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Models of late-type stellar photospheres

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Summary. In this review we discuss recent work and progress in the modelling of photospheres of stars of spectral types F and later. Special emphasis is laid on advances as regards the consideration of atomic and molecular blanketing, non-LTE and convection and other dynamic processes. In a special chapter we discuss the possibilities of semi-empirical modelling of late-type photospheres. In the conclusions we find that much important work remains in this field, but that a considerable part of this work may in fact be carried out in a near future.

Key words: Stars: atmospheres of – Stars: late-type – Stars: general

1 Introduction

The stellar photosphere is the layer of the star from which most of its energy flux is emitted, and where most of its line spectrum is formed. Any analysis of spectroscopic or photometric observations of a star depends therefore in principle on our, more or less primitive, understanding of this layer. Thus, the determination of the fundamental parameters of stars, including their chemical composition, is to a large extent based on models of stellar photospheres.

The stellar photosphere is also the boundary to the invisible stellar interior, and serves in several respects as the link between models of stars and stellar evolution and observations. The phenomena of stellar evolution manifest themselves as surface phenomena through photospheric fundamental parameters and changes of chemical composition due to dredge-up of processed material. The models of photospheres may be needed as boundary conditions for the models of stellar interiors. The understanding of the photospheric phenomena and their relation to interior processes

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are moreover important in semi-empirical modelling of stars using stellar oscillations (astro-seismology) and in studies of stellar magnetic fields and their origins.

However, the stellar photosphere is also an inner boundary: to the outer atmospheric regions, the chromosphere, corona, and wind (including a stellar envelope). In this way the effects of the stars on their environments – through radiation or mass loss, with far reaching effects on the interstellar medium and the dynamical and chemical evolution of galaxies – reflect the physics of stellar photospheres. It is important to note that although the photospheric density may well be many orders of magnitude greater than that of the outer stellar atmosphere, the division of the atmosphere into these different layers (which is usually made at the temperature minimum, just inside the chromospheric temperature rise) is rather artificial, in view of the spatial inhomogeneities of the atmospheres with several different layers existing at the same distance from the stellar centre, and the physical interaction between these layers. In spite of the overwhelming energy output and heat capacity of the photosphere, this interaction is not solely directed outwards – e.g., the backscattering of radiation from a dusty envelope of a cool giant may have severe effects on the photospheric structure and the spectrum.

One should also note that although the modelling of stellar photospheres is generally motivated by the need for such models in various applications, there are also good reasons to study the photospheres as such. Contemporary observations of the solar photosphere demonstrate a highly dynamic and fascinating landscape of complicated structures, cf., Fig. 1 and e.g., Title et al. (1989) and several reviews in Rutten and Severino (1989). Nature here provides systems which develop from (close to) thermal equilibrium to a state very far from equilibrium as one proceeds to greater atmospheric heights. Through these systems an intensive energy flux is transported, and the intricate world of structural patterns results. Obviously, the stellar photospheres resemble what Ilya Prigogine has called "dissipative systems", and might be worth careful study as examples of structure formation. However, the lack of spatial resolution in stellar observations severely limits this possibility – an obvious exception from this being the study of the solar photosphere. Whereas rather advanced models of early-type stars have existed for some years (Kudritzki and Hummer 1990), the models of late-type stars have lagged somewhat behind. There are natural explanations for this, as will be further discussed below, such as the massive blanketing from an enormous number of atomic and molecular spectral lines, the very important effects of convection, and the uncertainties as regards the origin of the winds. However, as will also be illustrated below, a number of significant improvements in these and other respects have taken place in recent years, and in our opinion this should open up this research field for much more ambitious systematic approaches towards physically reasonably consistent models of late-type atmospheres. A major motivation for writing this review is to stimulate such approaches.

We follow the usual definition of "late type stars", i.e. meaning all stars with Harvard class F and later, including S and N-type giants, M dwarfs, and even brown dwarfs. This includes a wide variety of objects, from normal F, G and K stars, so important in applications to the study of galactic structure and evolution, to the late giants and supergiants whose photospheres may be used as test sites for stellar evolution theories and where about half of the atomic elements may be produced and progressively visible, to the M dwarfs and brown dwarfs whose number density may be so high that they dominate the baryon mass of the universe. Physically these objects have almost only one property in common – their effective temperatures are lower than about 8 000 K – and it would be impossible to cover all important aspects

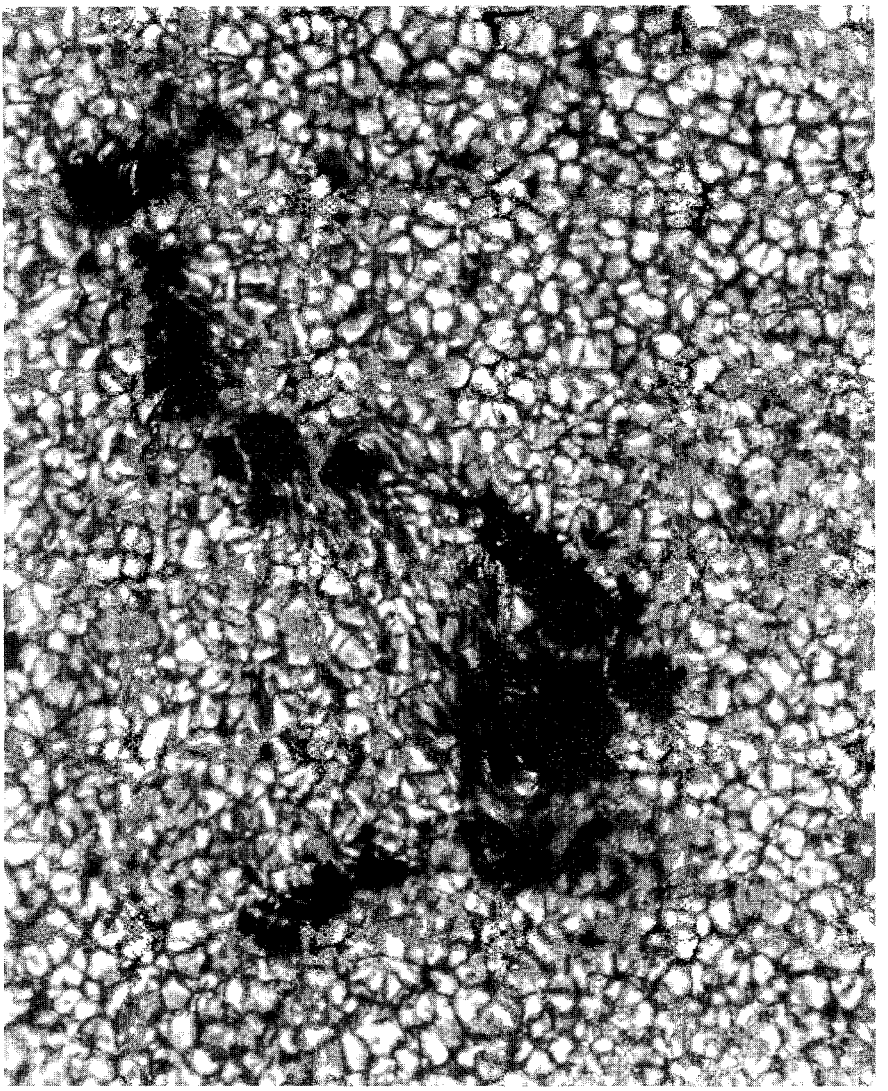

Fig. 1. A region of the solar photosphere in the spectral continuum around 4680 Å. The image, obtained with the Swedish Solar Telescope on La Palma by Göran Scharmer in 1993, shows a fragmented sunspot and many granules in different stages of evolution, including a number of elongated granules that probably are affected by the magnetic fields near the sunspot, and some dark centres (so called exploding granules) close to disintegration. Typical granules are about 1 000 km across, but many considerably smaller structures can also be seen. Among those are the bright filigree in the intergranular lanes in certain regions. These structures, which also show strong photospheric magnetic fields, are at the diffraction limit of the telescope ($0.''25$) and are thus not resolved

of their photospheres in one review. Our selection of topics will necessarily be biased towards our own interests and prejudice. Fortunately, a number of other reviews have been published on related topics. A number of aspects of late-type photospheres are discussed in different volumes of the NASA Monograph series on Nonthermal Phenomena in Stellar Atmospheres (Cram and Kuhi 1989; Johnson and Querci 1986), in the proceedings from the Cambridge Workshops on Cool Stars, Stellar Systems and the Sun (Wallerstein 1990; Giampapa and Bookbinder 1992) and from IAU Symp 145 (Michaud and Tutukov 1991), IAU Coll 106 (Johnson and Zuckerman 1989) and IAU Coll 137 (Weiss and Baglin 1993). Important methodological and physical problems and progress in modelling were discussed at a NATO workshop in 1990 (Crivellari et al. 1991). Determination of fundamental parameters from photospheric spectra was reviewed by Gustafsson and Jørgensen (1985) and chemical analysis of cool stars by Gustafsson (1989). The role of molecules was described by Tsuji (1986), and existing grids of model photospheres by Johnson (1985, 1986). Available atomic laboratory data was reviewed by Martin (1992) and molecular data by Jørgensen (1992a).

