. Such study has been carried out using jointly the ATLAS9 and MARCS softwares (Mészáros et al. 2012).

Computed model data can be used and have been applied as starting guesses for models nearby in  $T_{\text{eff}}$  and  $g$ . Usually the data are saved in the form of initial data table files for each choice of stellar model atmosphere parameters. In order to reduce the necessity of using the different bulky data bases, we try to generalize some physical features of stellar atmospheres, describing the atmospheres based *a priori* on simple local main thermodynamical parameters, thus trying to avoid, for instance, the extensive use of the Rosseland mean absorption coefficient. We show that it is possible to derive simple analytical approximation formulae for hot model stellar atmospheres of O, B and partially A stars, i.e. for the stars, which do not have any convective zone in their atmospheres and where only some species of molecules occur.

We start from the equation of the hydrostatic (gasostatic) equilibrium for the matter in the plane-parallel stellar atmospheres

$$\frac{dP}{dz} = \rho g_{\text{eff}}, \quad g_{\text{eff}} = g - a_{\text{rad}}. \quad (1)$$

Here we have ignored the microturbulence,  $g$  is gravity,  $a_{\text{rad}}$  is the radiative acceleration and the radial coordinate  $z$  is directed to the stellar centre, i.e.  $dz = -dr$ . The gas pressure  $P$  and the number density of nucleons  $N$  are given by

$$P = nkT = (1 + X_e)NkT, \quad N = \frac{\rho}{M}. \quad (2)$$

Here  $X_e$  is the mean ionization fraction and  $M$  is the mean mass of atomic particles, including electrons. Now we can express the gas density  $\rho$  by formula

$$\rho = \frac{MP}{(1 + X_e)kT}. \quad (3)$$

Consequently, from (1) it follows, that the logarithmic pressure gradient is expressed via the (exponential) pressure scale height  $h$  by

$$\frac{dP}{Pdz} = \frac{1}{h}, \quad h = \frac{(1 + X_e)kT}{M g_{\text{eff}}}. \quad (4)$$

## 2. CHOICE OF THE REDUCED PARAMETERS

Formula (4) shows that the logarithm of gas pressure is suitable to use as the depth variable in modeling of stellar atmospheres. We use it in the dimensionless scaled (reduced) form

$$\beta = \frac{P}{P(T_{\text{eff}})}, \quad (5)$$

which is suitable for comparing different model atmospheres among themselves.

Thus, Equation (4) can be written in the form

$$\frac{d \ln \beta}{dz} = \frac{1}{h}. \quad (6)$$

The differential element of the monochromatic optical depth  $\tau_\nu$  is defined in the form  $d\tau_\nu = k_\nu dz = k_\nu h d \ln P = k_\nu h' d \log \beta$ , where  $k_\nu$  is the monochromatic opacity coefficient [ $\text{cm}^{-1}$ ] and the decimal scale height  $h' = h \ln 10$ . Thus we obtain for the dex-gradient of the monochromatic optical depth the equation

$$\frac{d\tau_\nu}{d \log \beta} = k_\nu h'. \quad (7)$$

This formula enables us to find by integration the monochromatic optical depths, needed for solution of the equation of the radiative transfer of energy in stellar atmospheres.

Solution of the equation of the radiative transfer determines the temperature run in the stellar atmospheres. It is useful to describe this 'temperature profile' in the stellar atmospheres in units of the effective temperature  $T_{\text{eff}}$ , i.e. by the reduced temperature  $\theta$ , defined as the ratio

$$\theta = \frac{T}{T_{\text{eff}}}. \quad (8)$$

Further, we introduce the optical depth  $\tau$  similarly to the case of the quasi-grey atmospheres in the form

$$\theta^4 = \theta_0^4 + \frac{4}{3}\tau. \quad (9)$$

This expression can be used as the initial expression for finding of the thermal optical depth. It can be written in the form

$$(\theta^2 + \theta_0^2)(\theta + \theta_0)(\theta - \theta_0) = \frac{4}{3}\tau. \quad (10)$$

This equation specifies explicitly the temperature run at small argument values as  $\theta - \theta_0 = \tau/(3\theta_0^3)$ . In order to find the coupling of the formulae for radiation and for matter, an expression for the mean optical depth  $\tau$  is defined by

$$d\tau = \kappa \rho dz, \quad (11)$$

where  $\kappa$  is the mean opacity cross-section [ $\text{cm}^2/\text{g}$ ]. Thus, the derivative of the gas pressure from Equation (1) takes the form

$$\frac{dP}{d\tau} = \frac{g_{\text{eff}}}{\kappa}. \quad (12)$$

Now we define the column density, corresponding to pressure, by

$$m_g = P/g. \quad (13)$$

This quantity we use instead of the usual mass column density. Now we can write

$$\frac{d\tau}{dm_g} = \frac{\kappa g}{g_{\text{eff}}}. \quad (14)$$

This equation shows, that the relation ‘temperature versus gas pressure’ is determined mainly by the mean absorption coefficient. The aim of using  $m_g$  is to describe model atmospheres by local pressure and temperature, as it is general practice for the Earth atmosphere. In this way we avoid more complicated quantities, such as the Rosseland mean optical depth or the mass column density.

We start to demonstrate that in the reduced units (5) and (8) the model atmospheres can be described by simple expressions. As such an expression we choose for fitting in the outer layers the power-law formula

$$\theta = A(\beta + \delta)^b, \quad (15)$$

where we choose  $\delta = 10^{-7}$  in the role of the small quantity, which specifies the boundary temperature. On the outer boundary of model stellar atmosphere, i.e. if  $\beta = 0$ , holds

$$\theta_0 = A\delta^b. \quad (16)$$

Taking into account that  $\beta$  varies in wide limits, it is reasonable to specify the model layers in its logarithmic scale, as it is common practice for scaling the optical depth layers in the model stellar atmosphere computations. Thus, for fitting in the outer stellar atmosphere layers, we choose the formula

$$\log \theta = \log A + b \log(\beta + \delta). \quad (17)$$

Similarly, for the deeper layers we choose the power-law formula

$$\theta = D\beta^f, \quad (18)$$

from where it follows that in the logarithmic scale

$$\log \theta = \log D + f \log \beta. \quad (19)$$

For a smooth fit of these two expressions we introduce the weight function

$$W = \frac{1}{1 + \beta}. \quad (20)$$

Thus, finally we obtain for fitting the expression

$$\log \theta = W(a + b \log(\beta + \delta)) + (1 - W)(d + f \log \beta), \quad (21)$$

where  $a = \log A$  and  $d = \log D$ . Adapting the link of the  $\beta < 1$  and  $\beta > 1$  curves at  $\beta = 1$ , it follows that  $d = -a$ , giving  $\log \theta(T_{\text{eff}}) = 0$ , as needed.

