

# New extended atomic data in cool star model atmospheres

## Using Kurucz's new iron data in MAFAGS-OS models

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### ABSTRACT

*Context.* Cool star model atmospheres are a common tool for the investigation of stellar masses, ages and elemental abundance composition. Theoretical atmospheric models strongly depend on the atomic data used when calculating them.

*Aims.* We present the changes in flux and temperature stratification when changing from iron data computed by R.L. Kurucz in the mid 90s to the Kurucz 2009 iron computations.

*Methods.* MAFAGS-OS opacity sampling atmospheres were recomputed with Kurucz 2009 iron atomic data as implemented in the VALD database by Ryabchikova. Temperature stratification and emergent flux distribution of the new version, called MAFAGS-OS9, is compared to the former version and to solar flux measurements.

*Results.* Using the Kurucz line lists converted into the VALD format and new bound-free opacities for Mg I and Al I leads to changes in the solar temperature stratification by not more than 28 K. At the same time, the calculated solar flux distribution shows significantly better agreement between observations and theoretical solar models.

These changes in the temperature stratification of the corresponding models are small, but nevertheless of a magnitude that affects stellar parameter determinations and abundance analysis.

**Key words.** atomic data – Sun: abundances – stars: abundances – stars: atmospheres – stars: fundamental parameters – stars: late-type

## 1. Introduction

*Theoretical model atmospheres* are the most basic tool in the investigation of stellar parameters such as temperature, mass, age and of the element abundances present in stellar atmospheres. Thus the accuracy in determining all these stellar properties strongly depends on the accuracy and reliability of the underlying stellar atmosphere.

Many studies based on model atmospheres have shown the usefulness of model atmospheres for stellar parameter and abundance work. The work of Fuhrmann and colleagues (Fuhrmann 1998, 1999, 2002, 2004, 2008) on nearby stars of the galactic disk and halo might serve as an example of the validity of this approach. While Fuhrmann stays with the assumption of local thermal equilibrium (LTE), many precision studies of element abundances in cool stars remove this simplification and calculate element abundances based on full radiative and collisional equilibria (Non-LTE). For examples, see e.g. Mashonkina et al. (2008b,a), Shi et al. (2008) and Mashonkina et al. (2009).

For basic work on stellar parameters, that also enters the abundance analysis via the selection of the proper model, Megessier (1998), Castelli & Kurucz (1994), Castelli (1999), Grupp (2004b) and Grupp & Mashonkina (2008) show the

influence of different model atmospheres on various stellar parameter determination methods.

As a basic ingredient, bound-bound and bound-free atomic processes dominate the absorption properties of late type stellar atmospheres over a wide spectral range. Taking into account as complete as possible datasets for these major opacity sources is shown to be vital for accurate stellar parameter and abundance analysis work.

## 2. The model atmosphere code

Our study is based on the MAFAGS-OS theoretical model atmosphere code described by Grupp (2004a). Based on the ODF version of T. Gehren in the reprogrammed version of Reile (1987), this code relies on the following basic assumptions:

- Plane-parallel 1D geometry;
- chemical homogeneity throughout the atmosphere;
- hydrostatic equilibrium;
- convection is treated according to the formalism of Canuto & Mazzitelli (1991,1992);
- no chromosphere or corona;

- local thermal equilibrium;
- flux conservation throughout all 80 layers.

While these assumptions might break down for hot stars, stars with very extended atmospheres and the coolest stars, they are valid for stars in the range of  $T_{\text{eff}} \approx 4000\text{--}15\,000\text{ K}$  and for gravities from the main sequence down to  $\log(g) \approx 0$ .

### 3. Atomic data

The main target of this study is to investigate the effect of the new Kurucz iron line data on models and energy distributions. These data were compiled for us in a private data extraction run using the VALD (Kupka et al. 1999) database in January 2009 by Tanya Ryabchikova. This private extraction run was performed including predicted levels in all elements of the iron group.