2 Basic assumptions and present trends in "classical modelling"

Often the term "classical model atmospheres" is used, with a meaning that changes with time as the art of calculating model atmospheres proceeds. It usually refers to the underlying basic assumptions – at present those assumptions that one often attaches to the term "classical" are those of hydrostatic equilibrium, plane-parallel or spherically symmetric stratification, LTE and an energy equilibrium which only includes the radiative flux and a convective flux as approximated with the mixing-length theory. The term "classical model atmosphere" almost always refers to the photosphere only.

This field of research has long been characterized by an on-going discussion concerning the validity of these assumptions, and thus of the classical models, or "speculative-classical theory" to cite a critic (Thomas 1989). No doubt the critics are correct in the sense that the models are not correct they do not even include many of the most important physical properties of these interesting systems, and moreover, they are intrinsically inconsistent – the latter is true both as regards the properties of the radiation field (LTE) and the velocity field (hydrostatic equilibrium, neglect of mass flows, mixing length theory, microturbulence). However, the only way to improve the models is to abandon the basic assumptions, and that leads – at least in the general case – to formidable technical and physical problems. On the other hand, such models may be supposed to lead also to self-consistent descriptions of chromospheres, coronae and winds, and this would certainly be a very fundamental step forward in stellar physics, with significance for a wide field of new applications for stellar atmosphere theory. Thus, it seems clear that any steps that can be taken in that direction should be taken, and we shall in Sect. 4 describe a number of such steps towards more "unified" models of all the atmosphere. Until this can be achieved, however, it is reasonable to denote the results of the efforts of those who attempt modelling photospheres "model photospheres" instead of the usual term "model atmospheres" – in particular since semi-empirical modelling of chromospheres, coronae and winds is also being performed, although these are still treated as systems separate from the photospheres.

In our opinion, it is meaningful to improve the classical models today in at least two respects – (1) the introduction of spherical symmetry (where this has not yet been done) for the geometrically extended stars, and (2) the inclusion of more realistic line

blanketing. The first of these steps has recently been taken and is in fact relatively simple, while the latter step is very cumbersome. Here, we shall first comment on the "sphericity effects" and then give some more general comments on the blanketing. The detailed discussion on the line data needed for the blanketed models is deferred to Sect. 3.

Recent studies of the role of sphericity in cool stars include the studies of Scholz (1985), Bessell et al. (1989a,b), and Plez et al. (1992) for oxygen-rich giants and super giants, and the studies by Scholz and Tsuji (1984) and Jørgensen et al. (1992) for carbon-rich giants. In these studies, models of cool supergiant and giant stars with spherical rather than plane parallel symmetry are presented. Compared to the plane-parallel case, the radiation field in the spherical models becomes diluted in the upper photospheric layers. The dilution is dependent on the relative extension, d, i.e. the thickness of the photosphere divided by the stellar radius, which (for hydrostatic equilibrium) scales as $L^{1/2}M^{-1/2}T_{eff}^{-2}$, where L is the stellar luminosity and M the mass. Thus, for a given locus in the HR diagram, the sphericity effects increase with decreasing stellar mass which may potentially be used for direct spectroscopic determination of masses of cool stars. Whether it is necessary or not to compute a model in full spherical symmetry is dependent on the problem considered and the accuracy required in the analysis. In practice the temperature structure effects are considerable for $d > 0.1$, while the spectrum effects may be significant for smaller d, i.e. for most M and N giants. The structural effect is usually a decreased temperature of the surface layers in the spherical models compared to the plane-parallel ones, which affects both the chemical equilibrium and the synthetic spectra. The surface pressures are decreased in models of M giants and increased in N star models.

The second order effects, due to intensified molecular formation when the temperature decreases, may be very considerable, as was pointed out by Watanabe and Kodaira (1978, 1979) and further stressed by Schmid-Burgk et al. (1981), who also noted the possibility to independently determine both radius and stellar mass for M giants from the consequences of these structural effects on the stellar spectra. Such attempts have, however, not yet led to any reliable results due to the complexity of the situation, including the fact that the extension of these tenuous photospheres is not only the result of radiative transfer and hydrostatic equilibrium – velocity fields are probably also of decisive importance for determining their structure. For stars of higher gravity and for deeper layers in the photospheres the spherical models approach the plane parallel ones.

Since the plane parallel models usually are hotter than corresponding spherical models in the region of line formation, calculated neutral lines will often (if no second order effects dominate the situation) be weaker, and ionized lines stronger, for plane parallel models than for spherical ones. Consequently, abundances derived from neutral lines will often be greater when plane parallel models are used than when spherical models are used, and vice versa for the ionized lines. Drake et al. (1993) investigated the effects on K and early M giant abundances of Na, Al, O, Ca, and Fe, as derived from both neutral and ionized lines when spherical and plane-parallel models were used. They found relatively small differences (up to 0.1 dex) in all cases studied. Similar results were obtained in the study of molecular lines of CO and CN (Plez 1990). Plez et al. (1993), however, found a somewhat larger effect of up to 0.4 dex higher abundances when spherical models of M giants were used in the analysis of Li I and K I lines. In this case, however, the abundances derived from neutral Li and K lines are highest when based on spherical models. This is due to a more complex situation, where not only the computed metal line intensities, but also the

surrounding molecular line veil due to a huge amount of weak TiO lines, is dependent on the sphericity.

The consequences of line blanketing in stellar photospheres are basically two, cf. Mikelas (1978):

1. a backwarming which compensates the flux fraction, η, blocked by spectral lines by increasing the temperature $T(\tau)$ in the continuum-flux forming layers by $\sim \eta \times T(\tau)/4$, and
2. a cooling or a heating of the surface layers, depending on the depth variation of the opacity and where in the spectrum, relative to the peak of the local Planck function, it is located.

The situation can be analysed by using the Strömgren equation (assuming radiative equilibrium and LTE),

$$\Phi = \int_o^\infty \kappa_\nu J_\nu d\nu - \int_o^\infty \kappa_\nu B_\nu(T) d\nu = 0, \tag{1}$$

remembering that the angular mean intensity J_ν departs from $B_\nu(T)$ at $\tau_\nu \lesssim 1$ where it decreases towards $0.5 \cdot B_\nu(T(\tau_\nu = 1))$ since incoming radiation gets small. However, J_ν may still be $> B_\nu$ for high frequencies since the outward directed intensity comes from inner and hotter atmospheric regions, and the temperature sensitivity of the source function is considerable. In this case the right hand side integral in Eq. (1) may catch hot radiation from below and thus warm the surface. This is particularly the case if the absorption is not too strong or occurs suddenly at the surface, so that J_ν is not thermalized, as may be the case with molecular absorption, e.g., from TiO (cf. the effects found by Krupp et al. 1978). However, if the absorption is strong and persistent to greater depths it cools even if it is located at high frequencies when τ_ν gets < 1; the standard example of this is the effect of atomic line absorption in G and K stars (see e.g., Gustafsson et al. 1975). On the other hand, if the line absorption is located at low frequencies where the temperature sensitivity of $B_\nu(T)$ is much less, the first integral of Eq. (1) usually decreases when lines are introduced in the model, and $B_\nu(T)$ and T decrease. One example of this is the cooling in K star models due to the rotation-vibration bands of CO, found by Johnson (1973) and verified by Gustafsson et al. (1975) with a more realistic blanketing treatment. The general effects of blanketing were further discussed by Carbon (1979) and Gustafsson and Olander (1979).

The numerical treatment of blanketing in classical models is not a major obstacle today. Two methods are in current use – the Opacity Distribution Function (ODF) Method (Labs 1951; Gustafsson et al. 1975; Kurucz 1979) and the Opacity Sampling (OS) Method (Peytremann 1974; Sneden et al. 1976; Brown et al. 1989; Plez et al. 1992; Jørgensen et al. 1992). In the first of these, one transforms the rapidly varying absorption coefficient into smoothly varying functions within limited wavelength intervals, in order to keep the number of quadrature points in integrals such as those in Eq. (1) down to less than 10^3. In the second, one samples the absorption coefficient in on the order of 10^4 frequency points. Advantages and drawbacks of these and other methods are summarized by Carbon (1984) and by Jørgensen (1992b). In the ODF method a basic assumption is made: one assumes that there is a correlation in the absorption of different strengths at different depths – this may be a poor approximation for cool stellar photospheres where different sources of line absorption dominate at different depths. In this respect, and in several others, the OS method is more flexible,

and it is in common use now as the computer power has increased to such a level that classical model photospheres can be routinely calculated with about 10^4 frequency points representing the radiation field.

The most difficult problems with line blanketing in late-type star modelling are instead the need for very large amounts of atomic and molecular data, the fact that the LTE assumption is invalid (at least in principle), and the effects of velocity fields on the line profiles. The first of these problems will be discussed in Sect. 3, and it will be seen that very considerable progress has been made in recent years but that much work remains. The second problem is important, in particular for the modelling of the surface layers. We shall return to the problems of non-LTE in Sect. 4, but we note in passing that scattering terms of the source function cancel at the derivation of Eq. (1), i.e., if spectral lines are mainly formed in scattering processes, the radiation field is decoupled from the local temperature and the surface effects discussed above are much reduced. Also, the velocity field may affect the blanketing, but this has hardly been studied at all in stellar photosphere research.