In this expression the model stellar atmosphere parameters  $T_{\text{eff}}$  and  $\log g$  enter only implicitly.

### 3. ABOUT DEEP LAYERS OF MODEL STELLAR ATMOSPHERES

Let us now discuss the physics of deeper stellar atmosphere layers in more detail. In these deeper layers of stellar atmospheres, where the diffusion approximation for the radiation intensity is valid, the opacity coefficient  $\kappa$  has been specified as the Rosseland mean opacity coefficient. The diffusion approximation for the flux is

$$H_\nu = \frac{dB_\nu}{\kappa_\nu dz}. \quad (22)$$

The Rosseland mean opacity is defined by

$$\frac{1}{\kappa_R} = \int_0^\infty \frac{1}{\kappa_\nu} \frac{dB_\nu}{dT} d\nu \bigg/ \int_0^\infty \frac{dB_\nu}{dT} d\nu. \quad (23)$$

Now we take into account that the thermal gradient of the Planck function

$$\frac{dB_\nu}{dT} = \frac{dB_\nu}{dz} \frac{dz}{dT} = \kappa_\nu H_\nu \frac{dz}{dT}. \quad (24)$$

Thus, we obtain

$$\frac{1}{\kappa_R} = \frac{dz}{dT} \frac{H}{dB/dT}, \quad (25)$$

from where finally

$$\frac{dB}{dz} = \kappa_R H. \quad (26)$$

For the flux mean opacity we obtain the same expression, namely

$$\kappa_H H = \int_0^\infty \kappa_\nu H_\nu d\nu = \frac{dB}{dz} = \kappa_R H. \quad (27)$$

Equality  $\kappa_H = \kappa_R$  is an important constraint for deep atmospheric layers of stellar atmospheres, where the diffusion approximation holds.

Now we can write for deep stellar atmosphere layers

$$dB = \kappa_H H dz. \quad (28)$$

From (28) and (1), we obtain

$$dB = \frac{\kappa_H H}{\rho g_{\text{eff}}} dP. \quad (29)$$

Using the column density  $m_g$ , defined by (13), which can be also treated as the specific pressure, we can now write

$$\beta = \frac{m_g}{m_g(T_{\text{eff}})}. \quad (30)$$

Further we introduce the reduced Planck function

$$\varpi = \frac{B}{B(T_{\text{eff}})} = \theta^4 \quad (31)$$

and specific cross-section [ $\text{cm}^2/g$ ]

$$k_H = \kappa_H/\rho. \quad (32)$$

From (29), (31) and (5) it follows that

$$d\varpi = k_H C(T_{\text{eff}}) d\beta, \quad (33)$$

where we have introduced the notation

$$C(T_{\text{eff}}) = \frac{H m_g(T_{\text{eff}})}{B(T_{\text{eff}})} \frac{g}{g_{\text{eff}}}. \quad (34)$$

Thus, the connection between  $\varpi$  and  $\beta$  is specified by opacity coefficients  $k_H$  and  $k_R$ . We choose also here for absorption coefficient a power-law approximation, but now in the form of double power law, depending on temperature and pressure

$$k_H = C_H \varpi^\eta \beta^\varsigma. \quad (35)$$

Multiplying both sides of this expression correspondingly by (33) and thereafter integrating from the lower limits  $\varpi = 1$  and  $\beta = 1$  we obtain

$$(1 - \eta)^{-1} (\varpi^{1-\eta} - 1) = C_H C(T_{\text{eff}}) (\varsigma + 1)^{-1} (\beta^{\varsigma+1} - 1). \quad (36)$$

From here we find

$$\varpi^{1-\eta} = Y \beta^{\varsigma+1} - Y + 1, \quad (37)$$

where

$$Y = \frac{1 - \eta}{\varsigma + 1} C_H C(T_{\text{eff}}). \quad (38)$$

From physical considerations we choose  $\varsigma = 1$  and  $\eta = -1$ . In this approximation

$$\varpi^2 = Y \beta^2 - Y + 1. \quad (39)$$

Now there is the possibility in deep atmospheric layers to take into use a new argument

$$\beta' = \varpi = (Y \beta^2 - Y + 1)^{1/2}. \quad (40)$$

In this way we could obtain approximately  $\beta'$  in the role of the optical depth, if  $\beta > 1$  and  $8500 \text{ K} < T_{\text{eff}} < 11000 \text{ K}$ . Thus, for these model stellar atmospheres the expression

$$\log \theta = W(a + b \log(\beta + \delta)) + (1 - W)(-a + f \log \beta') \quad (41)$$

could be used. We can approximate  $Y$  with the expression

$$Y = \frac{1 + G_{\text{eff}}^\epsilon + \Theta_{\text{eff}}^\gamma}{1 + \Theta_{\text{eff}}^\gamma}, \quad G_{\text{eff}} \approx g/100, \quad \Theta_{\text{eff}} \approx T_{\text{eff}}/10^4. \quad (42)$$

In this expression  $\gamma \approx 4$  guarantees the needed smooth cutoff at higher temperatures and  $\epsilon \approx 1/3$  gives the needed shift of the larger gravity curves to the left. For computed model values of  $\beta$  we can now find the corresponding argument values

$\beta'$  and also the model values  $\theta$ . The dependence  $\log \theta$  versus  $\log \beta'$  could be considered as the curve to be optimized. However, we tried to avoid the two-dimensional ( $T_{\text{eff}}$  and  $\log g$ ) optimization and chose a different way.

#### 4. THE BEST FIT PARAMETERS

We decided to check the appropriateness of our concept, using for the purpose the ATLAS9 model stellar atmosphere database files computed by Kurucz (1994) which from the beginning have been publicly available via his CD-ROM 19. In this database the Rosseland optical depth has been used as the depth variable. Transforming the model data into our reduced quantities, we obtained the curves  $\log \theta$  versus  $\log \beta$  given in Figures 1 and 2. From Figure 2 it follows that in hot stellar atmospheres the best fit parameters  $a$ ,  $b$  and  $f$  turn out to be almost independent of  $\log g$ , but the curves depend somewhat on  $T_{\text{eff}}$ .

Checking the boundaries of applicability of our concept, we found that for outer atmospheric layers, up to  $T_{\text{eff}} = 5000$  and  $T = T_{\text{eff}}$ , the curves  $\log \theta$  versus  $\log \beta$  at different gravities are almost overlapping. This means that the convective zone in the deeper atmospheric layers does not affect the structure of the outer layers even by overshooting.

