PART I

INFLUENCE OF ABUNDANCES UPON STELLAR ATMOSPHERE CALCULATIONS

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Abstract. The basic equations for constructing a stellar atmosphere (hydrostatic equilibrium, flux constancy, radiative transfer, convective instability) are briefly summarized. While the parameters T_{eff} (effective temperature) and g (surface gravity) are directly contained in these equations, the element abundances ϵ_i enter only indirectly through the thermodynamic properties (such as electron pressure, entropy, ...) and the absorption and scattering coefficients of stellar matter.

The equation of state, convection, the effects of the absorption coefficients (particularly of line absorption) on the temperature stratification, and the role of velocity fields (microturbulence) are discussed in some detail, emphasizing their dependence on the abundances.

From a given model atmosphere, a 'theoretical spectrum' (colours, bolometric correction, line strengths etc.) can be calculated. The (relative) fluxes emerging at the surface are essentially determined by the temperature gradient and the absorption coefficients at the frequencies under consideration. The basic goal of quantitative classification, however, is the inverse problem, namely to deduce the stellar parameters from selected observed spectral criteria. Aspects relevant to this problem such as the question of uniqueness and the occurrence of possible systematic errors (even when using differential analysis techniques) are briefly sketched and illustrated by some examples.

1. Introduction

Spectral classification is based on the observation of selected spectral criteria (such as intensity ratios of lines, colours etc.) which are compared with those of a set of standard stars defining the classification system. The ultimate goal is to derive the basic stellar parameters, including the abundances of the elements. This requires a quantitative calibration of the criteria in terms of these parameters so that observed spectra can be compared with theoretical spectra. The most detailed and reliable procedures to achieve quantitative spectral classification make use of model atmosphere techniques.

As this Symposium is devoted to the discussion of abundance effects in classification, it seems useful to give a brief summary of the theoretical background for calculating stellar atmospheres with particular emphasis on the influence of the *element abundances* upon the atmospheric structure. In order to illustrate the basic effects of the abundances no detailed discussion is required. It suffices to use fairly simple – long known – approximations. Of course, any actual reliable calculation of theoretical spectra should involve very elaborate models. Details of the physical and numerical problems of stellar atmospheres can be found, for example, in the books by Mihalas (1970) or by Unsöld (1955). Effects of abundances have recently been considered by Pecker (1973) in a discussion of the use of model atmospheres for temperature-gravity calibration.

In the following, the basic equations governing the structure of the atmosphere will be summarized, followed by a discussion of the effects of the abundances on the structure

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(through the thermodynamic properties and the absorption of stellar matter). Finally, the relationship between theoretical and observed spectra and some other aspects relevant to spectral classification will be briefly discussed.

2. Basic Parameters and Equations

We consider a 'standard model atmosphere' which is assumed to be homogeneous, planeparallel, in hydrostatic equilibrium with constant (radiative plus convective) flux. Furthermore, local thermodynamic equilibrium (LTE) is assumed to hold (continuous scattering may be allowed for, but is not included here). The atmospheric structure and hence the emergent radiation is then determined by the parameters (some 94, in principle):

(i) effective temperature T_{eff}

(ii) surface gravity g, and

(iii) relative element abundances ϵ_i (usually expressed as atomic numbers, normalized to $\log \epsilon_H = 12.00$).

The structure of the atmosphere, i.e. $T(\tau)$, $p_e(\tau)$, $p_g(\tau)$ etc., is obtained by solving the equation of hydrostatic equilibrium,

$$\frac{\mathrm{d}p_g}{\mathrm{d}\tau} = \frac{g}{\kappa} - \frac{\pi}{c} \frac{1}{\kappa} \int_0^\infty \kappa_\nu F_\nu \mathrm{d}\nu \tag{1}$$

together with the condition for *flux constancy*,

$$F = \int_{0}^{\infty} F_{\nu} d\nu + F_{\text{conv}} = \frac{\sigma}{\pi} T_{\text{eff}}^{4} = \text{ independent of } \tau .$$
 (2)

Here τ is the optical depth at an arbitrarily chosen reference frequency ν_0 , κ is the corresponding absorption coefficient $\kappa \equiv \kappa_{\nu_0}$, p_g is the gas pressure, p_e the electron pressure, F_{ν} are the monochromatic radiative fluxes, and $F_{\rm conv}$ is the convective flux.