Existing grids of classical model photospheres in current use are summarized in Table 1. For a discussion of most of them, and some intercomparison, see Johnson (1985, 1986). Some intercomparison is also made in the references given in the table. The general outcome of these comparisons indicates a good, and sometimes very good, mutual agreement for the more detailed grids. The differences that exist, which may typically amount to 100 K at a given optical depth, can usually be explained as the result of differences in atomic or molecular data, in convection theory or in blanketing treatment. With the more detailed grids, where the ODF or the OS method have been used, the latter effect tends to be small. Computations based on independent model-photosphere codes have, however, partly been based on the same opacity data, and in this respect it is worth pointing out the danger in drawing too strong conclusions from the mutual agreement between "independently" computed model structures – the crucial test is obviously confrontation with the real stars through computed spectra and colours.

A long-standing problem has been that the late-type models have been too bright in the ultraviolet (see, Holweger 1970, Gustafsson et al. 1975). Kurucz (1992b) included a huge amount of new atomic lines in the model and spectrum computations, by which he was able to obtain agreement between observed and computed low resolution visual and UV spectral features. However, Bell et al. (1994) demonstrated that high resolution solar spectra calculated with Kurucz's line list show numerous far too strong lines. When these lines are subtracted the model fluxes in the ultraviolet seem still too great, and the U-B indices of solar-type stars too small, and Bell et al. (1994) conclude that a veil of weak atomic lines is therefore not the (full) explanation of the discrepancy. For the cooler models there are certainly still missing opacities. Considerable progress has been made recently in the modelling of early M giant spectra (cf. Plez, Brett and Nordlund, 1992) as well as M dwarf spectra (cf. Allard, 1994, Kirkpatrick et al. 1993). However, substantial improvements are still needed for the dwarfs and for the upper layes of the giant models. For the N stars progress has been made in matching the ultraviolet spectra (Johnson et al. 1988) but a severe problem remains in that the polyatomic bands tend to become too strong (Lambert et al. 1986, Jørgensen 1989) and for Miras there is still disagreement between models and observations, as well as between different grids (Bessell et al. 1989a). Synthetic spectra from the models often show spectral features formed in the upper photospheres (H_2O, HCN, TiO, Na D, H_2) to be too strong in cool stars.

Table 1. Grids of model photospheres in current use for late-type stars

Sp	$T_{\rm eff}$	log g	[M/H]	Notes	Reference
G-O	5500–50 000 K	0.0–4.5	−2.0–0.0		Kurucz (1979)
K-O	3500–50 000 K	0.0–5.0	−5.0–1.0	1	Kurucz (1992c)
K-G III	3750–6000 K	0.75–3.0	−3.0–0.0		Bell et al. (1976)
K-G V	3750–6000 K	3.75–4.5	−3.0–0.0	2	Eriksson et al. (1980)
K-G	5000–8500 K	2.0–4.5	−0.0		Peytremann (1974)
M I-III	2600–4200 K	−2.0–2.5	0.0		Tsuji (1978)
M III	3000–4000 K	0.0–2.0	0.0		Brown et al. (1989)
M I-III	3000–4000 K	−0.5–1.5		S	Plez et al. (1992)
M III	2500–4000 K	0.0–2.0	0.0		Johnson et al. (1980)
M V	3000–4250 K	4.75–5.75	−2.0–0.0		Mould (1976)
M V	2000–3750 K	4.0–6.0	−4.0–0.0		Allard (1990)
M V					Ruan (1991)
N, R	3400–4500 K	−1.0–1.0		C/O = 3.2	Querci et al. (1974)
N	2600–3800 K	−1.0–1.0		C/O=3.2, etc	Querci and Querci (1975)
N, S	2500–3500 K	0.0		C/O=0.6–2.0	Johnson (1982)
N	2500–3400 K	−1.0–0.5	−1.0–0.0	S, C/O = 1.02–2.0	Jørgensen et al. (1992)
N	2500–3500 K	−1.0–0.0	−1.0–0.0	3, C/O = 1.01–1.5	Eriksson et al. (1986)
R	3800–4800 K	2.0–3.0	0.0	C/O = 1.02–3.5	Olander (1981)
R	4200–5400 K	2.0–3.0	0.0	C/O = 1.74	Johnson and Yorka (1986)
Miras	2300–3530 K	$L \sim 10^4 L_\odot$	0.0	S	Bessell et al. (1989a)
Brown dw.	1000–4500 K	3.5–5.5		no metals	Saumon et al. (1994)

1) Available on CD-ROMs from author, prel. description in Kurucz (1992c)
2) Unpublished, used in numerous studies, description see Gustafsson et al. (1975)
3) Unpublished, description see Lambert et al. (1986)
S) Spherically symmetric models

We shall not review the extensive use of these classical models for the determination of fundamental parameters of stars but refer the reader to our previous review on that subject (Gustafsson and Jørgensen 1985, see also Gustafsson 1989). Let us just emphasize that recent abundance determinations, built on extensive and accurate observational data and strictly differential approaches, may give very consistent results for solar-type stars (see, e.g., Edvardsson et al. 1993) and that the improvements in molecular data for cool stars also make these accessible for high accuracy analyses (cf., e.g., Plez et al. 1993 for a nice example). Concerning the determination of effective temperatures, radii and surface accelerations of gravity for the coolest stars some unresolved problems, as well as some recent promising developments, may be worth noting:

In recent years several important improvements have been made as regards the temperature scale of red giants, in particular due to progress in the measurement of angular diameters by lunar occultation techniques (cf. Ridgway et al. 1980; White and Feierman 1987; Richichi et al. 1992, and references cited therein), speckle interferometry, and (particularly during the latest decade) Michelson interferometry (cf. Di Benedetto and Rabbia 1987; Mozurkewich et al. 1991; Quirrenbach et al. 1993; and McAlister 1985 for a general overview). These measures must be combined with measures of apparent bolometric fluxes and predictions of centre to limb variations from model photospheres in order to be transformed to effective temperatures; this is non-trivial for cool giants and in particular for Miras and other pulsating stars where the photospheres are severely affected and extended by progressing shocks. Also, note that the effective temperature is dependent on the wavelength at which the diameter measurement was made, since the apparent size of the extended photosphere

is wavelength dependent. A general clarifying discussion of this problem was given by Baschek et al. (1991).

Quirrenbach et al. (1993) found that stars of spectral types M3 III-M5 III tend to be typically 10% larger in the strong TiO band around 7120 Å than in the less contaminated region around 7540 Å. For Mira stars these effects are even greater. The use of wavelength dependent diameter measures as a test of model photospheres was discussed by Scholz and Takeda (1987) and should be further explored with newer models and observations. It should be noted, however, that the extension effects of M and N giants and supergiants are complex phenomena, even within the framework of static classical models (cf. Schmid-Burgk et al. 1981), that are sensitive to input molecular data, and their uncertainties.

We note in passing that the value of high spatial resolution studies of the apparently largest stars is not limited to the question of the effective-temperature scale, but is also relevant as regards giant surface structures and limb darkening (cf., e.g. the work on Betelgeuse and Mira by Wilson et al. 1992).

The overall agreement between the effective temperatures for F to early M stars between the effective temperatures derived from angular diameters (cf. Ridgway et al. 1980) and those of the Infrared Flux Method (cf. Blackwell et al. 1991, and references therein) is satisfactory in view of expected errors, and so is the agreement between the temperature scale based on red and infrared colours of Bell and Gustafsson (1989) and that of Blackwell et al. The calibration of visual colours by Buser and Kurucz (1992) also agrees reasonably well with this calibration. (For some remaining problems, in particular for metal-poor subdwarfs, see King (1993).) For stars significantly cooler than 4 000 K, however, the situation must be regarded as more unclear, as yet. Any photometric index is so affected by molecular absorption that the calibration of the photometry in terms of temperature needs detailed and accurate spectral modelling. For a promising attempt of this type, see Fluks et al. (1994) who derive effective temperatures from low-resolution spectral fits to recent models for M giants, in good agreement with the Ridgway et al. scale for stars earlier than M6. Using similar models for dwarfs (Brett 1994), Brett and Plez (1993) find significantly higher effective temperatures of early M dwarfs than those of previous temperature scales. It remains to be seen whether the scale has to be revised; more detailed model comparisons are needed, in particular in the infrared. In the absence of detailed models, the Infrared Flux Method is to be preferred, and that has been used by Tsuji (1981a, and b) for M giants and N stars, respectively. These calibrations tend to agree with the angular-diameter measurements, but the scatter is large and presumably reflects errors both in the measurements and in the model photospheres used in the calibrations. Modelling errors are more problematic since relatively small errors in $T_{\rm eff}$ ($\pm 5\%$) cause large effects in predicted molecular absorption, and thus in criteria for estimating surface gravities or abundances, as well as in the direct effects on the temperature structures of the molecular blanketing. This complication is illustrated in the analysis of N stars by Lambert et al. (1986), where errors in the effective temperature scale are among the most significant uncertainties for the error estimates in the abundances. For a discussion of the temperature scale of Miras see Bessell et al. (1989a). Renewed attempts to confront contemporary models for the cool giants with observations seem worthwhile.