New grids of models have been computed Heiter et al. (2002) using the ATLAS9 software with different versions of the mixing-length theory and with more elaborated convection theories. They found that stellar atmospheres, where  $T_{\text{eff}} > 8500$  K are fully free of convective energy transfer and that in model stellar atmospheres with convective zone at  $T > T_{\text{eff}}$ , the fraction of the convective energy transport and also the temperature profile depend strongly on the convection theory used. Thus, for such atmospheres hitherto no high-precision theory has been formulated and therefore also no serious attempts of high-precision modeling have been undertaken.

Being guided by the results, depicted in Figures 1 and 2, now we start to find the polynomial optimization coefficient values. First we consider the best polynomial fit of the higher effective temperature model stellar atmospheres,  $11\,000 \leq T_{\text{eff}} \leq 50\,000$  K, where the picture is somewhat simpler. In order to obtain reasonable polynomial coefficients, the effective temperature has been here scaled to

$$t_h = (T_{\text{eff}} - 11\,000)/39\,000. \quad (43)$$

Thus, the upper limit of  $t_h$  is equal to 1. Such a choice is based on the circumstance that many of the best fit methods work only in the  $[-1, 1]$  argument region.

The number of digits in the computed significand (mantissa) has been minimized to the length where no loss of precision was apparent on plots of the polynomials versus the models, even at high zoom and by the error estimates. In this way for  $a_h$  the 7th order best fit polynomial curve, for  $b_h$  the 6th order polynomial and for a  $f_h$  the 8th order polynomial were obtained. These polynomial coefficients of expressions

$$a_h = \sum_{i=0}^7 a_i t_h^i, \quad b_h = \sum_{i=0}^6 b_i t_h^i, \quad f_h = \sum_{i=0}^8 f_i t_h^i \quad (44)$$

are given in Table 1. The rough usable mean values of these polynomials are  $a_h = -0.06$ ,  $b_h = 0.04$ ,  $f_h = 0.21$ .

**Table 1.** Polynomial coefficients if  $T_{\text{eff}} \geq 11\,000$  K.

$i$	$a_i$	$b_i$	$f_i$
0	-6.1676e-2	3.7750e-2	1.9542e-1
1	-1.2587e-1	6.2951e-2	-2.0401e-1
2	1.6764e 0	-2.7077e-1	4.7984e 0
3	-1.5728e1	6.3483e-2	-3.0868e1
4	5.3982e1	1.1391e 0	9.3330e1
5	-8.2291e1	-1.6414e 0	-1.5229e2
6	5.8157e1	6.5702e-1	1.3788e2
7	-1.5646e1		-6.5138e1
8			1.2495e1

In order to study the lower effective temperature part of model stellar atmospheres, having  $8500 \text{ K} < T_{\text{eff}} < 11\,000 \text{ K}$ , we introduce the reduced temperature by

$$t_l = (T_{\text{eff}} - 8500)/2500 \quad (45)$$

and find in the same way the polynomial best fit coefficients for these model stellar atmospheres, obtaining the 5th order polynomials

$$a_l = \sum_{i=0}^5 a_i t_l^i, \quad b_l = \sum_{i=0}^5 b_i t_l^i. \quad (46)$$

The polynomial coefficients for  $a_l$  and  $b_l$  are given in Table 2.

**Table 2.** Polynomial coefficients if  $T_{\text{eff}} \leq 11\,000$  K.

$i$	0	1	2	3	4	5
$a_i$	-7.167e-2	1.565e-1	1.143e-1	-1.035e 0	1.078e 0	-3.683e-1
$b_i$	3.249e-2	5.496e-2	5.287e-2	-4.069e-1	4.369e-1	-1.533e-1

The most complicated in this effective temperature region are the deep layers, having  $T > T_{\text{eff}}$ , where the parameter  $f$  depends essentially both on  $T_{\text{eff}}$  and  $\log g$ . We chose the rough approximation that  $f$  depends linearly both on  $T_{\text{eff}}$  and  $\log g$ , i.e.

$$f = f_o + pT_{\text{eff}} + v \log g. \quad (47)$$

The best fit we found is  $f_o=1.167$ ,  $p=-1.175e-4$ ,  $v=7.534e-2$ . Thus, the best fit coefficient for the thermal profiles of model stellar atmospheres have been found.

The next aim is to find the polynomial best fit values for the total gas pressure at the effective temperature points, i.e. the quantities  $P(T_{\text{eff}})$ . These values we took to correspond to the Rosseland mean optical depth  $\log \tau_R = -0.25$  in the Kurucz (1994) tables.

The effective temperatures as parameters were reduced to dimensionless quantities according to formula

$$t_e = (T_{\text{eff}} - 8500)/41500. \quad (48)$$



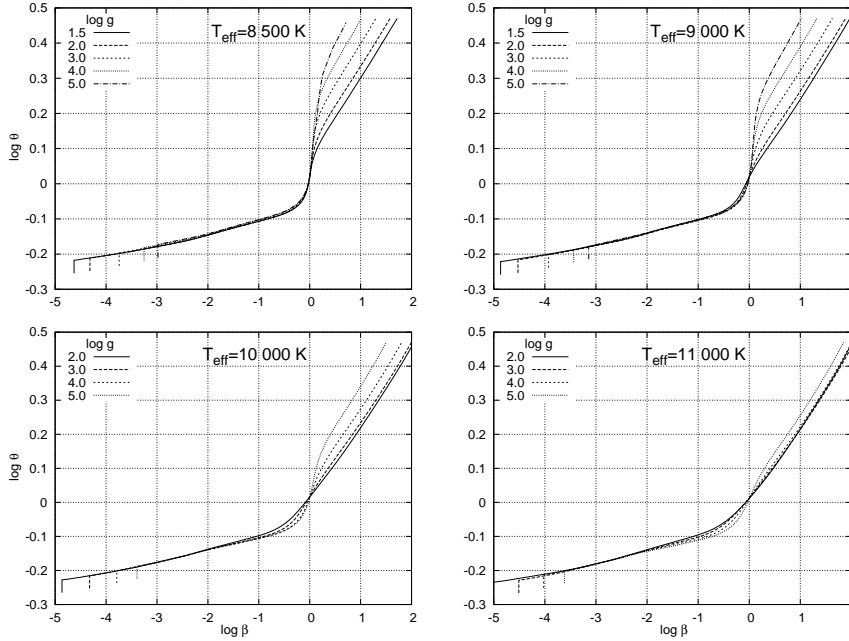


Fig. 1. The  $\log \theta$  versus  $\log \beta$  curves if  $T_{\text{eff}} \leq 11\,000$  K.

The upper value of the reduced parameter  $t_e$  is unity. After different attempts to choose the best fit formula for the pressure at the  $T_{\text{eff}}$  points, we concluded that the best choice is the ratio of rational polynomials of order 6 both in the nominator and in the denominator. Thus, the formula for  $\log P$  at corresponding value of  $\log g$  is

$$\log P(T_{\text{eff}}) - \log g = \beta_0(t_e) = \frac{D_6}{N_6}, \quad (49)$$

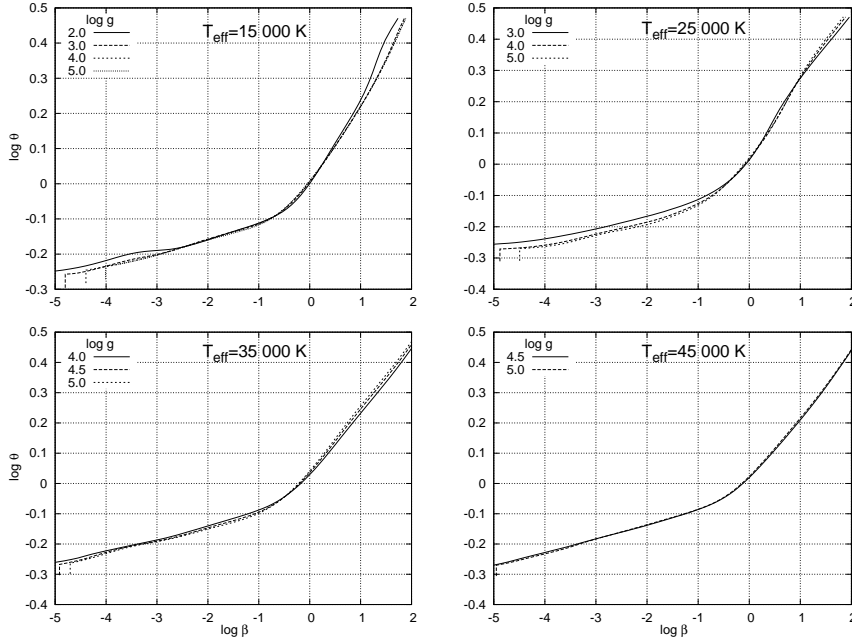
where the polynomial nominator and denominator are given by

$$D_6 = \sum_{i=0}^6 p_i t_e^i, \quad N_6 = \sum_{i=0}^6 d_i t_e^i. \quad (50)$$

The polynomial constant values obtained by best fit are given in Table 3. In the upper line for each gravity models are the denominator coefficients  $p_i$  and in the lower line are the nominator polynomial coefficients  $d_i$ . All the polynomial coefficients have been determined for the gravities with step  $\Delta \log g = 0.5$ . The number of significant digits of all polynomials, corresponding to a fixed  $\log g$  value has been minimized to the length where no loss of the precision was apparent on plots of the polynomials versus the models, even at high zoom, and by error estimates.

The curves  $\beta_0(t_e)$  versus  $T_{\text{eff}}$ , obtained from the Kurucz (1994) model data for different  $\log g$  values, are represented in Figure 3.

In order to use the best fit coefficients for any non-standard values of  $T_{\text{eff}}$  and  $\log g$ , the interpolation based on the computed best fit curves must be carried out.



**Fig. 2.** The  $\log \theta$  versus  $\log \beta$  curves if  $T_{\text{eff}} \geq 11\,000$  K.

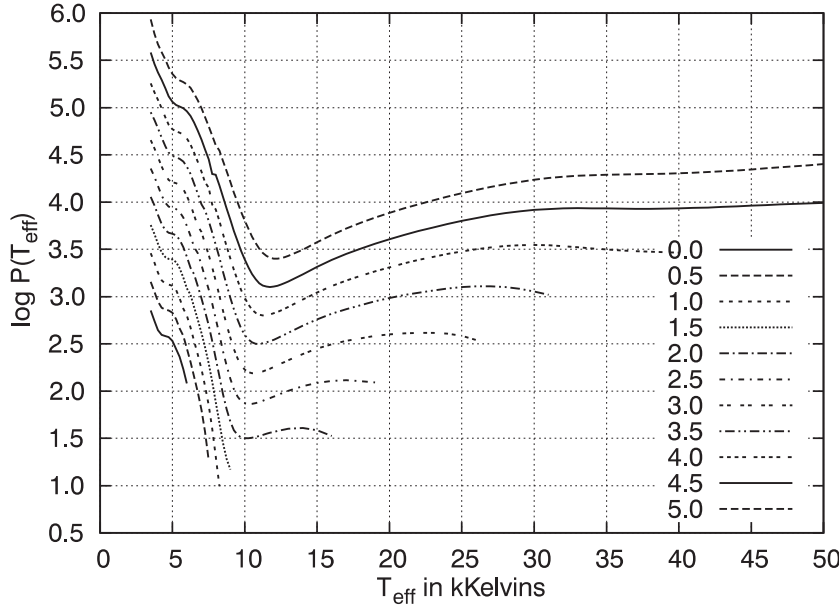
We have concluded that the standard solar mixture curves  $\log \theta$  versus  $\log \beta$  used here can be used well also as the initial model data in the case of any metallicities and apparently also any microturbulence velocities.

## 5. SPECIAL FEATURES OF MODEL STELLAR ATMOSPHERES

We have found the coefficients for best fit polynomials based on the grid of ATLAS9 model stellar atmospheres computed by Kurucz (1994). The grid is based on the opacity distribution function (ODF), and it has been computed almost two decades ago. There have been since then no drastic changes in the modeling results. Therefore, we concluded that, based on the obtained results, we can discuss adequately some main special features of model stellar atmospheres.

In the present study we had three main aims. First to study the possibility of reducing the initial model atmosphere data to short analytical initial data polynomials. The second was to use as the depth argument the logarithm of the local gas pressure instead of Rosseland mean. The third aim was to check the applicability of the derived formulae and proposed computation methods to obtain high-precision self-consistent results in modeling hot plane-parallel stellar atmospheres.

It turned out that in the hot O and B model stellar atmospheres the curves of reduced parameters,  $\log \theta$  versus  $\log \beta$ , at a fixed temperature almost do not depend on  $\log g$ . However, the computed model stellar atmospheres have different minimal  $\log \beta$  values at outermost atmosphere points of the almost overlapping curves. The smaller is the gravity, to the smaller  $\log \beta$  values extend the modelled curves. The difference is of the order of one dex and its maximal difference between giants and main sequence stars is about 1.5 dex. The outer endpoints on the curves



**Fig. 3.** The  $\log P(T_{\text{eff}})$  versus  $T_{\text{eff}}/1000$  curves. In legend are given the  $\log g$  values. Note the minimum points at  $T_{\text{eff}} \approx 11$  000 K. This means that in this region are the largest opacity coefficients in the stellar model atmospheres, caused primarily by hydrogen.

in Figures 1 and 2 are denoted by downwards directed markers.