The calculation of the radiative fluxes involves solution of the equation of radiative transfer for the intensity I_{ν} (at each frequency ν) into which the absorption coefficients κ_{ν} enter:

$$\cos\varphi \ \frac{\mathrm{d}I_{\nu}}{\mathrm{d}\tau_{\nu}} = I_{\nu} - S_{\nu} \ . \tag{3}$$

For simplicity, scattering is not considered in the present discussion, and the source function S_v is set equal to the Kirchhöff-Planck function $B_v(T)$.

Finally, Equation (2) has to be supplemented by the Schwarzschild criterion according to which *convective instability* occurs if

$$\left(\frac{d \log T}{d \log p_g}\right)_{\text{adiabatic}} < \left(\frac{d \log T}{d \log p_g}\right)_{\text{radiative}}$$
(4)

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Besides the absorption coefficients κ_{ν} , some *thermodynamic properties* of the stellar matter have to be known in order to calculate the atmospheric structure by Equations (1) through (4).

In particular, the equation of state

$$p_g = p_g(T, p_e), \ \rho = \rho(T, p_e)$$
 (5)

is needed for the integration of the equation for hydrostatic equilibrium. Furthermore, the entropy is required to evaluate the adiabatic gradient and convective flux.

With the assumption of LTE, the thermodynamic quantities and the κ_{ν} are determined (i) by T and p_e through the Saha-Boltzmann equations, and (ii) by the abundances ϵ_i of the constituents. If molecule formation is important the equations for the molecular equilibria have to be added.

The κ_{ν} comprise also *line absorption* besides continuous absorption. For its calculation, in addition to the population in the lower level, the profile function has to be known. It depends among others on the partial pressures of perturbing atoms (collisional damping, proportional to p_c or p_H in most cases) and on the velocity fields (microturbulence, see Section 3.4).

It should be remarked that line absorption is not only important for determining the temperature stratification (blanketing) but has to be considered (in the ultraviolet) also in the radiative pressure term of the hydrostatic equation for early-type stars.

3. Effect of Abundances on the Atmospheric Structure

The parameters $T_{\rm eff}$, g, ϵ_i which determine a model atmosphere are of different nature. While $T_{\rm eff}$ and g are directly contained in the basic equations, the abundances ϵ_i enter only through the thermodynamic properties and the absorption coefficients. An element which does not contribute to these quantities ('trace element') has no influence upon the structure of the atmosphere. However, before constituents can be neglected as trace elements in model calculations their possible influence has to be carefully examined. For example, potassium contributes about ≥ 30 per cent to the electron pressure in cool stars ($T \leq 3000$ K) despite its low abundance of only about 10^{-7} . ϵ_H (see, e.g. Bode, 1965).

3.1. EQUATION OF STATE

The thermodynamic quantities are sums of the contributions of the constituents so that the relative abundances ϵ_i simply enter as weights (when T and p_e are taken as independent variables). If $f_{ij}(T, p_e)$ is the fraction of element *i* in ionization state *j*, the equation of state for the case of negligible molecule formation can be written in the form (see, e.g. Mihalas, 1970):

$$p_{g}(T, p_{e}) = p_{e} \times \left(1 + \frac{\sum_{i} \epsilon_{i}}{\sum_{i} \epsilon_{i} \sum_{j} j f_{ij}}\right)$$
(5a)
$$\rho(T, p_{e}) = \frac{p_{g} - p_{e}}{kT} \mu m_{H} ,$$

where $\mu = \sum \epsilon_i \mu_i / \sum \epsilon_i$ is the mean molecular weight (μ_i = atomic weight of element *i*).

For high temperatures, $p_g/p_e \approx 2$ for hydrogen-dominated matter, and ≈ 1.5 for helium-dominated matter. For lower temperatures, when hydrogen and helium are largely neutral and the metals M mostly singly ionized, $p_g/p_e \approx (\epsilon_H + \epsilon_{He}) / \epsilon_M$.

In cases of partial ionization, essentially the abundance ϵ_i competes with the factor $e^{-\chi_{ion}/kT}$ of the Saha equation (χ_{ion} ionization potential). For example, in cool stars elements with low χ_{ion} such as K become important; or in the intermediate temperature range, the CNO group significantly contributes to p_e if hydrogen is strongly deficient (e.g. in the helium star HD 30353, Nariai, 1967).