As regards surface gravities (or masses *and* radii for extended stars) the situation is similar in the sense that the largest problems occur for the coolest giants, although already for K giants the problems are severe – well known is the long-standing debate on the gravity of Arcturus (cf. Trimble and Bell 1981), for which, however,

the arguments are now stronger for a relatively high value, see Bell, Edvardsson and Gustafsson (1985). These authors compared the use of ionization equilibria, pressure sensitive damping wings and lines of MgH. The latter method has been further studied and used by Bonnell and Bell (1993a), also for rotation-vibration OH lines in the infrared (Bonnell and Bell 1993b). For the coolest giants, where the spectra are so crowded that the wings of strong lines are impossible to trace and the number of suitable lines of ions is very small due to the low temperatures, the most promising spectroscopic method is the use of molecular lines or bands. These are, however, so sensitively dependent on the temperature and chemical composition, as well as on the atmospheric structure, that it is often most reasonable to estimate the gravity on the basis of the estimated stellar absolute bolometric magnitude and mass. Considerable improvements in the understanding of the photospheres will be needed before spectroscopic methods will be superior for M and N stars. For the nearby stars parallaxes from the Hipparcos data base will contribute important constraints on the surface gravities in the near future, and the proper motions may similarly strengthen estimates based on mean parallaxes for more distant stars.

3 Line absorption

As has already been emphasized, the line absorption is of key significance for the structures of late-type stellar model photospheres and for calculated model spectra. Many studies have illustrated the fact that not only the strong line absorption is significant for the temperature structure but, at a given geometrical depth and wavelength, all absorption such that the optical depth at that particular wavelength is in the range from the continuum optical depth to ~ 1. If, as is the case in extended regions in late-type spectra, many spectral lines contribute at each wavelength, the monochromatic absorption coefficients from these lines must be added, allowing for the different line profiles. This means that in the LTE case one needs to know the wavelength, the *gf*-value or transition probability, the excitation energy and relevant broadening parameters for each line significant in this way. This puts very heavy demands as regards atomic and molecular data, and often they just do not exist. One example is the broadening parameters for the molecular lines – for the atomic lines one often uses Voigt profiles with some damping constants while molecular lines are as a rule modelled with Gaussian profiles without extended damping wings, merely due to lack of pressure broadening data, although that is presumably totally erroneous for the high density cool dwarf photospheric models.

Very extensive data is also needed due to the fact that the statistical distribution of number of transitions versus *gf*-value for atoms and molecules in late-type stellar gases is such that the structural effects on the deeper photospheres are very much dominated by the very numerous weak lines. This is the more significant since these deeper layers are just the layers one is most anxious to model in important applications, such as abundance analysis. A dramatic illustration of the significance of accumulating data for the many weak lines is given by Jørgensen (1994) who showed that the last 10% of the accumulated band strength, supplied by many millions of very faint lines, of the water vapour rotation-vibration bands have a qualitatively significant effect on the model photospheres of late M giants.

Alexander and Ferguson (1994) have made an impressive compilation of available opacity data for both continuum sources, atomic lines, molecular lines, and grains, and computed Rosseland mean and Planck mean opacities for these. At 1 000 K grains

dominate the Rosseland mean opacity, at 2 000 K H_2O and TiO are the dominating sources, whereas metal lines and H^- dominate at 5 000 K (for solar abundances and characteristic densities).

3.1 Atomic lines

For computations of not too heavily line-blocked spectra it is often best to use laboratory data. One should always keep in mind, however, the possibility that a veil of weak lines, not included in the line lists, depresses the stellar "continuum". Generally, the best laboratory data are more accurate than computed data, in wavelength as well as intensity.

The National Institute of Standards and Technology (NIST) conducts a long term extensive programme for critical evaluation of atomic laboratory data, and issues regularly the results in their publication *Journal of Physical and Chemical Reference Data.* Most of these data compilations are also available in computer readable form. Among the recent compilations we note Martin et al. (1988), who listed transition probabilities for nearly 10 000 lines of the elements Sc–Mn; Fuhr et al. (1988), who offer a list for a similar number of Fe–Ni lines; and Fuhr and Wiese (1990), who have compiled a list of 8 300 selected lines of all elements for which reliable data is regarded to exist. Reader et al. (1980), Zaidel et al. (1970), and Striganov and Odintsova (1982) all list wavelengths of 30 000 – 50 000 lines. Of astrophysical interest is also the compilation of "solar" oscillator strengths by Thévenin (1989, 1990) of more than 6 000 lines from 35 elements identified in the solar spectrum in the wavelength range 4 000 Å-8 000 Å.

For many computations of late-type synthetic spectra (and always in the computation of model photospheres) it is, however, insufficient to include only the few thousands of lines measured in the laboratory. For such more comprehensive computations the most widely used data is the so-called Harvard-Smithsonian, or Kurucz's line list (Kurucz 1994). The basic approach behind that is the Scaled Thomas-Fermi-Dirac method, which was described by Warner (1967). It is a semi-empirical approach where the inner (so-called Thomas-Fermi statistical ion) part of the potential is fitted to match an outer coulomb potential. The word "scaled" refers to the use of a scaled radial coordinate to compensate for a full description of the relativistic (magnetic) term in the Schrödinger equation. Whereas the first version (Kurucz and Peytremann 1975) of this data base was based directly on Warner's method, later more extended versions are based on improvements with complete Hartree-Fock calculations, including configuration interaction integrals (Kurucz 1994, private communication).

An advantage of semi-empirical methods is that they usually are computationally faster than full *ab initio* methods, and that they to various degrees can take advantage of experimental data. In Kurucz's line lists experimental data are used when fitting the observed energy levels via so-called Slater parameters (Slater 1960). Such fits depend heavily on good experimental data, and since it was found that many important missing lines of the Kurucz and Peytremann (1975) list could be due to Fe, a long-standing collaboration with experimental groups has aimed at improving the known experimental values of the energy levels for Fe I (Brown et al. 1988; Nave and Johansson 1993) and Fe II (Johansson and Baschek 1988). Comparison of the predicted gf-values, based on these improved energy levels, indicates that the predicted Fe II lifetimes are about 12% shorter than the observed ones (Biémont et al. 1991). An extensive comparison between predicted and computed individual lines in the UV solar

spectrum (Bell et al. 1994) also indicates that the computed lines are systematically somewhat stronger (and sometimes considerably stronger) than the observed ones, as noted above, even though the computed low-resolution solar UV spectrum matches the observed flux (Buser and Kurucz 1992; Kurucz 1992b; Edvardsson et al. 1993). A systematic comparison between the computed *gf*-values (and calculated transition energies) with laboratory values would be very interesting.

The Harvard-Smithsonian atomic data base is continuously being updated with new experimental data, and when experimental energy levels and/or *gf*-values are believed to be superior to the computed values, these are included on the tape instead of the calculated ones. In total, the latest version of the tape includes 56 million atomic lines, out of which 10 000 are experimental values. Most of the lines are due to the iron-group elements, and 42 million of the lines are from the first nine ions of Ca through Ni. Future plans to extend the data base include computation of more complete data for elements lighter and heavier than the iron group, and inclusion of hyperfine and isotopic splitting of the lines.

For computations of opacities in the stellar interior, two data bases have been heavily used during the latest decades, namely the Los Alamos Astrophysical Opacity Library (LAOL, Huebner et al. 1977; Huebner 1985) and the compilation by Cox and Tabor (1976). Several astrophysical studies indicated that these data bases needed revisions (Simon 1982; Christensen-Dalsgaard et al. 1985; Swenson et al. 1990), which triggered the considerable effort of two independent groups to re-evaluate the complete set of atomic data. Seaton (1987) initiated the international Opacity Project (OP), and Iglesias et al. (1987) presented a project with the same aim (OPAL) at the Lawrence Livermore National Laboratory. Both projects have taken advantage of the increased computer power since the LAOL computations; they allow a much more realistic description of the atomic transitions, as well as a more sophisticated computation of the equation of state (EOS). Although these atomic data bases aim at evaluation of Rosseland mean opacities for stellar interiors (i.e., relatively high temperatures and pressures) they are also of importance for the modelling of stellar photospheres. Since they are based on independent techniques, mutual comparisons between their results, and comparison with the Kurucz' line list, are important. Comparison presented by Alexander and Ferguson (1994) shows that Rosseland opacities computed with the Kurucz line list generally agree well with the OP and OPAL tabulations in regions where atomic lines contribute to the Rosseland mean.

Both the OP and the OPAL operates with a basic atomic model where an atomic or ionic system of N+1 electrons is described as a "target" consisting of the nucleus and the N electrons, plus the "colliding" or "running" or "photo" electron that moves in the field of the target under influence of the radiation field, but the method for solving the problem is different. The OP computations are based on a pure, and well tested, *ab initio* method known as the close-coupling (CC) approximation (Burke and Seaton 1971). One of the advantages of this method is that it allows a homogenous and fairly accurate treatment of both bound and continuum states, and can be made numerically efficient (using the so-called R-matrix method). The *ab initio* approach is flexible since it is completely independent of the availability of laboratory data. Also, the project produced a systematic survey of the photoionization of excited states, which led to the discovery of many hitherto unknown resonances in the corresponding cross sections. The methods used for computations of the line-broadening were developed and described by Seaton (1988, 1990). Fine-structure splitting was included for selected ions of Fe. Transition probabilities for a total of 1.6 million transitions between 52 000 states in 18 atoms (with Z = 1–14, 16, 18, 20, and 26) and their ions

have been computed, for $n \leq 10$ and $l \leq 4$. In general, the agreement with other theoretical results and with experimental data has been found to be good. Recent reviews of the method as well as comparisons with experiments have been presented by Yu Yan (1992) and Mendoza (1992; with emphasis on presentation of the OP data base), and by Seaton et al. (1994).

