PHYSICAL INPUT FOR THE DETERMINATION OF STELLAR ABUNDANCES

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ABSTRACT. The fundamental parameters and the physical modelling and data used in the analysis of high-resolution high S/N spectra of stars are discussed. Particular emphasis is led on recent developments in these respects and the importance of further improvements is stressed.

1. INTRODUCTION

For weak stellar spectral line the equivalent width is approximately proportional to the chemical abundance of the element in question and the oscillator strength. The factor of proportionality is, however, dependent on stellar parameters, atmospheric structure and other data and processes that directly affect the line formation.

The equivalent widths can today, in high S/N spectroscopy at sufficient resolution, be measured with an accuracy of 10% or better. The f values can in many cases be determined with an even higher accuracy (cf. Huber's review in the present volume). Thus, one could hope that abundances could be estimeted with a corresponding accuracy. This is, in general, not possible; typical external errors in abundances are in good cases about 30%, and often greater than that. The reason for this is our lack of precise knowledge about the fundamental parameters, atmospheric structures and line formation. A clear-cut separation between the errors in chemical abundances caused by uncertainties in these different respects is rather artificial. In particular, the approximation of the atmospheric structures by a grid of standard model atmospheres also affects the choice of fundamental parameters (if made spectroscopically or photometrically

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by comparisons with model spectra or colours) and the data and approximations involved in the line calculation may affect both models and choices of fundamental parameters. Moreover, the choice of f values may also be affected by these circumstances; namely, if the f values are obtained in a differential analysis with respect to some other star, such as the Sun. Nevertheless, we shall here follow a schematic approach and in separate sections discuss the abundance effects of errors in fundamental parameters, in model atmospheres and in synthetic spectra, respectively. The vital problem of the uncertainties in f values is not treated here; the reader is referred to Huber's paper in the present volume for a discussion of those.

2. FUNDAMENTAL PARAMETERS

The determination of fundamental parameters for stars was discussed at IAU Symposium 111 (Hayes et al., 1985); for an overview of the use of models for deriving such parameters, see Gustafsson and Jørgensen (1985). Here, I shall only list some recent developments and comment on the abundance errors resulting from errors in the parameters.

A number of recent studies have contributed to a significantly increased accuracy in effective-temperature determinations. Among these studies are the lunar-occultation measurements of red giants by Ridgway and collaborators (see Schmidtke et al. 1986, and references given there), the systematic application of the infrared-flux method of Blackwell and Shallis (1977) to different types of stars (early-type stars : Underhill et al. 1979, Underhill 1982, Remie and Lamers 1982; solar-type dwarfs: Saxner and Hammarbäck 1985, Magain 1987; G-K giants: Bell and Gustafsson 1987; M and C giants: Tsuji 1981 a and b), the use of line spectra and ionization equilibria, supported by non-LTE calculations for O-stars by Kudritzki and collaborators (e.g. Kudritzki et al. 1983) and the use of Balmer-line profiles for solar-type stars by Cayrel et al. (1985). With optimal methods the temperatures are now obtainable with an accuracy of about 2-3% for early-type stars and even better for solar-type stars. For the O-type stars and for the coolest stars, of spectral type M and N, the errors are, however, about two times greater.

Which are the consequences of the errors in effective temperatures on the abundance analyses? Very schematically, we find from a glance at recent analyses that the temperature errors lead to errors in the interval 0.00 - 0.10 dex in absolute abundances. Exceptions from this are the CNO elements in early-type stars and in the M stars, where the errors may amount to two times as much or even more than that (cf., e.g., Smith and Lambert, 1985). Note also the more indirect coupling between temperature errors and errors in log g, which may in turn cause severe errors in abundances; examples thereof are provided by the O and B-type stars, and also by cooler stars if molecular lines with their great temperature sensitivity are being used for gravity determination (cf. Bell et al. 1985).

The surface gravities may be determined from Balmer lines for early spectral types, from the Balmer discontinuity (e.g. measured by the Strömgren δc_1 index) for late A and F-type stars, from pressure-broadened lines for solar-type dwarfs and sub-giants (cf. Edvardsson 1987) and from estimated absolute bolometric magnitudes (and guessed masses) for cool giants. (The non-LTE overionization effects could lead to severe systematic errors in determinations based on ionization equilibria, see below.) Typical errors in current gravity estimates amount to 0.1 - 0.2 dex for early-type stars, 0.3 dex for G-K-type giants and 0.5 dex for cooler giants. This corresponds to typical errors in abundances of 0.00 - 0.10 dex; exceptions are the CNO elements for red giants where the errors are about 0.2 dex, and the metals for late K, M and N giants where the errors range in the interval 0.1 - 0.2 dex.