3.2. CONVECTION

Element abundances affect the Schwarzschild criterion (4) since they enter into the adiabatic as well as into the radiative gradient. For the adiabatic gradient, abundant elements and the electrons have to be taken into account according to the expressions for the specific heats or the derivatives of the entropy. The radiative gradient on the other hand is determined essentially by the mean absorption coefficient and its pressure dependence, so that the ϵ_i enter through the equation of state and the κ_p .

An important application is the comparison of the hydrogen convection zone in cool metal-poor population II stars with that in normal stars. The lower metal abundances imply lower H⁻ absorption and hence, from the hydrostatic equation, a higher gas pressure at a given optical depth. This results in convection zones extending higher up into the atmospheres of metal-poor stars, and in flatter temperature gradients (Krishna Swamy, 1969).

3.3. Absorption coefficients and temperature stratification

The structure of the atmosphere, essentially $T(\tau)$, depends critically on the distribution of the absorption coefficients with frequency, i.e. on the non-grayness of the κ_{ν} . Most weight is given to the frequency range where, roughly speaking, the maximum flux occurs. This fact can be taken into account, for example, by referring the τ -scale to the Rosseland mean opacity,

$$\frac{1}{\overline{\kappa}_R} = \int_0^\infty \frac{1}{\kappa_\nu} \frac{\partial B_\nu}{\partial T} \, \mathrm{d}\nu \bigg/ \int_0^\infty \frac{\partial B_\nu}{\partial T} \, \mathrm{d}\nu \,. \tag{6}$$

This is a good approximation (diffusion approximation) in the deeper layers, whereas

near the surface other mean values, e.g. the Planck mean, are more appropriate.

Insight into the dependence of $T(\tau)$ upon the κ_{ν} , especially when line absorption is important, can be gained by simple approximations, e.g. the picket-fence model of Chandrasekhar (see Mihalas, 1970), or the approximation by Hunger and Traving (1956). The latter makes use of the moments of κ_{ν} , weighted by the Planck function,

$$M_{s} = \int_{0}^{\infty} \kappa_{\nu}^{s} B_{\nu} d\nu; \ s = -2, -1, 0, 1$$
(7)

The coefficients Q, k_{α} and L_{α} in the *approximate* expression for the temperature stratification

$$T^{4}(\bar{\tau}_{R}) = \frac{3}{4} T^{4}_{\text{eff}} \left(\bar{\tau}_{R} + Q - \sum_{\alpha=1}^{m} L_{\alpha} e^{-k} \alpha \bar{\tau}_{R} \right)$$
(8)

can be characterized by only two moments, M_{2} and M_{1} (M_{0} is essentially the normalization of B_{ν} , and M_{1} is used up for the definition of the Rosseland scale). While M_{2} is determined by the lowest κ_{ν} , M_{1} (corresponding to the Planck mean) takes account of the peaks of the absorption, e.g. of the absorption by strong lines. The surface temperature depends essentially on M_{1} , approximately $T^{4}(0)/T^{4}_{\text{eff}} \propto M_{1}^{-\frac{1}{2}}$.

Besides the distribution over frequency ('crowding of lines'), the effect of abundances on $T(\tau)$ depends also on the distribution of the line strengths on the curve of growth. For example, many overlapping faint lines or wings of strong lines will behave like a quasicontinuous absorption, and have an influence which is different from that of more isolated medium-strong lines. The general effect of *line absorption* on $T(\overline{\tau}_R)$ ('blanketing') is to increase the temperature in deeper layers ('backwarming') and to decrease it near the surface; the flux is redistributed: the decrease by the lines ('blocking') is compensated by an increase in relatively line-free ranges of the spectrum.

For a crude orientation about the order of magnitude of the contribution of various elements to the line absorption, we may make use of the fact that bound-bound and bound-free transitions steadily merge at the absorption edge, so that the height of the edge can be taken as some measure for the line absorption. In the hydrogenic approximation (principle quantum number *n*, effective charge Z), the absorption coefficient a_n per atom in state *n* is about $8 \times 10^{-18} nZ^{-2}$ cm² at the edge (see e.g. Allen, 1973). Thus we may expect line absorption of element *i* to be important for the structure of the atmosphere, (i) if the abundance ϵ_i is sufficiently high and the frequency ν_n of the edge falls in a range where the continuous absorption $\kappa_{\nu,c}$ is low, i.e. if $\epsilon_i f_{in} a_n^{(i)} / \Sigma \epsilon_i$ becomes comparable to $\kappa_{\nu,c}$ (f_{in} : fraction of element *i* in state *n*), and (ii) if ν_n falls in a range where the Rosseland weight function is large.

Although the inclusion of line absorption is straightforward in principle, the large number of lines which in many cases have to be taken into account, causes problems (lack of atomic data, question of completeness for lines considered, numerical treatment). Calculations with a direct inclusion of the stronger lines have, for example, been performed for the ultraviolet blanketing in early-type stars by Morton and his collaborators

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(e.g. Mihalas and Morton, 1965; Adams and Morton, 1968). Besides the direct approach, statistical methods have (in particular using opacity distribution functions) been developed to deal with a large number of lines (e.g. Labs, 1951; Röhm, 1954; Strom and Kurucz, 1966; Carbon, 1973; Peytremann, 1974; Gustafsson *et al.*, 1975), or the problem of calculating line-blanketing has been avoided by using scaled (solar) temperature stratifications in a restricted range of parameters. Particularly when the influence of abundances on the model is to be investigated, an accurate and consistent treatment of the line (and associated continuous) absorption is important, a schematic incorporation of line blocking does not seem sufficient. A detailed discussion and comparison of the different methods is, for example, contained in the recent paper by Gustafsson *et al.* (1975).

3.4. VELOCITY FIELDS

In spectral analyses, the atmospheric velocity field is mostly idealized as being composed of microturbulence and macroturbulence. One would expect that, in principle, the velocities can be calculated from the parameters which determine the atmosphere (and the layers below it). This view is supported by observed correlations between the microturbulent velocities ξ with T_{eff} , ε and the metal content (see, e.g., Baschek and Reimers, 1969; Nissen, 1970; Gustafsson and Nissen, 1972; Reimers, 1973). In practice, however, the microturbulence has to be treated as an independent additional parameter, which is derived empirically from the line spectrum, since the present theory of hydrodynamic phenomena does not allow its calculation with sufficient accuracy.

Microturbulence influences the structure of a stellar atmosphere through its contribution to the pressure and through the increase of the widths of the line absorption coefficients and hence of the line blanketing: (i) the left-hand side of Equation (1) has to be modified by adding a term $\frac{1}{2} d(\rho \xi^2)/d\tau$.* This term has to be taken into account if ξ becomes comparable to or larger than the velocity of sound, for example, in supergiants (see e.g., Groth, 1961) and possibly in some helium stars (low velocity of sound) such as HD 124448 in which Schönberner and Wolf (1974) find $\xi=10 \text{ km s}^{-1}$. (ii) The Doppler width entering the line absorption coefficient is increased according to $\Delta \nu_D / \nu = (\nu^2_{\text{ thermal}} + \xi^2)^{\frac{1}{2}}/c$. Note that the lines on the flat part of the curve of growth whose strengths are sensitive to ξ constitute an important contribution to the line blanketing in many cases.

We may expect that microturbulent velocities correlate with the velocities in the convection zones (e.g. Böhm-Vitense, 1971) which in turn depend on the element abundances. Although metal poor population II stars have hydrogen convection zones extending higher up into the atmosphere (see Section 3.2), the mixing-length theory predicts their microturbulent velocities to be smaller. This is because they are determined by non-local (overshoot) phenomena which originate from layers below the upper boundary of the convection zone (Böhm-Vitense, 1971) where the convective velocities

^{*} The contribution of macroturbulence to the pressure depends on the special structure of the velocity field.

are smaller in the metal-poor stars. The observed low microturbulence in population II stars, however, is as yet not quantitatively understood (Böhm-Vitense, 1975).

3.5. EFFECTS OF ABUNDANCES IN NON-STANDARD MODELS

So far we have discussed the essential effects of abundances on the atmospheric structure with the standard assumption of a homogeneous plane-parallel and flux constant atmosphere in hydrostatic and local thermodynamic equilibrium. Non-LTE calculations, for example, in general yield level populations different from those in LTE so that quantitative differences, say in the absorption coefficients, may arise. However, as the abundances influence the structure only indirectly through the thermodynamic properties and the absorption coefficients, no *basically* different effects occur when more general assumptions are made.

Finally, it should be mentioned that some stars such as the peculiar A stars have atmospheres which are *chemically inhomogeneous*. Inhomogeneities occur across the surface, as is more or less directly observed, but possibly also abundance gradients with depth have to be considered in view of the diffusion or the magnetic accretion hypothesis for A_p stars.

In the present discussion, only the basic effects of abundances on the structure of a stellar atmosphere are considered. No attempt is made to give a systematic discussion of results obtained for various regions of the HR diagram. Recently, investigations (containing also references to previous work) of the influence of metal abundances ϵ_M on model atmospheres have been carried out by Peytremann (1974) in the range $5000 \leq T_{eff} \leq 8500$ K and $2 \leq \log g \leq 4.5$, by Böhm-Vitense (1975) for $4000 \leq T_{eff} < 8000$ K and $L/L_{\odot} \leq 9000 M/M_{\odot}$, and by Gustafsson *et al.* (1975) for $3750 \leq T_{eff} \leq 6000$ K and $0.75 \leq \log g \leq 3$. For the cool giants considered by these authors, differences of the metal abundance within the range $-3 \leq \log(\epsilon_M/\epsilon_H)/(\epsilon_M/\epsilon_H)_{\odot} \leq 0$ do not lead to very pronounced effects on the *model atmospheres*, e.g. Böhm-Vitense finds that differences of only ≤ 200 K occur in the temperature stratification $T(\bar{\tau}_R)$. Gustafsson *et al.* find empirically that, at given $\bar{\tau}_R$, ΔT is proportional to $\Delta \log \epsilon_M/\epsilon_H$.

4. Theoretical and Observed Spectra

So far, we have followed the 'theoretician's point of view': a theoretical spectrum is calculated from the parameters T_{eff} , g, and ϵ_i . One can calculate grids of model atmospheres, calculate all desired spectral quantities with their dependence on the ϵ_i and hence obtain the calibrations for spectral classification. From the standpoint of applications, particularly of classification, however, the inversion of this procedure is of prime interest: observed, suitably chosen spectral criteria are to be fitted to a theoretical calibration which then allows to read off basic stellar parameters. It is desirable to know the sensitivity of the criteria to the parameters (i.e. the accuracy which can be achieved) or how far the parameters can be uniquely determined.

4.1. REMARKS ON THE BASIC STELLAR PARAMETERS

Since a (standard) stellar *atmosphere* is determined by T_{eff} , g and ϵ_i , the natural way to explore the influence of abundances on its structure and on the emergent radiation is to keep T_{eff} and g fixed, and to consider various ϵ_i . Comparing stars with the same T_{eff} and g is equivalent to comparing stars with the same T_{eff} and 'specific luminosity' L/M (*M* stellar mass).

On the other hand, the structure of the *entire star* is determined by its mass \mathcal{M}_0 and composition ϵ_i^{0} at birth, and by its age t (if rotation, magnetic fields, mass transfer from a companion etc. are neglected). Hence $\mathcal{M}, L, T_{eff}, g, \dots, and$ the atmospheric composition $* \epsilon_i$ depend on \mathcal{M}_0, e_i^{0} and t. (In practice, however, present theories of mass loss and mixing do not allow to calculate changes of \mathcal{M} and ϵ_i during the stellar evolution). The atmospheric parameters T_{eff}, g, ϵ_i may therefore be correlated as a consequence of the star's evolution, so that it may not always be appropriate to vary the abundances independently of T_{eff} and g.

As a special example we consider stars on or near the main sequence. Here $\epsilon_i = \epsilon_i^o$ (apart from exceptional cases) because the atmospheres still have the original composition, so that $T_{eff} = T_{eff}(\mathcal{M}_o, \epsilon_i, t)$ and $g = g(\mathcal{M}_o, \epsilon_i, t)$. Conversely, if we compare two main-sequence stars with different abundances (e.g. a population II star with a population I star), but identical T_{eff} and g, their masses and ages will be different.

4.2. REMARKS ON THE UNIQUENESS OF THE DERIVED ATMOSPHERIC PARAMETERS

As spectral classification should be applicable to a large number of stars, the number of independent spectral criteria is necessarily restricted. Obviously, the number of parameters which are to be derived has to be less than or at most equal to the number of criteria. In practice, this enforces a restriction in the number of elements which can be considered individually. Usually, the elements are grouped together and abundances for the metals or for the CNO group etc. are derived upon the assumption that within each group the relative element abundances are held fixed, e.g. at their solar values.