In contrast to the OP project, the OPAL computations are based on analytic parametrizations of the potential (described in detail by Rogers 1981), and use a number of constants which are fitted to experimental ionization energies (listed by Rogers et al. 1988). Necessary experimental values exist for all isoelectronic series up to zinc. The radial wavefunctions are computed from this potential, assuming either LS coupling or full intermediate coupling. By comparisons with *ab initio* results it has been demonstrated (Iglesias et al. 1992a; Iglesias et al. 1992b) that the accuracy obtained in the OPAL calculations is comparable to that of single-configuration self-consistent field (SCF) *ab initio* methods with relativistic corrections, and generally there is an excellent agreement between results from OP and OPAL computations. Also the approach for computation of the EOS is different in the OP and the OPAL, where OP has adopted the so-called "chemical picture" (Mihalas et al. 1990) and OPAL has adopted the so-called "physical picture" (Rogers 1986), but these differences are, although important in the deep stellar interior, of only little significance for the application to the photospheric problem. Recent descriptions of the two projects, with a comparison of their results and descriptions of astrophysical applications, have been given by Seaton et al. (1994) and by Rogers and Iglesias (1994). For transitions where configuration interactions are important, the OP results agree better with the experiments than do the OPAL results. The simpler parametric potentials used in the OPAL calculations allow, however, some more flexibility in certain respects. The number of transitions in the OPAL computations are varying from application to application, and could for example include 10 million lines of the first 10 ionization stages of iron at $\log(T) = 5.3$.

The OP and OPAL results are now being used for the construction of model photospheres. For the cool star photospheres, however, they need first to be combined with molecular data in order to give meaningful results.

3.2 Molecular opacities

As for the atoms, laboratory data for molecules are generally more accurate than computed data, but much too sparse to serve as the sole source for computation of a model photosphere or to represent the weak line veil in a cool spectrum. For detailed analysis of individual features where high accuracy is needed, it is therefore advisable to seek laboratory sources, but to remember also to include a satisfactory number of weaker lines from the theoretical calculations. The most extensive general laboratory data bases are the American HITRAN (High-Resolution Transmission Molecular Absorption) data base (Rothmann et al. 1987, 1992) which contains 648 000 lines from 31 different molecules, and the French GEISA data base (Husson et al. 1986, 1991), which strictly follows the HITRAN data base, but includes additional lines from molecules of particular interest for studies of the giant planets. The ATMOS (Atmospheric Trace Molecule Spectroscopy) catalogue, created in connection with the mission flown on Spacelab 3 (Farmer et al. 1985) is based on the HITRAN and GEISA data bases, but extended with additional molecules, such that in total it contains 400 000 entries for 46 species (Brown et al. 1987). Finally, the RADEN data base

(L.A. Kuznetsova and A.V. Stolyarov) is a user oriented service bank that on request can supply information on reviews, compilations, etc., on specific molecules, states and transitions. It contains information on about 300 diatomic molecules from more than 2600 publications. A data base of laboratory measurements, which is smaller but yet of central interest for stellar astrophysics, is the Berkeley Data Base (Davis 1994), containing measurements of the molecules TiO, ZrO, YO, CN, FeH, and LaO. All the mentioned data bases are available from their authors.

Typically, a reliable molecular opacity computation demands two orders of magnitude more lines than have been measured, and therefore be based on computed data. In contrast to the situation for atomic data, no homogeneous compilation of molecular data exists, and the quality, as well as the completeness, of the available data span a wide range. The two largest data bases in use for astrophysics are the Smithsonian database (Kurucz 1994) and the SCAN database (Jørgensen 1994). Both contain lists with identification, strength, frequency, and excitation energy for each spectral line. The Smithsonian list contains information for about 15 million lines from 11 different diatomic molecules, while the SCAN list contains about 70 million lines from 7 different diatomic and polyatomic molecules. Other molecular data bases include the lists by Piñeiro et al. (1987a,b, and references therein) for CO, CS, SiO and SiS, the list by Querci et al. (1974) for CN, C_2 and CO, the list by Littleton and Davis (1985) for ZrO and YO, the list by Goorvitch and Chackerian (1994) for CO, and the list by Langhoff and Bauschlicher (1994a) for SiO. They are all available from their authors on request.

Jørgensen (1992a) has compared the techniques used in generating these line lists. All are in a sense semi-empirical, because the calculations of the frequencies are based more or less directly on molecular constants, which are obtained directly from polynomial fits to measured energy levels. The theoretical part of a molecular line list compilation is mainly the computation of the dipole moment as a function of nuclear coordinates (i.e., vibration of the molecule). The band strength, S, is then computed from integrating the transition dipole moment between the initial (i) and final (f) states, $S \propto < i|\mathbf{d}|f >^2$. An often used *ab initio* method for this computation is the so-called Complete Active Space Self Consistent Field (CASSCF) approach (Roos et al. 1980; Langhoff and Bauschlicher 1994b). The accuracy of the results may be quite high if large enough basis sets and large enough active spaces are chosen, and the best computations for small molecules (i.e., molecules with two to three atoms) may exceed the experimental quality (Schamps 1994). Nevertheless, such computations are very CPU and disk space demanding. For example, the recent computation of the dipole surface for the water molecule by Jørgensen and Jensen (1993) required more than half a CPU year on a fast workstation (a DEC 5200, which has a computational speed equivalent to a Cray 1). For linear molecules (including diatomic molecules), the rotational line strengths can be computed from the vibrational band strengths by using simple Hönl-London factors, whereas more sophisticated (and CPU demanding) methods are required for top molecules. The frequencies may be computed directly from the experimentally determined molecular constants, which usually will give high accuracy for the lower states, but may differ substantially for the transitions involving high energy levels. A sophisticated (and very accurate, yet CPU demanding) method for computation of the transition frequencies is the so-called MORBID method (Jensen 1988), but that can only be applied to molecules where a substantial amount of experimental data is available to determine the fitting constants. It has therefore only been applied to astrophysically interesting molecules so far (Jensen 1994).

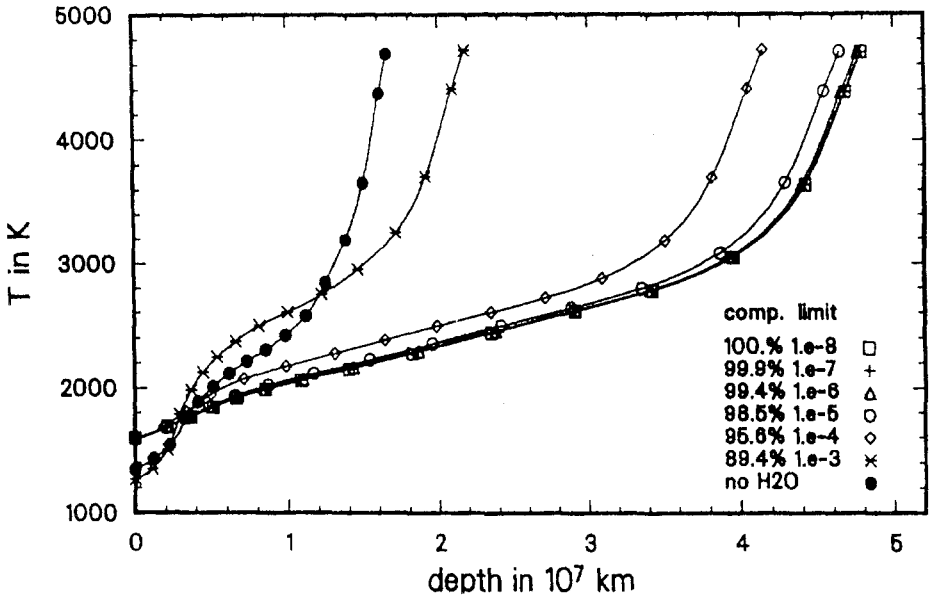

Fig. 2. The temperature vs geometrical depth of model photospheres of an M giant, $T_{\rm eff}$ = 3 100 K, $\log g = -0.5$, C/O= 0.43, when various degrees of completeness in the opacity of the water molecules is considered (from Jørgensen 1994)

In order to produce a good data base for the calculation of molecular absorption, we must, of course, be able to first figure out which molecules are to be considered. It turns out that even this basic question has non-trivial answers. The reason is that a model photosphere may not respond to one opacity before others are represented well enough. An insufficient number of diatomic lines, for example, may result in an insufficient cooling of our model, which in turn will result in an underestimate of the influence of the opacity of polyatomic molecules, which are only present at low temperatures. Also line data that include only the strongest lines of a given molecule may in itself lead to the misconception that this molecule is unimportant for the model. Often the weak lines are the most important ones for the energy balance! Jørgensen and Larsson (1990) analyzed the influence of the degree of completeness in the molecular data on the model photosphere structures. They introduced the ratio of the partition function, summed over all lines in the list, to the analytical partition function as a measure of the completeness of the line list. Jørgensen and Jensen (1993) elaborated this concept in their construction of a line list for the water molecule. They found that when including weaker and weaker H_2O lines in the calculation, the model photosphere converged towards a structure which, for M giant models, could be obtained by including all lines stronger than somewhere between 10^{-7} and 10^{-8} km/mol (about 20 million lines in total; see also Jørgensen 1994). When 90% of the absorption from H_2O was included the model photosphere structure still was closer to a model without any H_2O absorption than to the model with complete absorption (cf. Fig. 2) This emphasizes the overwhelming importance of the numerous weak lines for the energy balance, and it suggests that for many of the molecules for which

only a less complete line list exists today huge amounts of additional data must be calculated before we can claim having properly included the molecular opacity into the model photospheres.

