Modelling of Stellar Atmospheres
IAU Symposium, Vol. xxx, xxxx
N. E. Piskunov, W. W. Weiss, D. F. Gray, eds.

New Grids of ATLAS9 Model Atmospheres

Fiorella Castelli

Istituto di Astrofisica Spaziale e Fisica Cosmica, CNR, Via del Fosso del Cavaliere, 00133, Roma, Italy

Osservatorio Astronomico di Trieste, Via G.B. Tiepolo 11, 34131, Trieste, Italy

Robert L. Kurucz

Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA

Abstract. New opacity distribution functions (ODFs) for several metallicities have been computed. The main improvements upon previous ODFs computed by Kurucz (1990) are: (1) the replacement of the solar abundances from Anders & Grevesse (1989) with those from Grevesse & Sauval (1998); (2) the replacement of the TiO lines provided by Kurucz (1993) with the TiO lines from Schwenke (1998), as distributed by Kurucz (1999a); (3) the addition of the H_2O lines from Partridge & Schwenke (1997), as distributed by Kurucz (1999b); (4) the addition of the H I-H I and H I-H^+ quasi-molecular absorptions near 1600 Å and 1400 Å computed according to Allard et al. (1998). Other minor improvements are related with some changes in a few atomic and molecular data. New grids of ATLAS9 model atmospheres for $T_{\rm eff}$ from 3500 K to 50000 K and log g from 0.0 dex to 5.0 dex have been computed for several metallicities with the new ODFs. Preliminary comparisons of results from the old and new models have shown differences in the energy distributions of stars cooler than 4500 K, in the ultraviolet energy distribution of metal-poor A-type stars, in the U$-$B and u$-$b color indices for $T_{\rm eff}\leq$6750 K and in all the color indices for $T_{\rm eff}\leq$4000 K.

1. Introduction

Starting from 1992 Kurucz published new extended grids of model atmospheres for several metallicities [M/H] and several microturbulent velocities ξ. In each grid, the models cover a range in $T_{\rm eff}$ and logg from 3500 K to 50000 K and from 0.0 dex to 5.0 dex, respectively. All the models were computed with the ATLAS9 code, which handles line opacity with the opacity distribution function method (ODFs).

Later on, Castelli extended Kurucz's models by computing some more grids for metallicities with enhanced α elements abundances (+0.4 dex) and for ξ values different from those adopted by Kurucz. Furthermore, she recomputed the cool models in a few Kurucz grids by assuming the overshooting option for the convection switched off (Castelli, Gratton & Kurucz, 1997).

Both Kurucz and Castelli models were computed by using Kurucz's (1990) ODFs. They are all based on the solar abundances from Anders & Grevesse (1989), except for iron which is not the same in all the ODFs. In fact, the iron abundance $\log(N_{Fe}/N_{tot})$ is -4.53 dex from Holweger et al. (1995) when ODFs for enhanced α elements abundances were computed and it is -4.37 dex from Anders & Grevesse (1989) when ODFs for no enhanced α elements were generated. Therefore, it is not straightforward to state the net effect of the α elements abundances on the model structure.

Finally, the number of models is different in the various grids and also in some grids some models have 72 and some others have 64 plane parallel layers. These differences may give problems when interpolations in the models and in the grids are performed.

2. The Aim of this Work

The aim of this work is the computation of grids of homogenous ATLAS9 models, where "homogenous" means that:

(1) The number of models is 476 in all the grids. Table 1 shows which are the models.

(2) All the models have the same number of 72 plane parallel layers from $\log\tau_{Ross}=-6.875$ to $+2.00$ at steps of $\Delta\log\tau_{Ross}=0.125$.

(3) All the models are computed with the updated solar abundances from Grevesse & Sauval (1998) and therefore with updated ODFs, which now also include H_2O lines.

(4) All the models are computed with the convection option switched on and with the overshooting option switched off. Mixing-length convection with $l/H_p=1.25$ is assumed for all the models. The convective flux decreases with increasing $T_{\rm eff}$ and it naturally disappears for $T_{\rm eff}$ of the order of 9000 K.

3. The new Opacity Distribution Functions

The line opacity is included in the new ATLAS9 models through new-ODFs based on the Grevesse & Sauval (1998) (GS98) solar abundances. Table 2 lists the differences between GS98 abundances and those from Anders & Grevesse (1989) which were used in the Kurucz (1990) ODFs.