Also errors or uncertainties in the chemical abundances themselves cause errors in the abundance analysis, notably in studies where the analysis is confined to particular elements or is not brought to complete self-consistency. This effect occurs through blanketing in the models, through blends or "veils" in the spectra and, for late-type stars, through the electron pressure which is determined by the abundance of metal ions and which in turn determines the continuum opacity. A typical uncertainty in the over-all metal abundance of 0.2 dex leads, however, to errors less than about 0.05 dex in the abundances for most elements. Exceptions are the CNO abundances, in particular in cool stars; an error in [Me/H] of 0.2 dex thus leads to typical errors in the CNO abundances of K and N stars of about 0.1 dex.

The effects of uncertainties in the microturbulence parameter for contemporary high-quality analyses of many elements in solar-type stars are minor since weak lines, the equivalent widths of which are little affected by microturbulence, may be measured. For certain elements, however, such as rare earths, only a few and often saturated lines are available, and the resulting abundances may be in error by 0.2 dex or so. For hot stars, with fewer suitable lines, the microturbulence uncertainties may be more problematic. Baschek et al. (1982) ascribe the dominating uncertainties in their analysis of an early subdwarf to the uncertainties in the microturbulence parameter. For cool stars these uncertainties may also have severe effects, since blends and veils of weak molecular lines make the use of saturated lines necessary in the analyses. E.g.,from Smith and Lambert (1985) we find that uncertainties in the microturbulence parameter of 1 km/s lead to errors in their determinations of carbon and nitrogen abundances for M giants of about 0.2 dex.

In conclusion we find that the total abundance uncertainties, due to errors in the fundamental parameters, amount to typically 0.1 dex for many metals in most types of stars. Exceptions are the O and B stars, as well as the M and N stars, where a realistic error is about twice as great. For the CNO elements in stars of spectral type late G, K, M or N the errors are about two times greater than those of metal abundances. In particular, the error in the nitrogen abundances amounts to typically 0.4 dex for the M and N stars, which mainly reflects the temperature sensitivity of the CN line strengths.

3. MODEL ATMOSPHERES

As regards the modelling of stellar atmospheres it is worth noting that, even within the frame-work of classical plane-parallel LTE models with mixing-length convection it is not certain that specification of the fundamental parameters discussed above leads to a unique model atmosphere. A bifurcation in the upper solar photosphere, currently ascribed to the surface cooling of CO (cf. Ayres and Testerman 1981, Ayres 1986, Kneer 1983, Muchmore and Ulmschneider 1985, Muchmore 1986) may well be reflected in double solutions of the classical problem (cf. in particular Nordlund, 1985). A similar effect, due to SiO, may exist for cooler stars (cf. Muchmore et al. 1987). Recently, we have shown that polyatomic opacities in the upper layers of carbon-star models may, under certain conditions, lead to drastically different solutions to the model-atmosphere problem (Eriksson, Gustafsson and Jørgensen, unpublished research).

Evidently, we have two kinds of uniqueness problems to worry about for classical models. As was mentioned above, models with the same sets of fundamental parameters may be quite different and give quite different spectra. On the other hand, models with different fundamental parameters may have almost identical spectra. The classical example of the latter case is the very difficult problem of simultaneously determining helium abundance and gravity in late-type spectra.

The groups still calculating grids of classical models work on refinements of the blanketing treatment and synthetic spectra by including still weaker atomic and molecular lines (cf. Kurucz 1985) as well as, for the cooler stars, polyatomic absorption (Eriksson et al. 1984, Jørgensen et al. 1985, 1987). The polyatomic line absorption, being non-correlated in frequency with the diatomic absorption at greater depths, leads to errors when the Opacity-Distribution Function Method is used, while the Opacity Sampling Method requires very many frequency points to a considerable cost in computing time (Ekberg et al. 1986). Thus, a new efficient and more reliable blanketing algorithm is needed for the coolest stars.

A vigorous activity now takes place in work on models where at least one or more of the classical basic assumptions have been relaxed. Some examples will be given here. For the early-type stars Anderson (1985), using his multi-frequency/multigray algorithm, and Werner (1986), using Scharmer's operator perturbation technique, extend the non-LTE models of Mihalas and Auer (1972) and Kudritzki and collaborators (Kudritzki 1979) to include blanketing from carbon and, in on-going work, from other heavy elements. The effects of departures from LTE on solar-type models are now possible to study (an early attempt was that of Saxner 1985) but still rather uncertain due to uncertain cross sections for inelastic collisions between hydrogen and metal atoms and uncertain uv-fluxes. The wind-blanketing for early-type stars is considered successfully (cf. Abbott and Hummer 1986, Bohannan 1987) and found to lead to significant T_{eff} revisions for O-type supergiants. Anelastic convection is solar-type stars, with consideration of inhomogeneities in 3D radiative transfer and overionization effects for iron, is simulated numerically by Nordlund (1984). These models reproduce observed line widths and asymmetries in a gratifying way (cf. Dravins 1988, and references quoted therein). Nordlund estimates a correction to the solar iron abundance, based on planeparallel models, of about a factor of two but stresses the great uncertainty in this estimate. Spherically symmmetric models for red giants and super-giants have been studied extensively by SchmidBurg, Scholz, Wehrse and collaborators (see Scholz 1985, and references cited therein). These models show very interesting coupling between extension and molecular formation which not only complicates the task of the spectroscopist but also enables the determination of stellar gravities and radii (and thus masses) independently. Recently, Bessell et al. (1987) have also attempted calculations of blanketed spherially symmetric Mira models with shocks.

What are the errors made when grids of classical model atmospheres are used in abundance analysis? One may attempt to answer this question by comparing analyses made with classical models to those made with models with partly improved physics. One may also compare analyses with grid models to those made with temperature structures tailored to exactly reproduce observed strong-line profiles or continuous fluxes for the star in question. (Such semi-empirical models were, e.g., discussed by Ruland et al.

1980 or Magain 1985). An example of such a study of effects of model errors is that by Gustafsson (1983), who discussed the uncertainties in current analyses of Pop. II stars. Studies where effects of model uncertainties on abundances have been investigated seem to lead to typical model errors in abundances of 0.1 - 0.2 dex. For the N stars Lambert et al. (1986) find characteristically 0.3 dex. One may fear that these estimates, being more or less ad hoc but always incomplete, are underestimates.

4. CALCULATION OF SPECTRA

Even if departures from LTE would not be important for the atmospheric structures of certain types of stars, they significantly affect the spectra of many elements. This has been recognized since long for the early spectral types - more recently evidence for non-LTE effects in late-type stars has been accumulated. Thus, Ruland et al. (1980) found significant inconsistencies for Pollux (K 0 III) in abundances of Fe, Ti and Cr, when derived from lines with different excitation energies. This effect has been confirmed by several others for red giants (e.g., Kovacs 1983, 1985) and similar effects were found by Steffen (1985) for Procyon (F5 IV-V) and by Magain (1988) for several elements in Pop. II dwarfs. In fact, it cannot be excluded that trends in relative abundances with changing [Fe/H] for metal-poor stars could be ascribed to these effects (cf. Gustafsson 1987, Magain 1988). Brown et al. (1983) traced an inconsistency in the Zr/Ti ratio of red giants, when derived from neutral atoms and ions, respectively. The effects have been interpreted as primarily due to over-ionization in combination with different depths of formation for lines of different excitation, and some have been at least qualitatively reproduced in statistical equlibrium calculations (Steenbock 1985); although these are highly uncertain as a result of uncertainties in collision cross sections, in particular from inelastic collisions with hydrogen atoms (see also the study of Li by Steenbock and Holweger 1984).

For the early-type stars a great number of theoretical studies of specific elements and ions have been made (among the more recent ones are the detailed studies of Fe, Mg and Ba in Vega, AO V, by Gigas 1986, 1987). Much work is, however, needed before all important aspects of the physics of line-formation has been properly included and all relevant elements and transitions have been treated in such studies. In particular, the electron collision cross sections and the photo-ionization cross sections need to be known with a higher accuracy.

A number of more trivial aspects of the calculation of spectra should be remembered. The identification of lines, of blending lines and of veiling lines across the lines of interest and/or overlying the "continuum regions" is vital, not the least for cooler stars. Here, there are many severe uncertainties. The proper consideration of hyperfine structure and isotopic shifts may cause revisions of abundances by almost one order of magnitude in certain cases (as compared with if the line-splitting is neglected). The line broadening is not properly understood for many lines of interest for high-precision spectroscopy. Dissociation energies for the molecules may be uncertain by embarrassing amounts; a well-known example is D_o^o(CN) which is uncertain by more than 0.1 eV, leading to errors in the nitrogen abundances for the coolest red giants by 50% or more (cf. Lambert et al. 1986).

5. CONCLUSIONS

Our schematic discussion leads to the following conclusions:
(1) Errors in the estimated fundamental parameters introduce abundance errors $\geqq$ 0.1 dex. The errors are greatest for stars of spectral type O and for M and N stars, and greater for supergiants than for giants and dwarfs.
(2) The errors in model atmospheres, when studied, are found to lead to errors in abundance determinations of about the same order of magnitude as those caused by fundamental parameter errors.[1]
(3) The departures from LTE, not treated properly as yet, may again lead to systematic errors of the same order of magnitude as those discussed above.
(4) For the analysis of certain types of stars (not the least cool stars) and certain chemical elements (not the least those represented by few spectral lines) uncertainties due to blends and veils, hfs, dissociation energies etc. may again cause uncertainties of the same order of magnitude.

From this one may conclude that
(I) it is important to improve the determinations of T_{eff} and log g for most stars if improved abundance estimates are wanted;
(III) it is important to improve the model atmospheres and the calculation of spectral lines further. This also requires the determination of a vast number of cross sections and other atomic and molecular quantities of importance.

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[1] cf. the so-called Robin effect: Errors difficult to estimate are generally not supposed to exceed those more easily estimated.

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One should note that high S/N spectroscopy at sufficient resolution offers vital support to the development of methods for accurate T_{eff} and log g determinations, as well as to the improvement of model atmospheres and spectrum calculations. This requires, however, that accurate comparisons between observed and calculated spectra are made, not only for the quick determination of abundances and other parameters but also for tracing inconsistencies and studying these further (e.g., as a function of stellar parameters). Evidently, the development of the efficient high S/N spectrometers puts such extra obligations on the shoulders of the observer if he/she wants to contribute to a development where the accuracy in equivalent widths and f values can be fully exploited in the abundance determinations.

Fortunately, since most error sources discussed above are systematic, a very high accuracy may be reached in spite of these errors in differential studies where ratios between abundances for different but similar elements, or abundance differences for different but similar stars, are being measured. Although this fact is almost a truism and often quoted and used, the extent of these cancellation effects has not been studied very much and the differential studies are not very often designed such that the cancellation is maximized. With the presently rapidly growing qualitative understanding of model errors, departures from LTE etc., and the widening of the accessible frequency region of stellar spectra, such "self-compensating" high precision methods for stellar quantitative spectral analysis could be further developed.

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DISCUSSION

LINSKY Your point concerning thermal bistability or multistability is very important and we need to determine empirically whether or not this perverse phenominon occurs in different classes of stars. One method for doing so is to check whether the abundances derived from molecular spectra agree with abundances derived from neutral and ionized species.

GUSTAFSSON I agree.

BECKMAN Could you please re-state your estimates of the numerical values of the uncertainties into abundance analyses of solar type stars by inhomogeneities and by non-LTE effects ?

GUSTAFSSON Nordlund's calculations suggest that the iron abundance of the Sun may be overestimated by 0.2 dex or even somewhat more, if plane-parallel models are used instead of his 3D models. This estimate must be regarded as crude and preliminary.

M. SPITE You said that the error on the abundances, due to the models, in Pop II stars is about 0.1-0.2.
Is the error the same for the dwarf stars and for the giant stars ?

GUSTAFSSON It is hard to judge, indeed. One would expect that analyses of Pop II dwarfs were more affected by uncertainties in convection than the giants are while the converse may be fine as regards departures from LTE. None of these statements is free from reservations, however. Thus, the brighter UV fluxes of the dwarfs (assumed to be hotter) may lead to more severe departures from LTE there, and the lower densities in the giants may enable the convection-generated inhomogeneities to survive to higher layers in spite of the fact that the convective instability sets in at greater depths.