One consequence of the role of the weak lines is that it is not always obvious from the appearance of the spectrum which molecules are most important for the photospheric structure. Relatively weak continuum-like features (like C_3 or the weak bands of HCN or H_2O) can absorb more energy than spectroscopically strong (but discrete) absorbers (like CO and CS). C_3 seems to be the most important opacity source in the upper layers of carbon rich N star model photospheres, but the spectroscopic identification of this molecule in any carbon star is still disputable (no line-by-line identification exists), while the molecule C_2H shows the highest partial pressure of any molecule in the upper photosphere of certain types of our carbon star photospheric models, but still it has not been seen in any real star (two previous suggestions in the literature of its possible identification have both later turned out to be due to comparison with what is now known to be erroneous molecular data). The progress in cool-star atmospheric modelling therefore necessarily has to go through a tight interaction with spectroscopic observation, and theoretical and experimental molecular physics and chemistry. Lambert (1988) has given an illustrative review of the identification of some molecules in cool red giants through interaction between laboratory and astrophysical research, and Jørgensen (1994) has analyzed the relative importance of various known molecules in cool stars. We might well find in the future that molecules we have not yet thought of could be important for the structure of some types of cool stars.

There are at least five factors that determine the importance of a given molecule as an opacity source in a stellar photosphere:

1. the abundances of the atoms composing the molecule,
2. the dissociation energy of the molecule (relative to other molecules that compete for the same atoms),
3. the integrated absorption coefficient of the molecule at the relevant temperatures,
4. the number of lines in its absorption system, and
5. the wavelength of the bulk of the absorption relative to the maximum of the emitted energy in the layers of the photosphere where the molecule can form.

For a star of solar composition the number of hydrogen and helium atoms is approximately 1000 times greater than the number of all other atoms together. Nevertheless, these two atoms form no molecules among themselves that are of importance for the opacity (for the cool dwarfs there is a modification as regards this, see below). Of the remaining about 0.1% of the atoms, oxygen accounts for half of the amount (by number), carbon for half of the rest, and nitrogen for half of everything beside H, He, O, C and (the equally abundant, but inactive atoms of) Ne. The remaining atoms are mainly Mg, Si, S, and Fe. It is therefore in combinations of H, O, C, and N we find nearly all the molecules that seem to dominate the spectrum and/or the opacity of cool stars. The most important known of these are CO, CN, C_2, HCN, C_2H_2, C_3, and H_2O, although there are other candidates, e.g., C_2H, for which the absorption coefficient is still basically unknown in a form which would be useful for astrophysics. The most astonishing example where point (2), (3), (4) and (5) above completely outweigh point (1) occurs for red giants with $T_{\rm eff} \approx$ 3000 K–4000 K, where TiO completely dominates the opacity, although a typical such star with solar abundances has one million times more H_2 molecules than TiO molecules. CO, on the other hand, is an example of a molecule that has relative little influence on the model

structure, except for the uppermost layers of G and K stars, see Johnson (1973) and Gustafsson et al. (1975), in spite of its very high abundance (and dissociation energy) and relatively high integrated absorption coefficient and pronounced appearance in the stellar spectrum. This is because there are few but strong rotation-vibration lines slightly too far out in the IR compared to the stellar flux while the electronic band systems are located at too short wavelengths to be of significance.

Due to its high dissociation energy the CO molecule binds either all oxygen (if there is more carbon than oxygen nuclei) or all carbon (if there is more oxygen than carbon). This leads to the dramatic difference between the spectra of so-called carbon (-rich) (i.e., R and N-type) and oxygen-rich (i.e., K and M-type) stars. To our present knowledge the photospheric molecular opacity of carbon stars is dominated by CO, CN, C_2, CH, HCN, C_3 and C_2H_2 (although also C_2H, C_3H, CH_4, and other molecules may be important), whereas H_2O, TiO and SiO seem to be the most prominent in the oxygen-rich stars. For stars with C/O $\approx$ 1 (i.e., the S-stars), almost all carbon, as well as almost all oxygen, is tied up in CO, and a large fraction of the nitrogen is bound in the dipole-inactive N_2 molecule. Many atoms much further down the "abundance list" are therefore active in forming efficiently absorbing molecules in the photospheres of S-stars than in any other types of cool stars (for example ZrO, VO, LaO, YO, FeH, etc).

Beside the chemical division of the stars, also the division according to gravity (into giants and dwarfs) is also important for understanding which molecules will be important absorbers. The pressures in the photospheres of the giants are very low when compared to the pressures found in the atmospheres of the Earth and the other planets. For this reason we expect to find CO in giant stars, but not CO_2, and we do find NH and CH, but not NH_3 and CH_4, which latter are both very abundant molecules in the atmospheres of the giant planets, but have not been identified in stellar photospheres. These bigger molecules may exist in the dwarfs (since high gravities lead to higher pressures), and there are indications that CH_4 may play a dominating role for the opacity in the coolest of the dwarf stars (Tsuji 1994). Allard (1994) and Allard et al. (1994) have computed model atmospheres and synthetic spectra for M-type dwarfs and discussed the effects of various known molecular opacities in these stars. The adopted opacities of VO and FeH were based on approximate descriptions of the opacity distribution (by the JOLA method; cf. Tsuji 1994, Jørgensen 1992b) and the integrated band intensity was computed by adjusting the f-values until a best fit to the observed band intensities was obtained. The f-values for TiO used by Kirkpatrick et al. (1993) were based on fits to M giant spectra, whereas Allard (1994) and Allard et al. (1994) adopted the laboratory f-values, which in principle is to be preferred. The adoption of the laboratory f-values for TiO improved the fit for the cooler M dwarfs considerably, which illustrates the general risk of hiding problems in stellar modelling (in this case in the giant models used to obtain the first adopted f-values) by treating fundamental molecular parameters as fitting parameters. The importance of obtaining reliable laboratory f-values for VO and FeH is also obvious; these data are necessary before acceptable flux-constant models for the M dwarfs can be constructed. Different treatments of the water opacity were also tested, leading to quite different result as regards the synthetic spectra.

One of the primary and direct goals of the recently increased efforts in late M dwarf spectral analysis and modelling is to determine accurate effective temperatures which may ultimately lead to confirmation of the existence of brown dwarfs. Jones et al. (1994) used model photospheres to derive effective temperatures for M dwarfs, combined with a semi-empirical approach for the water band opacities. The model

photospheric studies mentioned above show a much improved agreement between effective temperatures deduced from observed flux distributions and those derived from stellar interior models as compared with earlier temperature scales simply based on black-body fluxes.

Considerations of the molecular opacities have primarily been concerned with the bound-bound (*b-b*) transitions (i.e., line lists). Recently, van Dishoeck (1994) discussed the possible importance of bound-free (*b-f*) transitions, and Borysow (1994) discussed the effects of collision induced absorption (CIA). Both effects deserve much more attention in future model photosphere computations.

b-f transitions occur when a photon brings a molecule into an electronically excited state above the dissociation energy of the ground state. If the upper electronic state is repulsive, the *b-f* opacity becomes continuous (direct photodissociation), whereas transitions into bound electronic states above the ground state lead to discrete absorption (predissociation and spontaneous radiative dissociation). Photodissociation of molecules in the stellar photospheres is most important for small hydrides, because they have a fairly low dissociation energy (typically 4–5 eV, corresponding to absorption at 3 000 Å). van Dishoeck and Dalgarno (1984) found that continuous absorption of OH could be important (and stronger than the discrete absorption) in the wavelength range of 1000–3000 Å, and van Dishoeck (1987) found the continuous absorption of CH to be comparable to the discrete absorption in the whole wavelength range of 1000 – 5000 Å. Johnson et al. (1988) found that continuous CH absorption contributes significantly in the near ultraviolet spectra of carbon stars.

The CIA takes place on a very short time scale when two atoms or molecules pass nearby ("collide" with) each other. During the passage the electronic orbitals of the two molecules disturb one another, and molecules that are dipole inactive when they are "alone" can therefore absorb dipole radiation during the short time of the "collision". At the low pressures found in the giants, electromagnetic (transient) interactions between the molecules are very rare, and pressure broadening and CIA can usually be neglected. For the higher gravities of the dwarfs (and in particularly in the white dwarfs and brown dwarfs) CIA may nevertheless be a dominant absorption mechanism (Borysow 1994).