#### 3.1. Old and new line list

Our new line list was compiled based on the abovementioned data extraction of VALD and includes the latest Fe I to III data of Kurucz (2009), taking into account observed and predicted transitions for each ion. These new calculations for iron included additional laboratory levels and more configurations than earlier work. Thus, the number of lines connecting the levels greatly increased. The line list are completed for the rest of the iron group using observed **and** predicted levels of Kurucz (1994a,c,b). Both the new data of iron *and* the data for the rest of the iron group elements from the stated Kurucz CD-roms is incorporated in the VALD database used for data extraction by Tanya Ryabchikova. All lines were processed using the data extraction algorithms of VALD (Kupka et al. 1999).

These data replace older data compiled in 1998 from Kurucz (1994a,c,b). For the old line lists lines between both observed and predicted levels have been extract making use of the files GFxxyy.GAM and GFxxyy.LIN where xx stands for the atomic numbers 20 through 28 and yy codes the ionisation states 00, 01 and 02. We used our own reduction software adopted from the software delivered with the CDs to process these files.

For the non iron group elements, Kurucz & Bell (1995) data were used in the old line list. Kurucz & Bell (1995) data was also included in the new list, but also its continuous updates incorporated in VALD. For detailed references to the new list see Kupka et al. (1999) and the compilations on the VALD Internet platform<sup>1</sup>. Both lists – old and new – contain diatomic molecules taken from Kurucz (1993, 1999).

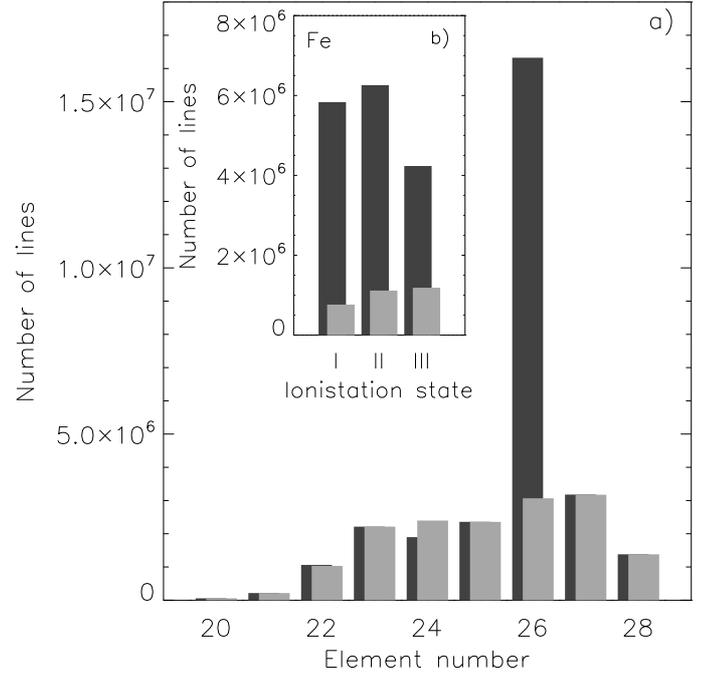
Figure 1a) shows the number of lines in the final list for the iron group elements. The enormous increase of iron lines is obvious. Small deviations in the number of Cr lines are due to the fact that in the old list, Cr lines had been included both below 500 Å and above 100 000 Å. These regions are unimportant for the solar line blending and the bug has been corrected in the new version of the line list.

The number of lines for the non iron group elements Li through Te is shown in Fig. 2. It becomes obvious that there are few changes for all elements but iron between both lists.

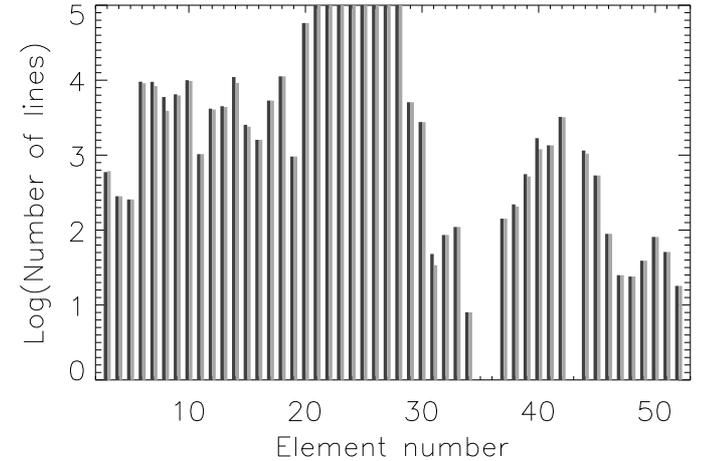
#### 3.2. Changes in continuous opacities

Another change of atomic data with respect to the 2004 model is the inclusion of TOPBASE (Cunto & Mendoza 1992) bound-free cross sections for AlI (Mendoza et al. 1995) and MgI

<sup>1</sup> <http://vald.astro.univie.ac.at/>



**Fig. 1.** Number of lines for iron group elements in new (black) and old (grey) MAFAGS-OS line lists. **a)** For the elements Ca through Ni, sum of ionization states I, II and III. **b)** For the first three ionization states of Fe.

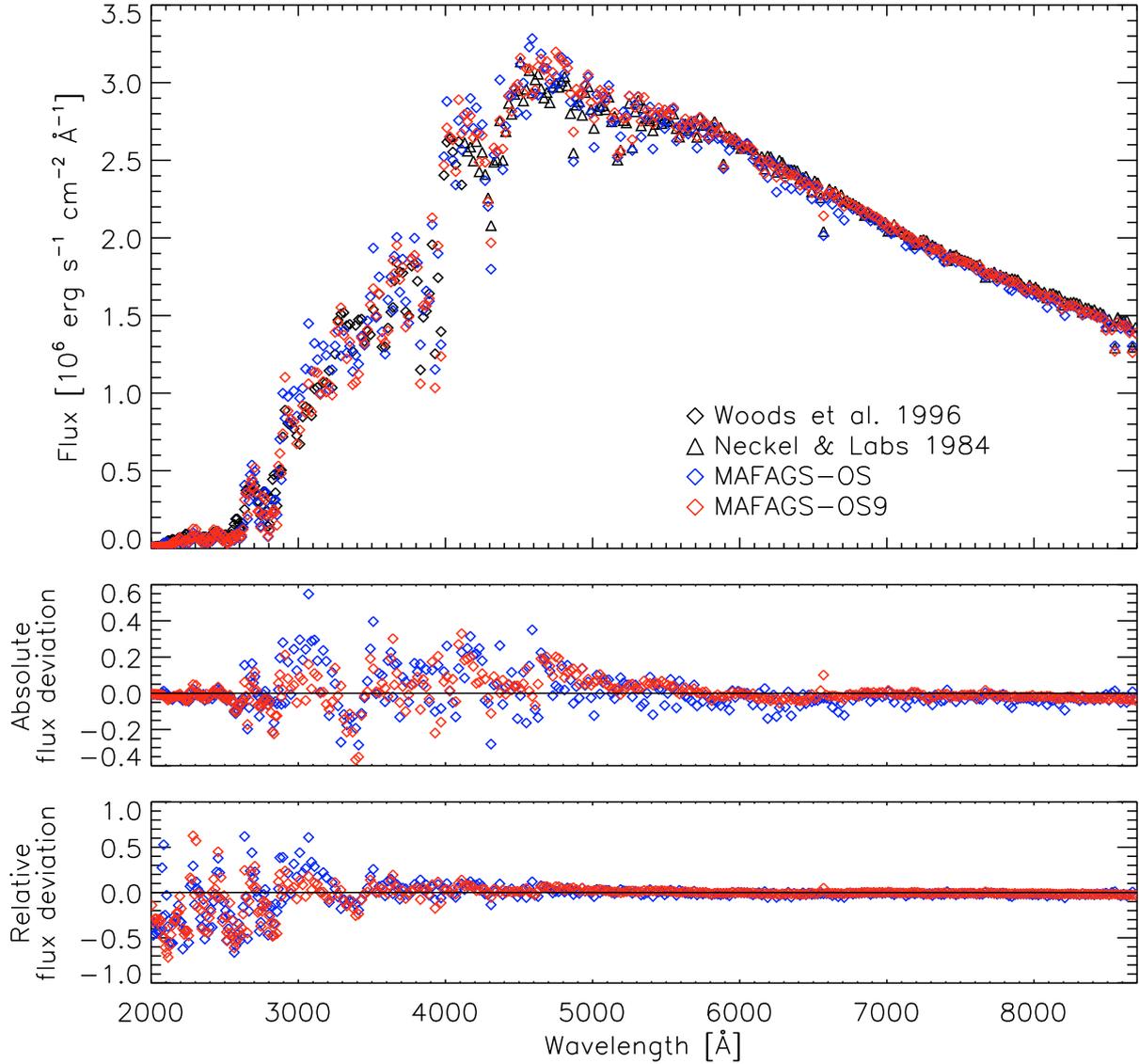


**Fig. 2.** Number of lines for the elements 2–52 on logarithmic scale. Color coding is the same as in Fig. 1.

(Butler et al. 1990). Old and new models make use of Bautista (1997) ionization cross sections for Fe I (See Fig. 4).

#### 3.3. Line selection

Our model considers the ionization states one, two and three and runs with  $\approx 86\,000$  wavelength points between 500 Å and 850 000 Å. Table 1 shows the number of bound-bound transitions in the new and old line-list together with the number of lines that were selected by the code to sample our standard solar model opacities (For a description of the selection criteria see Grupp 2004a). The number of selected lines corresponds to our standard solar model. Both line lists contain additional 4 247 857 lines related to transitions in diatomic molecules.



**Fig. 3.** Comparison of observed (black) and model solar flux for the old (blue) and new (red) solar models. Observations are taken from Neckel & Labs (1984) for the spectral range above 3300 Å and from Neckel & Labs (1984) for the near UV region below 3300 Å. *Top panel:* Direct comparison of solar flux data. *Mid panel:* Deviation of the models from the measured solar flux in absolute values. *Bottom panel:* Deviation of the models from the measured solar flux in relative values.

**Table 1.** Data for the new and old atomic linelist.

List	Total number of atomic lines	Number of selected lines for sampling
1998	16 012 015	322 040
2009	35 352 145	621 406

#### 4. Solar flux and temperature structure

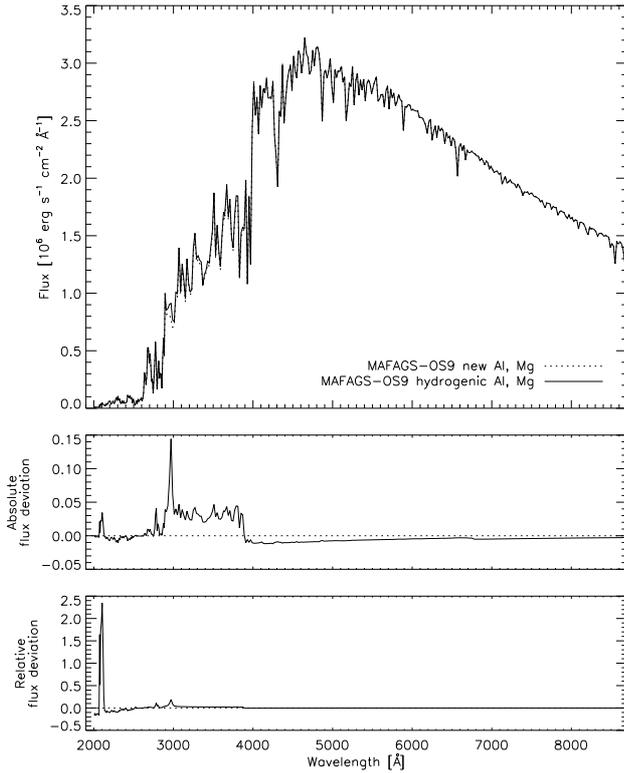
Figure 3 shows the comparison of the old and new models with observed solar flux data from Neckel & Labs (1984) and Woods et al. (1996). Despite remaining inconsistencies in the wavelength range blueward of 5000 Å, it is obvious that the model computed using the new iron data shows both less scatter and better absolute agreement with observed quantities.

Nevertheless, the region between 3000 Å and 5000 Å shows remaining shortcomings of about  $\pm 10\%$  in flux, that reach  $\pm 20\%$

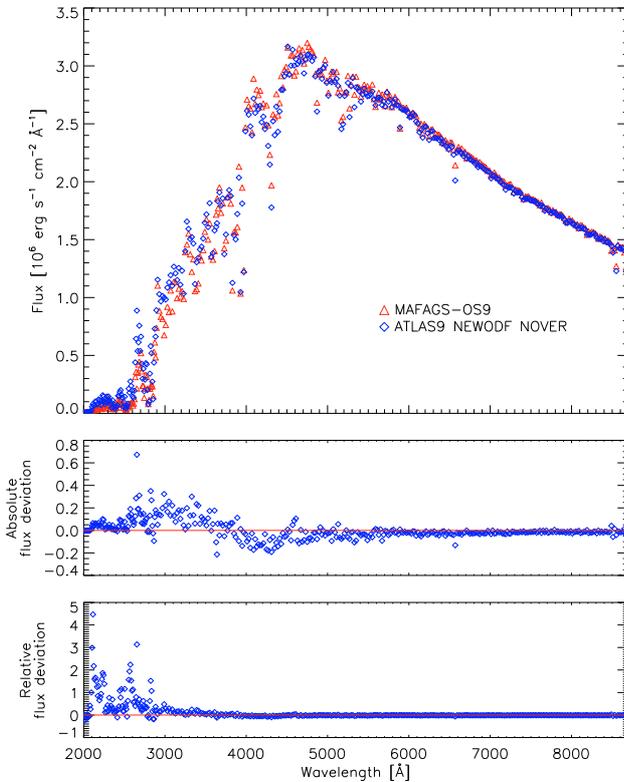
at some points. These discrepancies and the slight underestimation of the solar flux in the very scatter-dominated region below 3000 Å are present in both datasets. Still, the computations with the new iron data are closer to observation even in those regions.

The flux changes are mainly due to the new data for iron. The influence of new Al I (Mendoza et al. 1995) and Mg I (Butler et al. 1990) bound-free cross sections is shown in Fig. 4. The flux differences are small in the visible wavelength range and contribute only to some larger deviations in the near ultraviolet region. These changes in the UV do not significantly affect the atmosphere stratification, but they can be important for non-LTE calculations, as the departure coefficients of levels with transitions in the UV might well depend strongly on photon processes in this region (see e.g. Shi et al. 2008). The rest of the input atomic data concerning bound-free transitions is unchanged with respect to the “old” model.

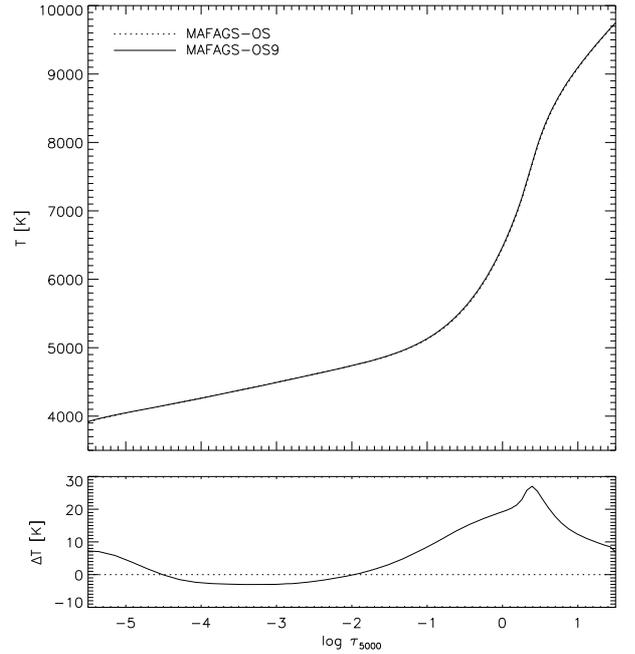
Figure 5 shows the comparison of our latest model to the ATLAS9 model of Castelli & Kurucz (2003). The selected



**Fig. 4.** Comparison of MAFAGS-OS model atmospheres using “old” bound free data for AlI and MgI and recent detailed calculations of Mendoza et al. (1995) and Butler et al. (1990).



**Fig. 5.** Comparison of the new MAFAGS-OS model (red) solar atmosphere with the recent ATLAS model with NewODF and the overshooting option switched off (blue). *Top panel:* Direct comparison of solar flux data. *Mid panel:* Deviation of the ATLAS model from the MAFAGS-OS9 model in absolute values. *Bottom panel:* Deviation of the ATLAS model from the MAFAGS-OS9 model in relative values.



**Fig. 6.** Comparison of the temperature structures of the old (dashed line) and the new (full line) model.

ATLAS model is the ASUNODFNEW model<sup>2</sup> computed with new ODFs and the overshooting option turned off.

The ATLAS model chosen uses the new ODF tables of Kurucz and has the overshooting option turned off. While both models show similar flux structure in the red and near IR region, with the ATLAS model having slightly less flux here, they significantly differ in the UV to green part. This leads to the ATLAS model underestimating the observed solar flux in the red and IR by  $\approx 5\%$  at  $9000 \text{ \AA}$  and to a good agreement between ATLAS and measured solar flux in the green spectral range. Looking at the picture as a whole, neither of the two versions fits the solar flux significantly better than the other, but both have good and not so good spectral regions. The difference between the models is quite likely to emerge from the lack of the new iron lines in the ATLAS9-NEWODFs and some different UV continuous opacity sources used in both models. In addition, the models use different formalisms to treat convection, which will also influence the overall flux distribution.

The changes in solar temperature structure due to the two different line lists are shown in Fig. 6. The overall effect is small, nevertheless changes of  $\approx 5\text{--}25 \text{ K}$  in the line forming regions will slightly affect line formation.

## 5. Discussion and conclusions

We have shown the influence of the new iron Kurucz data on the solar model and solar energy distribution. This new data shows significantly better agreement with the observed solar flux with respect to scatter and absolute values. Changing to the new data also slightly changes the solar temperature stratification. Therefore, the new data are shown to be a real improvement of the model and helps to better represent solar atmospheric observables.

Remaining discrepancies are mainly found to be in the short wavelength part below the solar flux maximum. They might

<sup>2</sup> <http://wwwuser.oat.ts.astro.it/castelli/grids.html>

be related to missing or inaccurate data in the resonances of strong bound-free absorbers or slight misplacements of the center wavelengths of strong lines.

Some major implications of the improved representation of the stellar flux are:

- changes in synthetic colors and line indices;
- changes in abundance analysis due to changes in temperature stratification of the model atmosphere;
- changes in non-LTE analysis due to changes in the UV fluxes that determine photo-ionization processes emerging from transitions in this spectral region;
- changes in stellar parameters if they rely on synthetic colors, line indices or individual lines;
- the lower scatter also allows better automatic comparison of synthetic and observed spectral data. A work field that shows increasing importance with large survey projects such as SDSS (York et al. 2000), LAMOST (Su et al. 1998) and GAIA (Perryman et al. 2001) on the way. For those projects the mere number of spectra acquired does not allow for manual inspection, requiring automated procedures of spectral analysis.

Although the impact on the temperature stratification is relatively small, changing to the new data significantly changes the flux of the solar model, placing it into better agreement with observations.

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