An important feature of the curves is that the influence of the radiative acceleration plays unimportant role even quite near to the Eddington limit. Only the curves with minimal value of gravity at each effective temperature in the outer atmospheric layers are somewhat shifted to higher temperatures values.

We try now to sum up the main peculiarities of the studied stellar model atmospheres, which follow from the Figures 1–3.

First the  $\log \theta$  versus  $\log \beta$  curves in Figure 1 represent the convection-free stellar atmospheres with effective temperatures,  $8500 \text{ K} < T_{\text{eff}} < 11\,000 \text{ K}$ . We see, that the low-gravity stellar atmospheres have the temperature profile, which is almost the same as in the hotter atmospheres. However, these curves are very different for high-gravity atmospheres in deep layers, where  $T > T_{\text{eff}}$ . Namely, the larger is the gravity of the model stellar atmospheres the shorter it is from both ends.

This shift on the figures can be estimated to be approximately proportional to  $\log g/3$ . The temperature rise in the region near  $T_{\text{eff}}$  is extremely steep for the main sequence stars. This can be explained by the steep change of the absorption coefficient in this region of stellar atmospheres due to ionization of hydrogen atoms. In the deeper model atmospheres layers the curves at different gravities turn out to have almost the same value of  $d \log \theta / d \log \beta$ , which means that these parts of the thermal profiles are parallel.

Figure 2 shows us the  $\log \theta$  versus  $\log \beta$  curves for higher temperatures and what is their outer stretch, denoted by downwards directed markers. In deep layers of the stellar model atmospheres the reduced curves stretch to common value of  $\beta$

**Table 3.** Polynomial coefficients of  $\beta_0(t_e)$ .

	$p_0$	$p_1$	$p_2$	$p_3$	$p_4$	$p_5$	$p_6$
5.0	-5.6792e-1	-1.0466e1	9.6309e0	-2.7722e1	3.6660e1	8.5931e1	-1.9666e2
$d_i$	1.0000e 0	-1.1246e1	1.6170e2	-6.6124e2	1.5710e3	-1.9899e3	1.1014e3
4.5	-4.5019e-1	-1.2998e1	-3.5031e1	3.8559e2	-9.2304e2	9.3107e2	-3.8431e2
$d_i$	1.0000e 0	-1.0971e1	2.2039e2	-9.6427e2	1.9133e3	-1.8685e3	7.8640e2
4.0	-3.3375e-1	-1.1052e1	5.7207e2	-1.0227e4	1.1426e3	7.7921e4	-1.0594e5
$d_i$	1.0000e 0	-3.4559e1	6.8919e2	-7.4930e3	1.0265e5	-2.9283e5	2.6581e5
3.5	-2.3484e-1	-1.4460e1	8.1548e2	-1.4303e4	1.0277e4	8.7418e4	-1.3209e5
$d_i$	1.0000e 0	-4.1055e1	8.6625e2	-1.1030e4	1.6554e5	-4.8400e5	4.2399e5
3.0	-1.4716e-1	-5.3802e1	-3.2545e3	1.2994e5	-1.9581e6	2.0103e6	1.5319e6
$d_i$	1.0000e 0	1.8030e2	-6.3349e3	1.5111e5	-2.0226e6	2.5835e7	-4.5027e7
2.5	-7.4783e-2	-2.5913e1	8.3280e2	-2.4043e4	1.8221e5	-6.0925e5	8.6628e5
$d_i$	1.0000e 0	-2.3952e1	7.6543e2	-7.3318e2	1.0964e5	-7.0600e5	9.5986e5
2.0	-2.9191e-2	-3.0777e1	-1.3106e2	-4.9271e4	4.8603e5	-1.7280e6	0.0000e0
$d_i$	1.0000e 0	2.3117e1	8.7432e2	7.5867e4	-4.6508e5	1.3406e6	0.0000e0

for all gravities. The form of these curves depends on the effective temperature.

In Figure 3 are given the  $\beta_0$  curves, i.e. the gas pressure values at the point of effective temperature, obtained for each Kurucz (1994) model stellar atmosphere at different values of  $\log g$  that are given in the legend. As seen, at  $T_{\text{eff}}$  about 11 000 K the curves have a minimum value point corresponding to maximal opacity coefficient. Obviously therefore we had to divide the model atmospheres into two regions relative to the value of  $T_{\text{eff}}$ . However, we succeeded to find the best fit polynomial coefficients of  $\beta_0$  for whole interval of  $T_{\text{eff}}$ .

In order to check the quality of the approximation formulae in the well visualized form, we have formed the mantissa (significand) precision estimators by

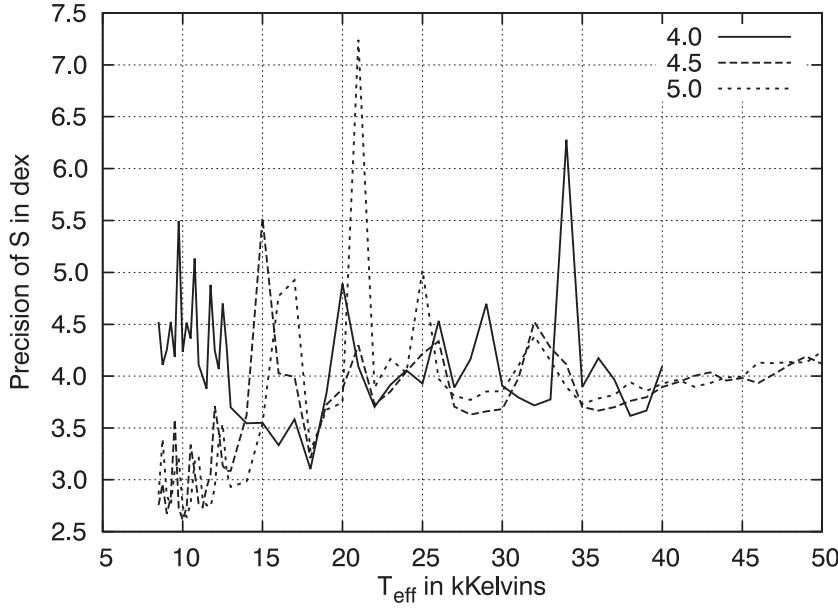
$$S(g_l, t_e) = -\log \left( \frac{|P_0 - P(g_l, \tau_1)|}{P(g_l, \tau_1)} \right), \quad \log P_0 = \beta_0(g_l, t_e) + \log g, \quad (51)$$

where  $\tau_1$  means the corresponding Kurucz (1994) model point at Rosseland mean  $\tau_R = 1$ . Further,  $g_l = \log g$  and the reduced effective temperature  $t_e$  is given by (48). Using this formula we have found that the precision of the obtained approximation formula for  $\beta_0$  is from 3 mantissa digits (1 ‰) at lower temperatures to 4 mantissa digits (0.1 ‰) at higher effective temperatures. The quality of this approximation formula, via precision estimator  $S(g_l, t_e)$ , is visualized in Figure 4, which demonstrates that the approximation curves are in good mutual accordance with original ATLAS9 model data.

## 6. CHECKING BY MODEL COMPUTATIONS

We have checked whether the polynomial expressions we have determined are suitable for starting of the model atmosphere computations. We studied the convergence of some radiative field characteristics in the Unsöld-Lucy iteration method. The model, which we study here, has main parameter values,  $T_{\text{eff}} = 12\,000$ ,  $\log g = 4.5$  and  $[\text{Fe}/\text{H}] = -2$ , i.e. the metal abundances are 2 dex lower than the solar values.

The precision estimator of the dex length of the mantissa of the flux we define



**Fig. 4.** The precision estimator  $S(g_l, t_e)$  versus  $T_{\text{eff}}/1000$  curves at  $T_{\text{eff}}$ . In legend are given the gravity values  $g_l$ . Note that at some temperatures there are the precision peaks. Larger differences between the curves are at lower  $T_{\text{eff}}$  values. Most typically the difference of the model data and of the approximation formula is about 0.1 ‰.

by

$$S_H = -\log(\max(|\delta H|/H_0)). \quad (52)$$

We define similarly the precision estimators of all other radiative field characteristics. Thus, the precision estimator of temperature

$$S_T = -\log(\max(|\delta T|/T)), \quad (53)$$

where  $\delta T$  is the current loop step temperature correction.

In addition the precision estimator of the emission and absorption terms ratio  $S_L$ , is defined by

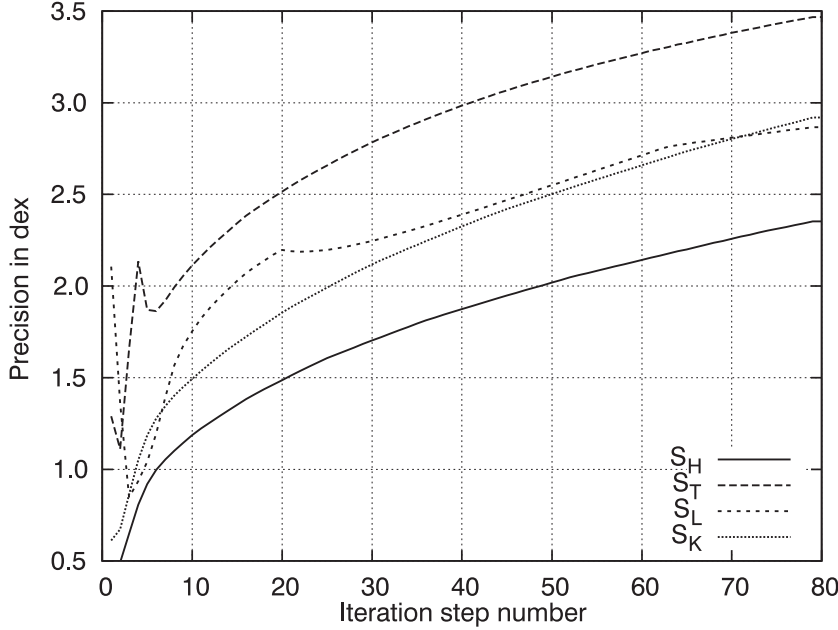
$$S_L = -\log(\max(a_J J/a_B B - 1)) \quad (54)$$

and the precision estimator of the second Eddington moment  $K$  is defined by

$$S_K = -\log(\max(|\delta K|/K)). \quad (55)$$

In spite of high precision in the approximation polynomials, the model computations of hot stellar atmospheres give initial total flux values, which in some layers can differ from the needed value corresponding to afore taken  $T_{\text{eff}}$  by factor of 2.

As an example the curves of all these precision estimators obtained by the Unsöld-Lucy method for model atmosphere, having  $T_{\text{eff}} = 12\,000$  K and  $\log g = 4.5$  for 80 iteration loop steps are given in Figure 5. The precision estimators  $S_L$  and  $S_K$  are placed approximately mean-way between the  $S_H$  and  $S_T$  curves.



**Fig. 5.** Growth of precision in the iteration loop, obtained applying the Unsöld-Lucy method. The precision estimators for flux  $S_H$ , for temperature correction  $S_T$ , for emission and absorption terms ratio  $S_L$ , and for the 2nd order Eddington moment of the radiative field  $S_K$ . The model atmosphere parameters are  $T_{\text{eff}} = 12000$  K and  $\log g = 4.5$ . The argument is the loop counter.

Our computations showed that in the traditional Unsöld-Lucy method the current relative temperature correction is essentially smaller than the relative flux error. As a rule  $S_T - S_H > 1$ , and thus  $S_T$  cannot be used as a criterion of the maximal flux error, which is essentially larger.

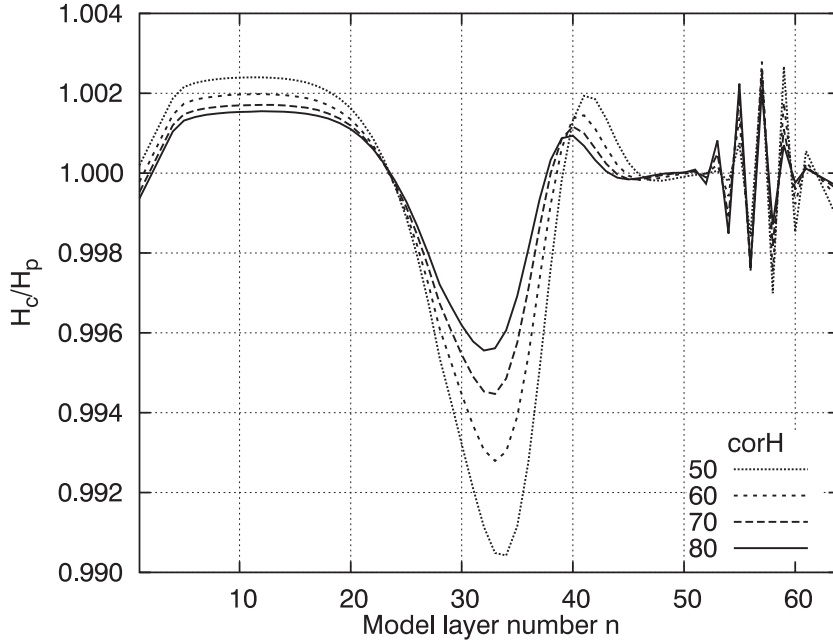
The computed relative flux deviations in each model correction loop have been reduced by the damping coefficient 0.6 and forbidden to exceed this value in early iteration steps. In less than 10 iteration steps the flux constancy reaches the level obtained if we start directly from the Kurucz model data. As the iterations progress, the improvement in the flux constancy slows and stops due to unremovable small zigzags in flux at very deep atmospheric layers. The curve of final computed relative flux deviations is plotted in Figure 6, from where the zigzags, being the precision delimiters, are well seen. In order to achieve high precision of the model flux, more elaborated iterative procedures are needed.

The computations for arbitrary values of  $T_{\text{eff}}$  and  $\log g$  have been initiated by the interpolation of the  $\beta_0$  curves. The value of  $t_e$  is specified by (48) and no interpolation relative to it is needed. Thereafter the  $\beta_0$  value must be interpolated between two adjacent gravity curves, the values of gravities of which are specified by

$$g_e^- = 0.5 \text{int}(2g_e), \quad g_e^+ = g_e^- + 0.5, \quad \delta g_e = g_e - g_e^- \quad (56)$$

and the interpolation is made by

$$\beta_0(g_e, t_e) = \beta_0(g_e^-, t_e)(1 - \delta g_e) + \beta_0(g_e^+, t_e)\delta g_e. \quad (57)$$

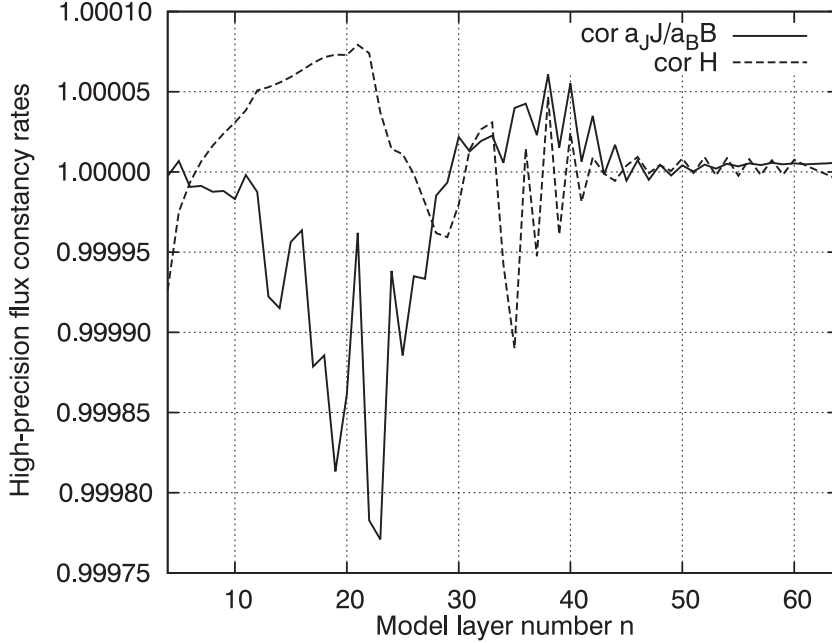


**Fig. 6.** The ratio of the corrected flux  $H_c$  relative to the precise model atmosphere flux  $H_p$  with  $T_{\text{eff}} = 12000$  K,  $\log g = 4.2$  and  $[\text{Fe}/\text{H}] = -2$ . In legend are given the iteration loop counters. Note that the zigzags at deep layers are probably unremovable. This also limits the achievable maximal value of the precision estimator  $S_H$ .

This interpolation formula works well for initialization of computations of model stellar atmospheres with non-standard model parameter values.

In order to get high-precision flux constancy, we studied the least squares optimization by the Levenberg-Marquardt method with the subsequent Broyden single parameter correction loop. Such a correction scheme for model stellar atmospheres was elaborated and applied by us (Sapar et al. 2013). A single Jacobian cycle turned out to give high-precision flux constancy, which is almost 2 dex better than the constancy obtained by the Unsöld-Lucy method. Some iterative curves of flux throughout the stellar atmosphere obtained for the same model data as the Unsöld-Lucy method are given in Figure 6. From it is seen the unremovable zigzags which determine the final attainable exactness. The corresponding curve for final relative flux deviations and for local ratio of the absorbed and emitted radiation, both obtained by Levenberg-Marquardt method is given in Figure 7. As seen, this method gives highly self-consistent exactness of modeling results.

In Figure 8 we represent the total relative temperature correction curve. The curve cannot be explained in an elementary way. The corrected boundary temperature turns lower, the central part turns hotter and in deeper layers the curve has a minimum, followed by a rise. As demonstrated by N. Sakhbullin in the 1st part of his monograph (Sakhbullin 1997), such a correcting difference generally corresponds to the transition from ATLAS9 to ATLAS12 modeling, accomplished by Kurucz (1992, 1994). This fits well also with the results of present study. From the paper by Castelli & Kurucz (2003) it follows, that the later improvements of



**Fig. 7.** The ratios of the final corrected radiative flux and of the local ratio of the absorbed and emitted radiation, for model atmosphere with  $T_{\text{eff}} = 12\,000$  K,  $\log g = 4.2$  and  $[\text{Fe}/\text{H}] = -2$ , corrected using in the least squares optimization the Levenberg-Marquardt method with subsequent Broyden correction loop. The flux constancy obtained is almost 2 dex better than obtained by the Unsöld-Lucy method. The highest precision has been obtained in the deep layers.

the opacity distribution functions have not changed them noticeably at hot temperatures and thus, the Kurucz (1994) model data used by us correspond quite well to the level of present knowledge.

## 7. OTHER WAYS IN LTE PLANAR ATMOSPHERES MODELING

The computations convinced us that the polynomial approximation formulae proposed and the usage of  $\log \beta$  as the argument are quite acceptable for iterative correction of any hot model stellar atmosphere. Using a more updated data base, say the ATLAS12 data, the polynomials can be improved.

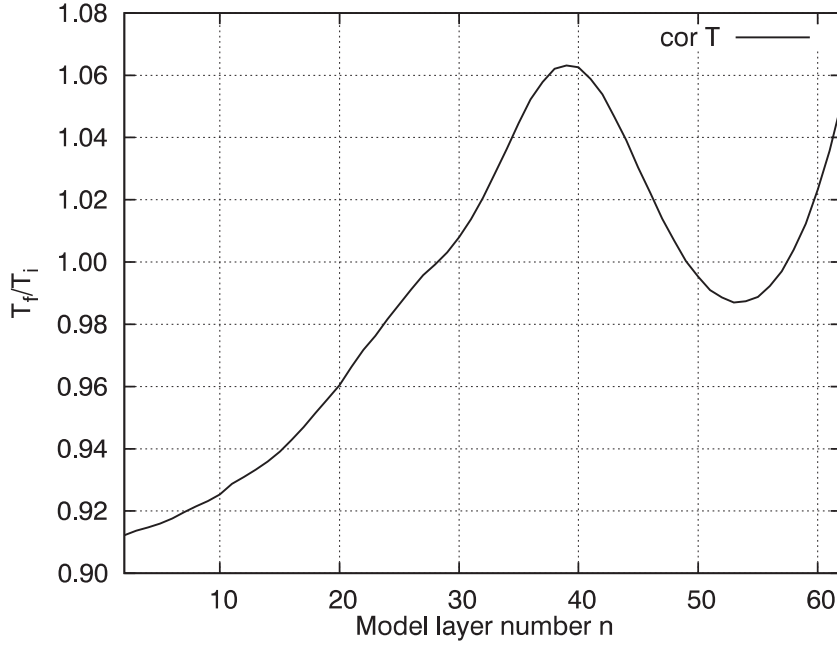
If there are no model stellar atmosphere at one's disposal, then the most straightforward way is to use the Rosseland mean absorption coefficient  $\kappa_R(T, P)$ , but to write the equation of hydrostatic equilibrium in the form where the roles of argument and function are interchanged, thus giving to the hydrostatic equilibrium the form

$$\frac{d\tau_R}{dP} = \frac{\kappa_R}{g}. \quad (58)$$

Differentiating (9) and eliminating the optical depth, we obtain

$$\frac{4dT^4}{3dP} = \frac{T_{\text{eff}}^4 \kappa_R}{g} \quad (59)$$





**Fig. 8.** The ratio of the final and initial temperature profiles for model atmosphere with  $T_{\text{eff}} = 12\,000$  K,  $\log g = 4.2$  and  $[\text{Fe}/\text{H}] = -2$ , corrected by the Levenberg-Marquardt method and the subsequent Broyden correction loop. Abscissa is the model atmosphere layer number.

Expressing this equation in reduced units by (8) and (13) yields

$$\frac{4d\theta^4}{3d\beta} = \kappa_R \frac{P(T_{\text{eff}})}{g}. \quad (60)$$

It is reasonable to start integration from the point  $T = T_{\text{eff}}$  and  $P = P(T_{\text{eff}})$  to both sides. Thus we can write

$$T^4 = T_0^4 + \frac{3T_{\text{eff}}^4}{4} \int_0^P \frac{\kappa_R}{g} dP. \quad (61)$$

In this way it is possible to find an initial thermal profile. Our computations have shown that the initial curve  $T$  versus  $P$  can be a quite rough approximation, if the least squares optimization by Levenberg-Marquardt method has been used. A similar method, but using the least squares integral in the form  $I = \int_0^P (\Delta H)^2 dP$  for optimization, has been tentatively studied by Napier (1970) and Napier & Dodd (1974). They also concluded that the initial curve for successful iterations can be chosen in very rough approximation.

It deserves to be mentioned that the Unsöld-Lucy temperature correction method has been modified in different ways, but no essential breakthrough has been obtained. As an example, the method of complete linearization, developed by Mihalas & Auer (1969), gave complicated equations for a bulky system of linear equations. An exhaustive description of this method and the formulae needed has been summarized by Sakhbullin (1997).

Cardona et al. (2007, 2009) and in a number of former papers have tried to simplify the iteration algorithms similarly to Unsöld-Lucy method, but extending the manifold of quasi-constant ratios used. Their proposal is to find the needed temperature corrections which satisfy the local energy conservation constraint, varying only the temperature of the Planck function in each layer separately and thereafter accomplishing the computation of the radiation transfer with corrected temperature values. Another method proposed by them is to carry out the iterative computations of the radiative field and temperature corrections with fixed opacities (the inner loop) and thereafter to carry complete computations in the outer loop. However, they checked the method only on simple pure hydrogen toy models.

They made also an interesting proposal to use in the equation of the radiative transfer the difference  $D_\nu = I_\nu - S_\nu$ . Then one obtains

$$\mu \frac{dD_\nu}{d\tau_\nu} = D_\nu - \mu \frac{dS_\nu}{d\tau_\nu}. \quad (62)$$

Integrating along light rays the reciprocally compensating large emission and absorption terms fall out and the new source term of the equation demonstrates its close parentage with the flux contribution. Thus, even if the number of digits in computer mantissa is short, essentially higher numerical precision can be obtained by this method.

## 8. CONCLUDING REMARKS

Here we have proposed a new method to start the iterative model stellar atmosphere computations and checked its adequacy. The idea is to use in the computations the logarithm of reduced gas pressure,  $\beta$ , as the depth variable and the logarithm of the reduced temperature,  $\theta$ , as the function to be determined. In such reduced quantities different model atmospheres are better comparable and adjustable to describe by analytical approximation formulae.

For hot convection-free stellar atmospheres the dependence  $\log \theta$  versus  $\log \beta$  has been approximated to simple polynomials. In cooler stellar atmospheres with convective zones in the deeper atmospheric layers, the outer non-convective part to  $T_{\text{eff}} > 5000$  K can be described in the same manner. The initial model data-base has been substituted by functions  $\log(P(T_{\text{eff}})/g)$ , described as the ratio of rational polynomials, which can be interpolated for any value of  $T_{\text{eff}}$  and  $\log g$ , but also used for non-solar metallicities and different microturbulence velocities.

The estimators of the correct digit-length in significands (mantissa) have been constructed and applied to check the obtained flux constancy and iterative correction steps in other radiation field characteristics.

Our present study was primarily aimed at elaborating some new and simple algorithms for high-precision model computations of stellar atmospheres and stellar spectra. The computations have been accomplished by our consumer-friendly and compact Fortran 90/95 software SMART, using parallel-processing on local small grid of multi-core personal computers.

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during about two decades to elaborate our version for study of hot stellar model atmospheres. We also appreciate his thoroughness as a referee. This work was supported by the research project SF0060030s08 of the Estonian Ministry of Education and Research.

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