The most important CIA in stellar photospheres seems to be due to the "collisions" between two hydrogen molecules, and so far the $0\rightarrow0$, the $0\rightarrow1$, and the $0\rightarrow2$ bands (but not the hot bands of the ro-vibrational bands) have been calculated. Spectral bands corresponding to other molecular complexes which have not yet been computed (for example, collisions between H and H_2) may also play an important role for the stellar photospheric structure. Lenzuni et al. (1991) and later Lenzuni and Saumon (1992) and Saumon et al. (1994) applied the CIA results to stars of zero metallicity. The effects on such stars are expected to be particularly great, because of the lack of "normal" molecules, and, not unexpectedly, CIA was found to be the dominating opacity source. Computations showing for which range in metallicity and gravity the CIA is of importance are still missing, as are data for some of the presumably important transitions (like the ro-vibrational hot-bands and $H-H_2$ interaction).

The *b-b* transitions typically occur in the visible and the infrared spectral range, the *b-f* transitions in the near UV, and the CIA in the infrared. The *b-f* transitions will therefore be important primarily for spectrum synthesis, and not for the atmospheric structure of the stars, since the main part of the stellar flux passes at much longer wavelengths. The CIA may, however, be expected to be of importance also for the photospheric structure itself, particularly for the coolest stars where most of the flux is emitted in the near IR. Whereas roto-translational CIA takes place at relatively

long wavelengths, compared to the stellar flux maxima, Borysow and Frommholdt (1990) estimated typical ro-vibrational CIA absorption, at temperatures of interest in stellar photospheres, to take place at wavelengths in the interval 1 to 5 μm. We can therefore expect ro-vibrational CIA to be of importance for stars cooler than about 3500 K, provided that the CIA opacity is large and/or the other opacity sources are small (for example, due to a low metallicity.)

Pressure broadening of the molecular lines (for example the CO lines) may also affect the photospheric structure substantially; however, no study has been performed of this, so far.

Although the molecular absorption data in many respects still are in an exploratory state compared to the atomic opacities, several investigations have shown that where high quality extensive *ab initio* computations of the molecular opacities exist, models based on such data often give radically different and more consistent results (e.g., when applied in abundance analysis or for judging the evolutionary status of the stars studied, cf. Lambert et al. 1986; Plez et al. 1993) than models based on less complete opacities. This leaves us today with the challenging task to revise a considerable amount of what was previously thought to be sufficient data for various molecules, to identify yet unrevealed molecular opacity sources (maybe C_2H, C_3H, FeH, CaOH, CH_4?), to include new opacity mechanisms (CIA, photodissociation processes, pressure-broadening), and finally (and not least) to study which revised pictures this will give us of the fundamental physical processes in stars, of stellar evolution, and of the chemical evolution of galaxies.

4 New methods and results in theoretical modelling

4.1 Departures from LTE

A basic reason why the populations of atomic and molecular states may well be out of local thermal equilibrium in late-type stars is the low energy of the collisions, as compared with the typical energy gaps between different atomic states. Therefore, radiative transitions often dominate over collisional ones. The non-local character of the radiation field, especially wavelengths where it may be considerably hotter than the local Planck function, is then of great significance.

However, it is not easy to establish quantitatively the significance of departures from LTE. The reason for this is that in the formation of, e.g., a metal line in a late-type spectrum, a very great number of atomic levels are involved through transitions to the upper or lower level of the line. Furthermore, the atomic data needed to calculate these transition rates (and in particular the collision rates) are often very uncertain. Moreover, the background radiation fields that cause the radiative transitions to depart from the local Planckian distribution are uncertain in themselves and dependent on other departures from LTE. Finally, the radiation fields are dependent on the structure of the photosphere, which in itself may be severely affected by such departures.

The literature on non-LTE effects in late-type stellar spectra is very extensive. For a review of the early work in this field, see Mihalas and Athay (1973). However, much of this work mainly concerns line formation for simple (or highly simplified) atoms in chromospheres and coronae. Pioneering theoretical studies of complex atoms (Fe) in the photosphere of the Sun and other late-type stars were made by Athay and Lites (1974) and Lites and Cowley (1975). Using model atoms with a small number

of levels and transitions they explored the effects and found rather extensive "over-ionization" (with respect to the local Saha equilibrium) to occur, in particular in metal-poor models. Steenbock (1985) was able to increase the size of the model Fe atom considerably in his calculations for the Sun and for Pollux (KO III). He found a qualitative agreement with empirical effects traced for Pollux by Ruland et al. (1980) – leading to systematically low abundances of Fe and Ti when estimated from low-excitation atomic lines. These effects, which may amount to 0.3–0.4 dex in the abundances, were interpreted as essentially reflecting an over-ionization in shallow atmospheric layers where the low-excitation lines form.

A major uncertainty in calculations of this type is the uncertainty in cross-sections for inelastic collisions of atoms and molecules with atoms and electrons. Steenbock and Holweger (1984) pointed out the significance of collisions with hydrogen atoms in the non-LTE study of Li in late-type stellar spectra. They estimated the collision rates from Drawin's (1968, 1969) simple expressions (essentially a generalization of the classical Thomson formula). Later applications of this recipe in non-LTE calculations for Pollux and the Sun seem to suggest that it leads to too great cross-sections and thus too small non-LTE effects (Holweger 1988; Watanabe and Steenbock 1986). Also Lambert's (1993) critical discussion of the observational indications and the meagre data available from quantum mechanical calculations suggests that the collision rates have been overestimated and that quantum mechanical calculations of the (quasi) molecular states formed by the two colliding atoms (H+ atom) should be carried out. As regards the electron collisions the uncertainties are also considerable; for a recent summary of the situation, see Inokuti (1993).

The complexity of the problem of spectral line formation in late-type stellar photospheres makes the availability of adequate numerical methods a key issue. One of the most important developments in the theory of stellar photospheres in the last decade has thus been the design of new techniques for solving the equation of radiative transfer and the statistical equilibrium equations iteratively, with so-called Approximate or Accelerated Lambda Iteration (ALI) methods. If we first calculate the monochromatic lambda operator $\Lambda_{\mu\nu}$, such that

$$I_{\mu\nu} = \Lambda_{\mu\nu}(S_{\mu\nu}) \tag{2}$$

where $S_{\mu\nu}$ is the total monochromatic source function, the intensity $I_{\mu\nu}$ may be inserted into the statistical-equilibrium equations. Iteration between Eq. (1) and the statistical-equilibrium equations, the Λ iteration, converges very slowly, basically because the information proceeds very slowly at great optical depths from iteration to iteration (cf. e.g., Mihalas 1978). Rybicki (1972, 1984) suggested an efficient way of speeding up the iteration by preconditioning the problem such that photon transfer at great optical depths is eliminated. This "core saturation method" gave rapid convergence but approximate solutions. It was applied in some complex problems, e.g., by Stenholm and Stenflo (1978) for multidimensional radiative transfer of polarized radiation in magnetic flux tubes and by Flannery et al. (1979) in multilevel calculations.

Approximate operators could, however, also be used to give an exact solution by operator splitting, introduced in radiative transfer problems by Cannon (1973). The idea here is to calculate the intensity with an approximate operator $\Lambda^*_{\mu\nu}$,

$$I_{\mu\nu} = \Lambda^*_{\mu\nu}(S_{\mu\nu}) + (\Lambda_{\mu\nu} - \Lambda^*_{\mu\nu})(S^+_{\mu\nu}) \tag{3}$$

where $S^{+}_{\mu\nu}$ is the source function from the previous iteration. Only the approximate operator has to be inverted, and the idea is now to design an operator as simple as possible, still however able to contain the physical character of the transfer process.

Scharmer (1981) combined the Rybicki and Cannon approaches and also devised a simple and effective non-local approximate operator Λ^*, essentially based on the Eddington-Barbier relation. He demonstrated the great flexibility of the approach by applying it to partial redistribution problems (Scharmer 1983), to moving atmospheres (Scharmer 1984) and with Carlsson to multilevel problems (Scharmer and Carlsson 1985; Carlsson 1986). Since then different versions of the ALI method with different approximate operators and different preconditioning of the statistical equilibrium equations have been explored (for overviews, see Rybicki 1991; see also Rybicki and Hummer 1991). Other significant improvements in these methods were the introduction of numerical acceleration techniques (see Auer 1987 and 1991 for overviews) and, for dynamic atmospheres, of adaptive frequency grids (Stift and Moser 1993).

Among the applications and developments of the ALI technique are studies of spherical expanding atmospheres by Hamann (1985, 1986, 1987) and by Hempe and Schönberg (1986), Schönberg and Hempe (1986) who constructed an efficient diagonal approximate Newton-Raphson operator. Other important developments concern multilevel radiative transfer with overlapping lines and continua (Rybicki and Hummer 1991, 1992), the development of local (diagonal) approximate operators suitable for multidimensional transfer (Olson et al. 1986) and the application of these to two-dimensional transfer with partial redistribution (Auer and Paletou 1994; Paletou et al. 1993).

The ALI methods have been applied to a number of problems of spectrum diagnostics of late-type stars, e.g., Bruls et al. (1992), Carlsson et al. (1992), Carlsson et al. (1994), Kiselman (1994), and Takeda (1991). These studies, and references given in them, present illustrative examples of the present possibilities of systematic and detailed non-LTE analyses of late-type stellar spectra.