A more subtle question concerning the uniqueness of derived parameters arises due to the fact that (as long as molecule formation is unimportant) the theoretical spectrum is determined if $T(\tau)$ and $p_e(\tau)$ are given together with the abundances ϵ_s of those elements s which exhibit observable structures (lines, absorption edges, ...) in the spectral range considered. This may be realized in some detail, e.g. by making use of the Eddington-Barbier approximation for the flux F_v emerging from the stellar surface,

$$F_{\nu} = 2 \int_{0}^{\infty} B_{\nu}(\tau_{\nu}) E_{2}(\tau_{\nu}) d\tau_{\nu} \approx B_{\nu}(\tau_{\nu} = \frac{2}{3}), \qquad (9)$$

where τ_{ν} is the optical depth at the particular frequency ν under consideration, and E_2 the exponential integral of order 2. Since in spectral classification we are more concerned

^{*}Note that not all kinds of observed abundance differences are directly related to stellar evolution. For example, the anomalies found in A_p stars or white dwarfs are probably due to processes which operate in the outer layers only.

with relative intensities, we consider the ratio of fluxes at two frequencies ν and $\nu + \Delta \nu$ with corresponding optical depths τ and $\tau + \Delta \tau$ (or absorption coefficients α and $\kappa + \Delta \kappa$). Let τ be the reference scale for which $B_{\nu}(T(\tau))$ is regarded as known, then, for small $\Delta \nu$ and $\Delta \tau$,

$$\frac{F_2}{F_1} \approx 1 - \Delta \tau \left(\frac{\partial \ln B_{\nu}}{\partial \tau}\right)_{\tau = \frac{2}{3}} + \Delta \nu \left(\frac{\partial \ln B_{\nu}}{\partial \nu}\right)_{\tau = \frac{2}{3}} + \dots$$
(10a)

with $\Delta \tau = \int_{0}^{\tau=2/3} \Delta \kappa / \kappa \, d\tau$. For a spectral line, the variation of B_{ν} with frequency can be neglected over the line, and $\Delta \kappa$ is to be identified with the line absorption coefficient 1, so that the depression in the line is

$$1 - \frac{F_2}{F_1} \approx \frac{2}{3} \left\langle \frac{1}{\kappa} \right\rangle \left(\frac{\partial \ln B_{\nu}}{\partial \tau} \right)_{\tau = \frac{2}{3}} .$$
 (10b)

Here $\langle 1/\kappa \rangle$ denotes the ratio of line to continuous absorption coefficient averaged over the layers down to $\tau = 2/3$.

We infer from Equations (10) that spectral features (such as line strengths, colours, bolometric corrections etc.) primarily depend (i) on the relative temperature gradient, and (ii) on the line and continuous absorption in the 'layers of formation'. $\langle l/\kappa \rangle$ is (a) directly proportional to the ratio of the abundance ϵ_s of the element producing the line to that of the main contributor to the continuum (in most cases hydrogen), and depends (b) on the level populations, i.e. excitation and ionization conditions which are determined by T and p_e . The $T-p_e$ relation is therefore more directly significant for discussions of stellar spectra than the fundamental parameters themselves. Incidentally, this was pointed out already in 1958 by Unsöld who discussed the effect of different ϵ_i in cool stars, within the framework of coarse analysis, by keeping mean values of T and p_e fixed.

Is it now possible that different combinations of the model parameters (T_{eff}, g, ϵ_i) result in the same $T-p_e$ relation and in the same spectrum? In this generality, this seems possible only for the rather academic case that the elements s having observable spectral features (lines) are not the same elements that significantly influence the atmospheric structure. If, however, only a selected number of spectral criteria (e.g. only continuum and Balmer lines) and/or only a restricted spectral range (e.g. only the visible for early-type stars) is considered, the problem of the uniqueness is not trivial, i.e. spectral classification is more vulnerable to ambiguities than more detailed spectral analyses.

For example, in cool stars helium does not exhibit lines in the visible and does not contribute to the electron pressure and the opacity. The structure of an atmosphere with such an abundant 'passive' constituent cannot be distinguished from that of a star with e.g. no helium and a different (higher) gravity. Another important example is the role of the ultraviolet line blanketing in early-type stars: it has been shown (e.g. Mihalas and Morton, 1965) that, for the same gravity, the $T-p_e$ relation of a star without metals is very similar in the formation layers of the visible spectrum to that of a star with metals (and hence with ultraviolet line-blanketing) which has a different effective temperature.

Related problems occur, for example, for the interpretation of the spectra of A_p stars (see e.g. Leckrone, 1973), or for the connection of classification of hot stars in the extreme ultraviolet with that established in the visible.

4.3. SYSTEMATIC ERRORS IN DIFFERENTIAL ANALYSES

A theoretical calibration of classification criteria is subject to systematic errors which seem unavoidable even in sophisticated model atmosphere calculations. Differences in the stellar parameters ΔT_{eff} , $\Delta \log g$, $\Delta \log \epsilon_i$, however, can be obtained with higher accuracy because all kinds of sources of systematic errors largely cancel when stars of similar structure are compared. Differential evaluation of calibrations obtained by model atmosphere techniques can be regarded as the most reliable procedure in theoretical stellar classification. (This, of course, does not mean that absolute calibrations are dispensable).

One should realize, however, that the range of interest for element abundances is so wide that even in differential work systematic errors cannot be excluded. Consider two stars with identical T_{eff} and g, then their atmospheric structures are similar only if all relevant $\Delta \log \epsilon_i$ are small enough, i.e. if a trace element (as defined in section 3) remains a trace element, and if, for example, an important contributor to the opacity remains important, etc.

For example, in solar-type stars a decrease of the metal abundance by a factor of 10 or more leads to a reduced line blanketing and hence a different $T(\tau)$. Furthermore, strong lines in the metal-rich star which depend on the van der Waals broadening will shift onto the flat part of the curve of growth which depends on the microturbulent velocity, so that also systematic effects in the relative strengths of the lines may arise. On the other hand, an increase of the metal content in solar-type stars raises the question how far the lines included for the blanketing calculations are complete. The overabundances of irongroup elements and rare earths are found in some peculiar A stars to be so large that they dominate the line absorption in the ultraviolet and hence lead to a different $T(\tau)$ as compared to normal stars of similar T_{eff} and g (e.g. Leckrone, 1973; Leckrone *et al.*, 1974).

5. Conclusion

Quantitative stellar classification relies upon the calculation of theoretical spectra which can best be obtained by using model atmospheres. In order to minimize the systematic errors inherent in model and line computations, differential methods should be preferred.

Besides the direct ('observable') dependence of spectral features (lines, colours etc.) on the abundances of the elements which produce the respective feature, the spectrum depends also implicitly on element abundances through their influence upon the structure of the atmosphere, i.e. essentially upon the $T-p_e$ relation.

While effective temperature and gravity are directly contained in the basic equations from which the model atmosphere is to be constructed, the abundances enter only

indirectly through the thermodynamic properties (mainly electron pressure and entropy) and through the absorption coefficients of the stellar matter. Since the emergent intensities depend crucially on the temperature stratification which in turn depends strongly on the absorption coefficients, the latter have to be consistent with the element abundances. In particular the inclusion of the absorption by numerous metal lines – which cannot be neglected for most types of stars – requires considerable numerical effort (even in the case of LTE). The microturbulent velocity has to be considered as an additional parameter since at present it cannot be expressed in terms of the basic parameters with sufficient accuracy.

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B. BASCHEK

DISCUSSION

R. Kandel: In connection with velocity fields, there are of course many problems. I would consider your 'second' effect, viz. the effect of line broadening, the fundamental one, since the 'velocity fields' are in fact derived from broadening observations. My remark is that, whenever the 'turbulent pressure' term in the HSE equation becomes important, it is very likely that dissipation terms also will become important. Some time ago Anthony Hearn in *A. and A.* found that the energy requirements of microturbulence were uncomfortably high in A stars. For Betelgeuse, many authors found a 'supersonic' microturbulence of 10 km s⁻¹; if one applies Hearn's calculations to this, one finds a mechanical energy flux of the order of the total flux of the star is required by the dissipation of such microturbulence. Thus there is a serious problem, and velocity fields must, if they are real, be included in the energy transfer too.

Baschek: I agree, as for the fairly hot stars studied by A. G. Hearn. For cooler stars with their strong hydrogen convection zones, the problem does not seem so serious to me.

Foy: This comment concerns the turbulence. I have checked the effect in the abundance determinations of the changes in stellar structure due to the turbulent pressure (Foy, thesis, 1974).

Consider a model defined by $T_{eff} = 4500$ K, log g = 2.50 and $[M/H]_0 = 0.0$. Ignoring turbulent pressure whereas the turbulent velocity changes from 0.0 to 5.0 km s⁻¹ induces errors in abundance determination less than 0.10 or 0.15 dex (depending upon the lines). So this is not very large, compared to the usual error bias (?) in such works (typically 0.20 dex).

Baschek: At T = 4500 K, the velocity of sound is about $v_s = 8$ km s⁻¹, so that in your example $(\xi/v_s)^2$ is at most about 0.4 and hence no drastic effects upon the structure are expected.

Bell. In the analysis of stars for which high values of ξ are found, was that high value of ξ included in the calculation of the atmosphere used for the analysis?

Baschek: In most cases, not. One should realize, however, that an inclusion of ξ in the hydrostatic equation would imply knowledge about its dependence with depth, e.g. should for some reason ξ be proportional to $\rho^{\frac{1}{2}}$, then $\frac{1}{2}\frac{d}{d\tau}\rho\xi^2 = 0$. In special cases, e.g. for the A supergiant aCyg, some information on $\xi(\tau)$ has been derived and its effect on the pressure has been taken into account (Groth, 1961 – see references).

Schatzman: One should be very careful about assuming that the chemical composition in the atmosphere is the same as the initial composition. Time scale of diffusion, even including macroscopic transport of some sort, is sufficiently short to produce changes in chemical composition.

De La Reza: We are studying in collaboration with Dr Querci the influence of abundances on the structure on the atmosphere of carbon stars. We chose a group of elements that constitute the principal electrons donors as K, Na, Ca, Mg. The point is to study the global problem, i.e. introduce an initial abundance of the element, see what is the effect on the atmosphere, with this calculate the theoretical profile and compare with the observations. If the fit is not good we continue with this iterative scheme up to obtaining complete agreement. From preliminary results for a giant star of T_{eff} = 3500°. The effect to put 10 times more number of K and Na atoms as in the sun is to raise the temperature to 200° K in a certain region of the atmosphere. We expect that this effect is even greater in lower values of T_{eff} .

Schatzman: It is difficult to make any predictions. For stars earlier than late F for example, the diffusion takes place mainly at the bottom of the convective zone. The velocity of diffusion varies very much with the depth of the lower boundary of the HCZ. We can expect age effects depending upon the spectral type. One more difficulty is due to the inhibition of diffusion under gravitational (or radiation pressure) drag by macroscopic motions (stochastic motions). Anyhow, differences are to be expected when comparing main-sequence stars of different age and of spectral type earlier than F8 for example.

Garrison: I would like to comment on a small, but extremely important misconception about spectral classification which stellar atmospheres theoreticians often express. While it is true that MK spectral classification uses a restricted number of line ratios as *Guidelines*, the ultimate criterion is that the entire blue-violet spectrum matches that of the standards. This considerably reduces the chance for error because it is very rare that in the entire spectrum, abundances will mimic T_{eff} and log g. Thus the star will be called peculiar by the perceptive classifier, even though he may not know exactly why

it doesn't match. If something is wrong, it usually doesn't match in detail and the classification is a signal to the high-dispersion spectroscopist of theoretician to investigate the star in more detail to determine why.

Baschek: I think there is a steady transition from classification based on very few parameters (e.g. two or three colours) over spectral classification to detailed model analyses. In my talk, I used the term 'spectral classification' or 'classification' in a general sense.

Kandel: Are electrons still important in cool stars? If so, as you pointed out, potassium is not a trace element, but then one has to worry about non-LTE effects. Auman and Woodrow in a recent Astrophysical Journal have shown departures from the Saha equation for cool giants and supergiants. The critical thing appears to be the collision of cross-sections with neutral atoms and molecules.

Baschek: At temperatures of about 3000 K electrons are still important. Regarding non-LTE effects, I agree that they have to be carefully examined whenever some indications for their importance show up.

Jaschek: You have mentioned some work relating to stellar atmosphere calculations done for different metal abundances. My question is if you could detail a little bit more which are the regions of the HR diagram covered by such studies.

Baschek. To my knowledge, systematic abundance studies are more or less restricted to the region (F-K) where the 'metals' as a group are important for the atmospheric structure. In early-type stars and in cooler stars, where molecules are important, investigations are complicated by the fact that more than one abundance has to be considered to vary.

Bidelman: Could you expand your remark concerning spectral classification in the far ultraviolet a bit?

Baschek: In early-type stars, the bulk of radiation is in the far ultraviolet. I wonder how far a classification system which has been introduced outside this range, i.e. in the visible, can be extended into the ultraviolet or how far it will match an ultraviolet classification scheme. Will it be too coarse, will ambiguities arise or ...?

De La Reza: As far as the influence of the changes in the electron density is concerned we have to consider not only the abundance effects but also the non-LTE effects. For instance, Auman and his collaborators are investigating the non-LTE effects for M stars and these are quite large. In the future we have also to investigate the abundance effect on this.