New-ODFs are computed for 57 values of temperature T (from 1995 K to 199526 K, i.e. for logT ranging from 3.30 to 5.30 at steps of 0.02 dex) and 25 values of gas pressure $\log P_g$ (from -4.0 to $+8.0$ at steps of 0.5 dex), while Kurucz (1990) ODFs were computed for 56 values of T (from 2089 K to 199526 K, i.e. for logT ranging from 3.32 to 5.30 at steps of 0.02 dex) and 21 values of $\log P_g$ (from -2.0 to $+8.0$ at steps of 0.5 dex). The larger ODF table should allow better modelling the upper layers of cool stars and of giant stars.

Table 1. The 476 models of each grid.

	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	No of models
3500	X	X	X	X	X	X	X	X	X	X	X	11
3750	X	X	X	X	X	X	X	X	X	X	X	11
4000	X	X	X	X	X	X	X	X	X	X	X	11
4250	X	X	X	X	X	X	X	X	X	X	X	11
4500	X	X	X	X	X	X	X	X	X	X	X	11
4750	X	X	X	X	X	X	X	X	X	X	X	11
5000	X	X	X	X	X	X	X	X	X	X	X	11
5250	X	X	X	X	X	X	X	X	X	X	X	11
5500	X	X	X	X	X	X	X	X	X	X	X	11
5750	X	X	X	X	X	X	X	X	X	X	X	11
6000	X	X	X	X	X	X	X	X	X	X	X	11
6250		X	X	X	X	X	X	X	X	X	X	10
6500		X	X	X	X	X	X	X	X	X	X	10
6750		X	X	X	X	X	X	X	X	X	X	10
7000		X	X	X	X	X	X	X	X	X	X	10
7250		X	X	X	X	X	X	X	X	X	X	10
7500		X	X	X	X	X	X	X	X	X	X	10
7750			X	X	X	X	X	X	X	X	X	9
8000			X	X	X	X	X	X	X	X	X	9
8250			X	X	X	X	X	X	X	X	X	9
8500				X	X	X	X	X	X	X	X	8
8750				X	X	X	X	X	X	X	X	8
9000				X	X	X	X	X	X	X	X	8
9250					X	X	X	X	X	X	X	7
9500					X	X	X	X	X	X	X	7
9750					X	X	X	X	X	X	X	7
10000					X	X	X	X	X	X	X	7
10250					X	X	X	X	X	X	X	7
10500					X	X	X	X	X	X	X	7
10750					X	X	X	X	X	X	X	7
11000					X	X	X	X	X	X	X	7
11250					X	X	X	X	X	X	X	7
11500					X	X	X	X	X	X	X	7
11750					X	X	X	X	X	X	X	7
12000						X	X	X	X	X	X	6
12250						X	X	X	X	X	X	6
12500						X	X	X	X	X	X	6
12750						X	X	X	X	X	X	6
13000						X	X	X	X	X	X	6
14000					X	X	X	X	X	X	X	7
15000						X	X	X	X	X	X	6
16000						X	X	X	X	X	X	6
17000						X	X	X	X	X	X	6
18000						X	X	X	X	X	X	6
19000						X	X	X	X	X	X	6
20000							X	X	X	X	X	5
21000							X	X	X	X	X	5
22000							X	X	X	X	X	5
23000							X	X	X	X	X	5

Table 1. cont.

	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	No of models
24000							X	X	X	X	X	5
25000							X	X	X	X	X	5
26000							X	X	X	X	X	5
27000								X	X	X	X	4
28000								X	X	X	X	4
29000								X	X	X	X	4
30000								X	X	X	X	4
31000								X	X	X	X	4
32000									X	X	X	3
33000									X	X	X	3
34000									X	X	X	3
35000									X	X	X	3
36000									X	X	X	3
37000									X	X	X	3
38000									X	X	X	3
39000									X	X	X	3
40000										X	X	2
41000										X	X	2
42000										X	X	2
43000										X	X	2
44000										X	X	2
45000										X	X	2
46000										X	X	2
47000										X	X	2
48000										X	X	2
49000										X	X	2
50000											X	1

Except for TiO, new-ODFs are computed with the atomic and molecular line lists as in the Kurucz (1990) ODFs, but some molecular lists have been extended to more bands (i.e. CN, OH, and SiO) and some bugs in the line lists have been corrected.