Bruls et al. (1992) studied the formation of solar K I and Na I resonance lines with detailed model atoms and discussed different intricate processes in interplay in the ionization equilibria, e.g., the "photon suction process", which here produces overpopulation of the neutral state by driving a population flow from the ion reservoir. The complex ionization balance affects the alkali resonance lines basically because the lines become effectively thin already in the photosphere, while, e.g., the strongest Mg and Fe lines are mainly in detailed balance.

Carlsson et al. (1992) analysed in detail the formation of highly excited Mg I emission lines in the infrared solar spectrum. They demonstrated the photospheric origin of these lines, being a consequence of replenishing of the population depletion of Mg I from the reservoir of Mg II, again by photon suction. This study opened up the diagnostic use of Rydberg emission lines, e.g., for study of solar and stellar magnetic fields.

Carlsson et al. (1994) systematically investigated the formation of Li I lines in a grid of late-type model photospheres with different fundamental parameters. They used a detailed model atom, extending up to the Rydberg regime, and analysed through experimentation how non-LTE processes of different types affect the resulting line strengths. They found corrections of LTE abundances of varying sign and size that may amount to about a factor of 3 and should be considered, e.g., in discussions of primordial abundances. Similarly, for solar type stars of different metallicities Kiselman (1994) discovered effects of similar magnitude on boron (B I) abundances from overionization and optical pumping in resonance lines.

Takeda (1991) studied the formation of iron lines in the spectrum of Arcturus (K2 III) by means of a comparatively elaborate model atom, taking into account the accumulative effect of many levels and transitions (81 and 50 transitions were explicitly represented for Fe I and II, respectively, while another 2965 and 1859 transitions were considered more statically. He found that departures in the excitation equilibria were small at depths $\tau(5000) > 10^{-3}$ and that departures from the LTE ionization were also rather limited, at least as long as the line blocking in the ultraviolet was calculated in the LTE approximation. However, observationally these effects seem to be significant (Takeda 1992) and this strengthens the need for further analysis of the empirical effects found for low excitation iron lines in Arcturus and by Ruland et al. (1980) in the spectrum of Pollux, and for more self-consistent modelling of metals in late-type stars, including the blanketing effects.

For molecules, the effects of departures from LTE are expected to be small for rotation-vibration bands, while the effects for electronic transitions may well be considerable (cf. Hinkle and Lambert 1975). The small effects for the ro-vibration lines have been verified by detailed calculations for CO (Ayres and Wiedemann 1989; Wiedemann and Ayres 1991) while little systematic work has been done as regards the electronic transitions. An important possible non-LTE effect on the molecules may also occur through the ionization equilibria of the parent atoms (Johnson 1994). The most obvious case where an effect of this type may be significant for the photospheric structure is that of TiO. Johnson (1994) has recently given a review of possible non-LTE effects in the spectroscopic systems of the most abundant molecules in late-type stars.

Reasonably selfconsistent non-LTE model atmospheres have been constructed for different types of early-type stars (cf., e.g., Gabler et al. 1989), but no corresponding efforts have as yet been made to solve the full non-LTE model-photosphere problem of late-type stars. Blanketed non-LTE model photospheres have, however, been constructed for the Sun (as well as for early-type stars) by Anderson (1985, 1989, 1991). Arguing that it should not be important to describe the details of the hundreds of thousands of radiative transitions that determine the structure of a late-type stellar photosphere, he developed a statistical method where the spectrum is divided into frequency bands and the quadrature points in each such band are grouped into different "radiation blocks". Each quadrature point is ascribed to a certain block, depending on whether the point represents a line core, or an inner or outer wing in the spectral line, and what type of transition the line corresponds to. The photons within each block should experience approximately the same physics – the probability for them to be created or destroyed, or scattered into other blocks, should be roughly the same. Corrections are calculated iteratively to the total energy density of radiation of each block, while the calculation of the distribution of radiation within each block is lagging behind one iteration in the algorithm. A number of simplified model atoms represent simple and complex atoms and molecules. The statistical equilibrium equations, describing the populations in these states, are eliminated analytically from the linearized equations. The method used for solving the transfer problem is a standard Feautrier technique with variable Eddington factors, constrained by the equations of radiative and hydrostatic equilibrium. Two assumptions made are those of line profiles independent of temperature and pressure for the complex atoms, and of complete redistribution. At least the first of these may in principle be possible to relax.

A main feature of Anderson's solar model (Anderson 1989), in comparison with corresponding LTE models, is that when the strong metal lines decouple from the local temperature above their thermalization depth, surface cooling by CO (which is

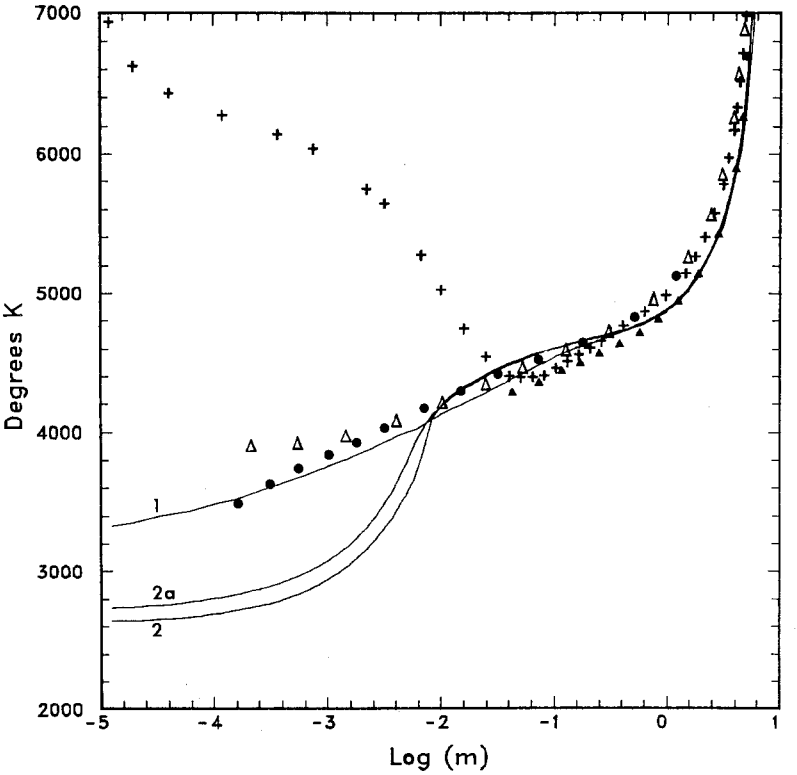

Fig. 3. Temperature vs depth, measured as integrated column mass for some solar model atmospheres. The open triangles denote the semi-empirical Holweger and Müller (1974) model photosphere, while the crosses correspond to a semi-empirical non-LTE model by Maltby et al. (1986) and the filled circles the semi-empirical model constructed by Ayres and Testerman (1981) to match the CO rotation-vibration line observations. The filled triangles denote the flux-constant (theoretical) LTE-model of Kurucz (1979) and the curve denoted by 1 a corresponding LTE-model by Anderson (1989). Model 2 is the first full theoretical non-LTE model for the solar photosphere (also from Anderson 1989) while in Model 2a atomic and molecular transitions between similar states were treated in LTE. Note the large effect of CO cooling of the surface layers in the non-LTE models. From Anderson (1989)

still in LTE) gets much more dramatic than for LTE models (cf. Fig. 3). However, this does not occur until depths smaller than those of the solar temperature minimum. In fact, for most depths below the temperature minimum the complex atoms like Fe tend to stay close to LTE, partly as a result of the UV line haze, which allows the continuum to thermalize. (A stimulating discussion of the basically astonishing result that the classical assumptions of LTE and radiative equilibrium seem to work so well for the solar photosphere is given by Rutten (1990)). Models of more metal-poor stars can, for this reason, be expected to show departures from LTE at greater depths. Such models have, however, not been constructed, except for the pioneering but schematical attempts by Saxner (1984), in spite of a strong scientific case for this project.

4.2 Convection

Until recently, the model photospheres relied on some version of the traditional and often questioned mixing-length theory, first developed for terrestrial convection by Taylor (1915) and Prandtl (1925) and applied to stellar problems by Biermann (1932) and Vitense (1953). Recent grids of models with convection of this type show hydrogen ionization convection zones in the surface layers for early F star models. These zones deepen and their uppermost layers (defined by the Schwarzschild stability criterion) sink below the visible photosphere as the effective temperature diminishes. The visible layers of the solar model photospheres are thus hardly affected by convection at all, which is contrary to what the solar granulation pattern seems to indicate. For still lower effective temperatures the hydrogen ionization convection zone goes further inwards untill, for $T_{eff} \lesssim 4000K$, H_2 dissociation again makes the surface layers convectively unstable, in particular for dwarfs. The convective flux is proportial to the density and is thus (relative to the radiative flux) more significant in dwarfs than in giants, and more significant in metal-poor stars than in metal rich ones, at a given optical depth.

The mixing-length approach not only contains several free parameters, but is also, in its local approach where a "convective element" after having moved a certain distance l halts and immediately gives its thermal energy to the local surrounding, highly unphysical for describing convection in stellar atmospheres with their small depths (on the order of l) and their rapid transition from optically thick to optically thin gas. Although more or less similar but more physically satisfactory recipes have been suggested (see, e.g., Lyndon et al. 1992; