IMPROVED RESULTS FOR EQUILIBRIUM ABUNDANCES FROM DIFFUSION CALCULATIONS

S.L SCHUH, S. DREIZLER AND J.L. DEETJEN
Institut für Astronomie und Astrophysik, Universität Tübingen, Sand 1, D–72076, Tübingen, Germany
email: schuh@, dreizler@, deetjen@astro.uni-tuebingen.de

1. Previous work

Due to high surface gravities, element segregation by gravitational settling is of great importance in white dwarf atmospheres. In hot white dwarfs, as in other hot stars, radiative levitation can efficiently counteract the downward diffusion of heavy elements, and the interplay between these forces governs the atmospheric chemical composition. Incorporating the competition of these processes into stellar atmosphere model calculations provides predictions for the vertical stratification and absolute abundances of metals, and is therefore an important task. An overview of the work done in the field of such diffusion calculations, with a focus on white dwarfs, is given in a recent review (Dreizler and Schuh, 2003), which contains the relevant references to both the articles where these ideas where first mentioned as well as to very recent papers which describe current implementations and their applications. Within these latest approaches, the equilibrium formulation (Chayer *et al.*, 1995) is of special interest since it permits a relatively simple description of the balance between gravitational settling and radiative levitation. It therefore allows a self-consistent solution of the chemical stratification within state-of-the-art, fully line blanketed non-LTE stellar atmospheres with many elements, incorporated via detailed model atoms (Dreizler, 1999).

Applications to hot DA white dwarfs have shown that synthetic spectra derived from such chemically stratified models can quantitativly describe the EUV spectra observed from these objects (Dreizler and Wolff, 1999; Schuh *et al.*, 2002). The abundance calculations as used for the analysis of EUVE spectra have since been extended to a larger model grid and are currently being prepared for publication. Abundance predictions will be tabulated for a large range of optical depths for models covering the range of $38{,}000\,\mathrm{K} < T_{\mathrm{eff}} < 71{,}000\,\mathrm{K}$ and $7.2 < \log g < 8.4$.

But while superior to homogeneous models in the EUV range, the stratified models have so far not been elaborate enough to truthfully reproduce all of the very abundance-sensitive metal lines in the UV spectral range simultaneously. Using the above-mentioned stratification profiles, Chayer *et al.* (these proceedings), for example, succeed in simultaneously reproducing the observed oxygen lines of different ionization stages in FUSE and HST STIS spectra of GD 984, RE J1032+532 and WD 2152-548 but fail to obtain similarly well-fitting results for nitrogen.

To investigate whether these discrepancies are mostly due to limitations in the way the models have been set up, or whether they arise mainly from additional, or different, physical processes happening in the stellar atmosphere but not incorporated in the modelling process, tests for improvements of the models by Schuh *et al.* (2002) have been carried out and are being presented here.

2. Improvements

The changes with respect to the old models fall into two categories: A generally more efficient stellar atmosphere code in conjunction with a new implementation of the opacity sampling method for the iron group elements, and a different set-up of the model atmosphere calculations by extending them to include more elements than previously used.

The advances in the formulation of the code are as detailed in Dreizler (2002), while the principles underlying the opacity sampling for iron group elements used can be found in Rauch and Deetjen (2002). In both cases the methods are not radically new with respect to comparable previous calculations, but the combined effect of their changed numerics leads to the differences in predicted equilibrium abundances as shown in Fig. 1. These results are for a model with $T_{\rm eff}$ =56,000 K and $\log g$ =5.6; compare the full and the dotted line to estimate the combined impact of the changes in the code and the method of preparation of atomic input data.

One important reason to switch to the modernised opacity sampling offered by IrOnIc (Rauch and Deetjen, 2002) was the obvious need to include more than just a handful of the most important elements. Due to their sigificant opacities, the missing iron group elements from Ca to Ni were additionally taken into account first, in a continued effort to push the models to a more sophisticated level. This addition leads to changes in the structure of the model that finally result in new abundance profiles as illustrated by the dashed lines, also in Fig. 1, for the elements common to all three models, and to abundance predictions for the add-on elements as shown in the last panel of this figure.

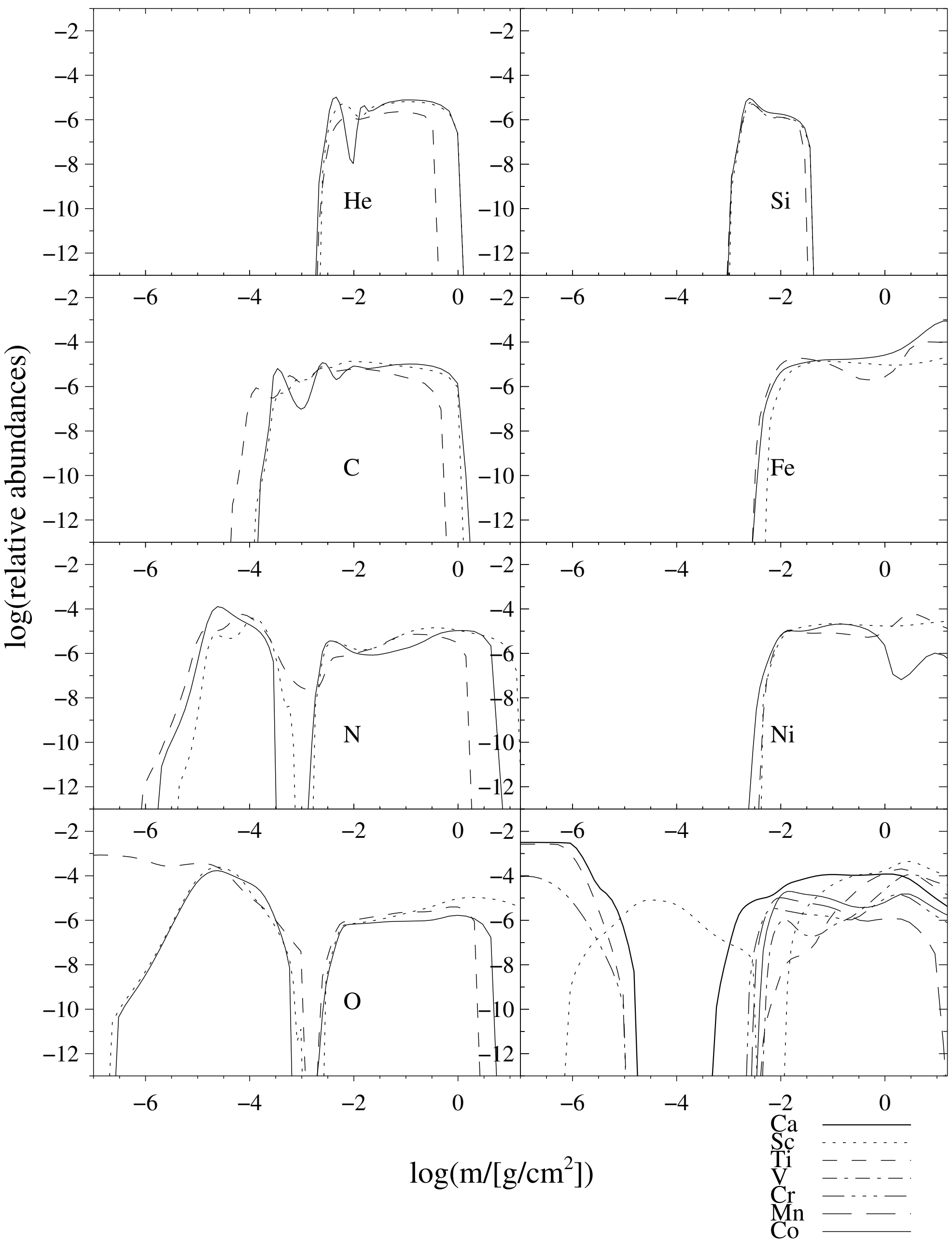

Figure 1. The first seven panels show the abundance stratifications predicted by a model calculated with the old code and containing less elements (full line), and by a model calculated with the new atmosphere and sampling codes but containing the same resticted number of elements (dotted line), in comparison to the ones predicted by a model calculated with the new codes and containing more elements (dashed line), with the respective element name indicated directly in the appropriate panel. The last panel shows the predictions of that last new model for the additional elements included there, with a code to the individual species printed on the lower right hand side.

3. Discussion

While for all elements that are common to both models the shapes of the equilibrium profiles are fairly similar in all cases, the absolute abundances in numbers at a given depth point can differ substantially, mainly due to the steep gradients involved. It therefore will depend heavily on the formation region of any given line how much its shape will be affected.

The impact of the extention to the full iron group elements is explored next. The main differences in the atmospheric structure are caused by two of the newly added elements that display surprisingly large equilibrium abundance values: Ca and Ti. Both additionally hit the artificially introduced upper limits of a mass fraction of 10^{-2} in the outmost parts of the atmosphere. Such high abundances are not corrobated by observations, see Holberg (these proceedings).

It is one possibilty to interpret the outward increase as the sign of a selective wind – prohibited by the static character of the model – which might in principle help to decrease the excessive overall abundance of the affected elements. A more elegant interpretation seems to be availabe by adopting results from Fontaine and Chayer (1997) for He in sdB stars, who included weak mass loss in their models and find that equilibrium profiles tend to be maintained in the atmosphere until the reservoir is emptied from bottom up, at which point the element quickly disappears. Using equilibrium profiles when an element is obviously present in a specific object, and completely discarding it otherwise, may therefore be an acceptable choice.

Acknowledgements

This work is supported by the Deutsche Forschungsgemeinschaft under grants DR 281/13-1 and 13-2.

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