In new-ODFs, the TiO lines computed by Kurucz (1993) with semi-empirical methods have been replaced by the TiO lines from Schwenke (1998), as distributed by Kurucz (1999a) on the CD-ROM No 24. Furthermore, the H_2O lines from Partridge & Schwenke (1997), as distributed by Kurucz (1999b) on the CD-ROM No 26, were added to the other lines. New-ODFs also include H I-H^+ and H I-H I quasi-molecular absorptions at 1400 Å and 1600 Å, respectively, due to the collision of neutral hydrogen in the ground-state with ionized hydrogen and other neutral hydrogen atoms (Castelli & Kurucz, 2001). These absorptions are observed as broad features in λ Boo stars and in metal-poor A-type stars.

The treatment of the overlapping lines at the end of the term series was also improved in the new-ODFs.

Table 2. Solar abundances different in Anders & Grevesse (1989) (AG89) and in Grevesse & Sauval (1998) (GS98). The abundances are given as $\log(N_{elem}/H_H)$.

	He	Li	Be	B	C	N	O	Ne	S
AG89	−1.01	−10.84	−10.85	−9.40	−3.44	−3.95	−3.07	−3.91	−4.79
GS98	−1.07	−10.90	−10.60	−9.45	−3.48	−4.08	−3.17	−3.92	−4.67

	Ar	Sc	Ti	Fe	Se	Kr	Sr	Cd	Xe
AG89	−5.44	−8.90	−7.01	−4.33	−8.65	−8.77	−9.10	−10.14	−9.77
GS98	−5.60	−8.83	−6.98	−4.50	−8.59	−8.69	−9.03	−10.23	−9.83

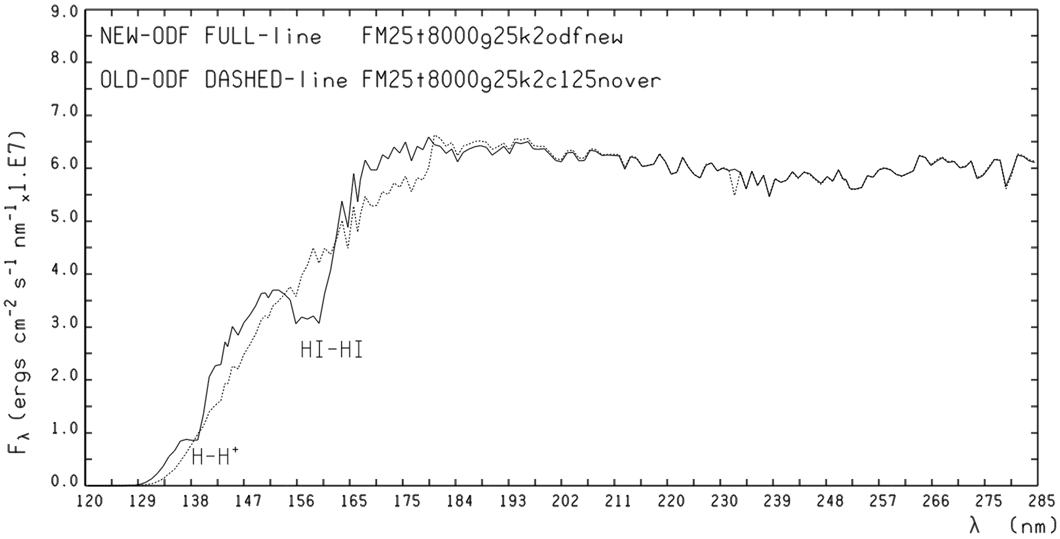

Figure 1. Comparison of the ultraviolet flux from the old-ODF model (thin dashed line) and the new-ODF model (thick full line) with parameters $T_{\rm eff}$=8000 K, logg=2.5, [M/H]=−2.5, ξ=2.0 km s^{-1}

New-ODFs are computed on an Alpha Digital Personal Workstation running OPEN VMS using the codes XNFDF and DFSYNTHE. The XNFDF code pretabulates number densities and continua opacities. The DFSYNTHE code computes a line opacity spectrum for each T,P_{gas} couple from 89.7 Å to 100000 Å at 500000 resolution. Line opacities are then sorted in the same wavelength intervals as in the Kurucz (1990) ODFs.

4. The New Grids and Future Work

New full grids of model atmospheres computed up to now are those for:

[M/H]=0.0, −0.5, −0.5a, −1.0, −1.5 and ξ=2 km s^{-1}

where "a" means that the abundances of the α elements O, Ne, Mg, Si, S, Ar, Ca, and Ti are enhanced by +0.4 dex over the solar or solar-scaled abundances.

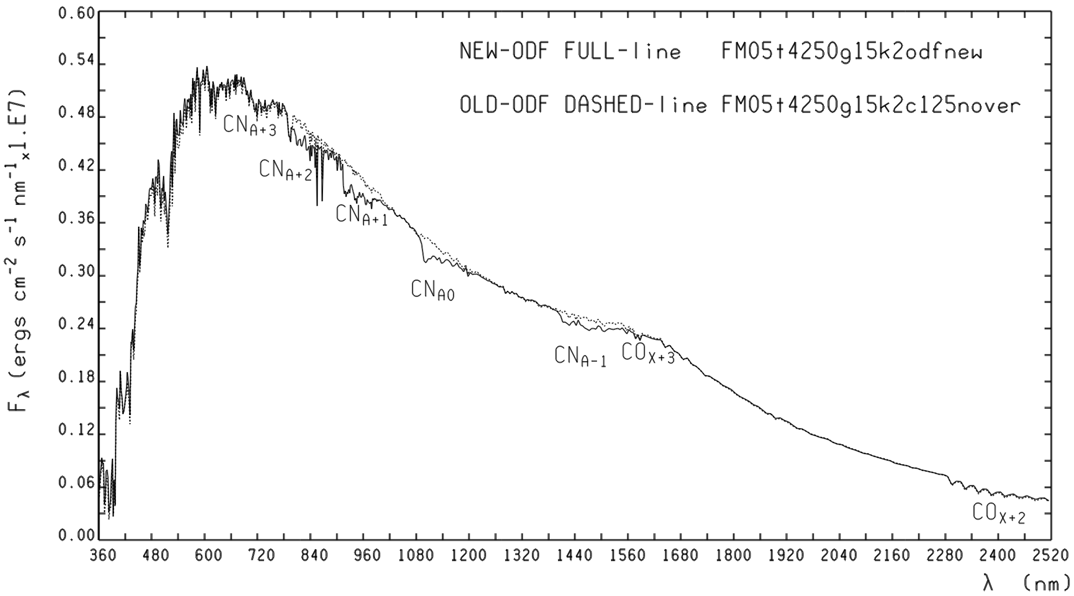

Figure 2. Comparison of fluxes from the old-ODF model (thin dashed line) and the new-ODF model (thick full line) with parameters T_{eff}=4250 K, logg=1.5, [M/H]=−0.5, ξ=2.0 km s^{-1}. The bands of CN and CO are indicated in the figure.

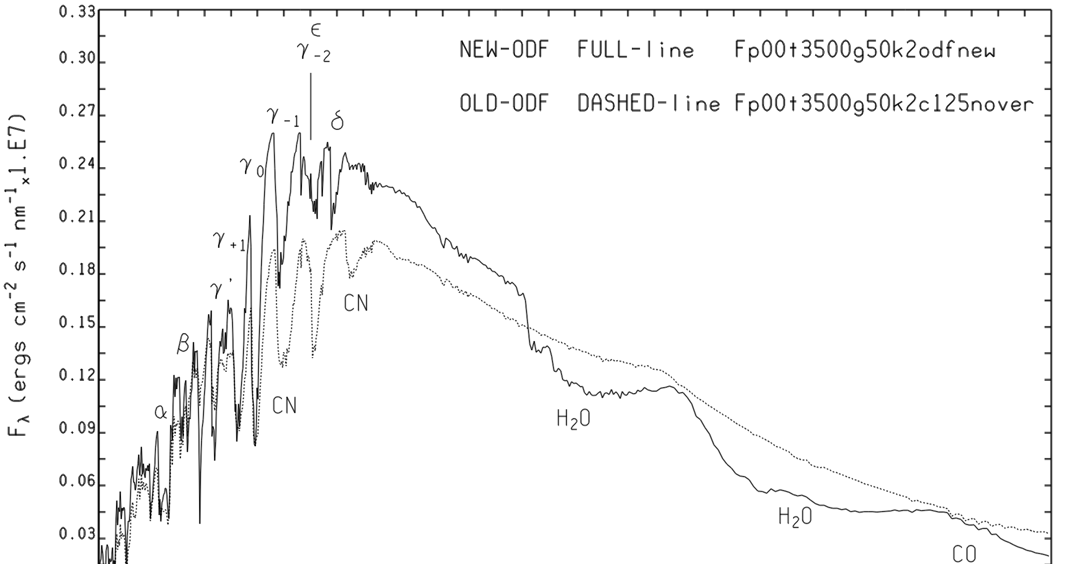

Figure 3. Comparison of fluxes from the old-ODF model (thin dashed line) and the new-ODF model (thick full line) with parameters T_{eff}=3500 K, logg=5.0, [M/H]=0.0, ξ=2.0 km s^{-1}. The bands of TiO, CN, H_2O, and CO are indicated in the figure.

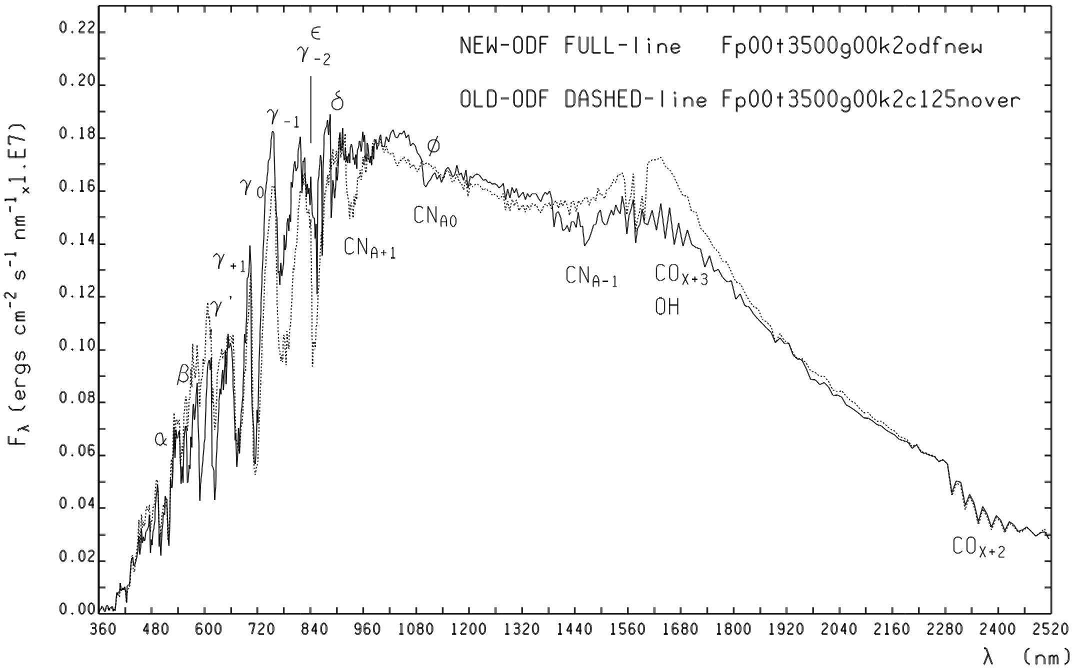

Figure 4. Comparison of fluxes from the old-ODF model (thin dashed line) and the new-ODF model (thick full line) with parameters $T_{\rm eff}$=3500 K, logg=0.0, [M/H]=0.0, ξ=2.0 km s^{-1}. The bands of TiO, CN, OH, and CO are indicated in the figure.

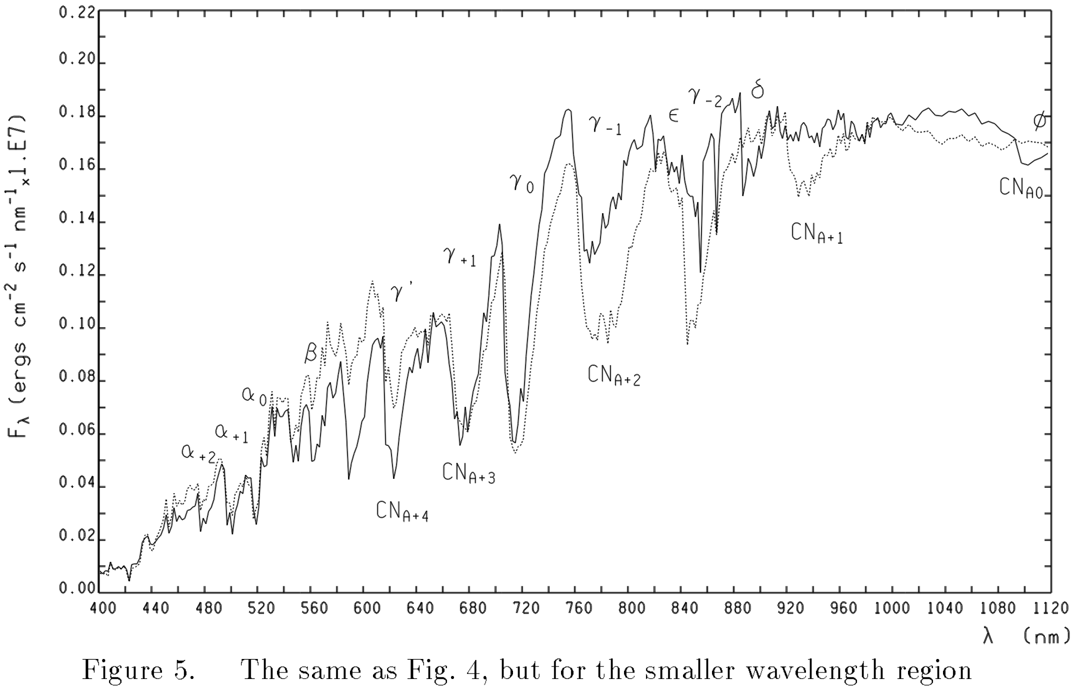

Figure 5. The same as Fig. 4, but for the smaller wavelength region 400-1120 nm plotted on a larger wavelength scale.

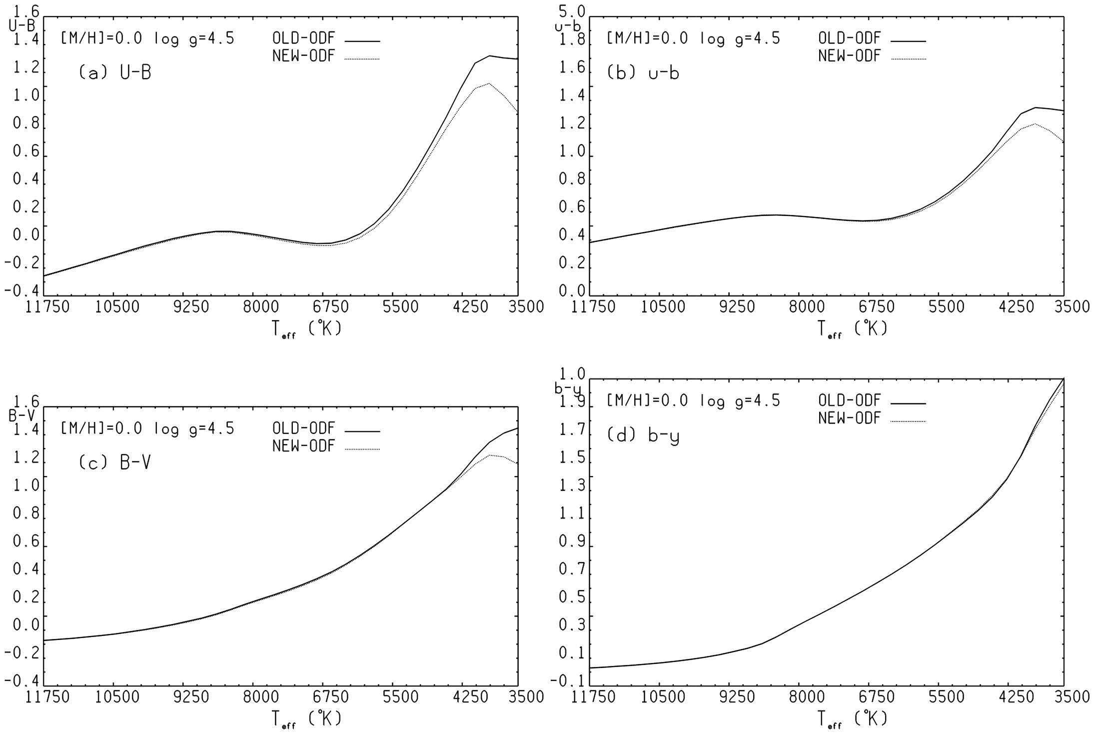

Figure 6. $T_{\rm eff}$-color relations for logg=4.5 and [M/H]=0.0 when old-ODF models (thick line) and new-ODF models (thin line) are used: (a) for U−B; (b) for u−b; (c) for B−V; (d) for b−y.

Together with the models we have computed corresponding grids of fluxes and color indices in the UBV and RIJKL Johnson system, in the VRI Cousins system, and in the uvby Strömgren system. The new grids are available at http://kurucz.harvard.edu/grids/gridxxxodfnew.

Small new-ODF grids for a few values of $T_{\rm eff}$ and logg have been also computed for [M/H]= −1.5a, −2.0, −2.0a, −2.5, −2.5a, and −3.0a (Castelli & Cacciari, 2001). We plan to extend these small grids to all the models listed in Table 1. In addition to models and fluxes computed for ξ=2 km s^{-1} we plan to compute models and fluxes for ξ=0, 1, 4, and 8 km s^{-1}. Color indices in several photometric systems will be also computed.

5. Comparison between Old and New Models

Preliminary comparisons of energy distributions have shown that the different solar abundances do not affect the models very much. In fact, the differences between old-ODF and new-ODF models are significant only when additional absorptions introduced in the new-ODFs play an important role.

Remarkable differences which increase with decreasing gravity and/or metallicity can be observed in the 1250-2000 Å region for $T_{\rm eff}$ between 9000 K and 7000 K. They are mostly due to the H I-H$^+$ and H I-H I quasi-molecular absorptions. Fig. 1 shows the energy distributions from old-ODF and new-ODF models for T_{eff}=8000 K, logg=2.5, [M/H]=−2.5, ξ=2 km s^{-1}.

The new TiO line list, the addition of H_2O lines and some improvements in the molecular data have greatly modified the energy distributions of models cooler than 4500 K. Examples are given in Figs. 2, 3, 4, and 5. Figure 5 shows in more detail the TiO and CN absorptions in the range 4000-11200 Å for the model T_{eff}=3500 K, logg=0.0, [M/H]=0.0, ξ=2 km s^{-1}.

Color indices U-B and u-b from new-ODF models are redder than the indices from the old-ODF models for T_{eff}<6500 K (Fig. 6a,b). The difference increases with decreasing T_{eff}. For instance, the difference for U−B amounts to 75 K when the model T_{eff}=5750 K, logg=4.5, [M/H]=0.0, ξ=2 km s^{-1} is considered.

Both (B-V) and (b-y) from new-ODFs are redder than those from old-ODFs for T_{eff}<4500 K, but the differences for (b-y) are almost negligible (Fig. 6c,d).

References

Allard, N.F., Drira, I., Gerbaldi, M., Kielkopf, J., & Spieldfield, A.,1998, A&A, 335, 1124

Anders, A., & Grevesse, N., 1989, Geochim. Cosmochim. Acta, 53, 197

Castelli, F., & Cacciari, C., 2001, A&A, 380, 630

Castelli, F., Gratton, R. G., & Kurucz, R. L., 1997, A&A, 318, 841

Castelli, F., & Kurucz, R. L., 2001, A&A, 372, 260

Grevesse, N., & Sauval, A. J., 1998, Space Sci. Rev., 85, 161

Holweger, H., Kock, M., & Bard, A., 1995, A&A, 296, 233

Kurucz, R. L., 1990, "Stellar Atmospheres: Beyond Classical Models", NATO Asi Ser., ed. L. Crivellari et al.,441

Kurucz, R. L.,1993,"Diatomic Molecular Data for Opacity Calculations", CD-ROM No 15

Kurucz, R. L., 1999a, "TiO Linelist from Schwenke (1998)", CD-ROM No 24

Kurucz, R. L., 1999b, "H_2O Linelist from Partridge and Schwenke (1997), no IDs", CD-ROM No 26

Partridge, H., & Schwenke, D. W., 1997, J. Chem. Phys., 106, 4618

Schwenke, D. W., 1998, Faraday Discuss., 109, 321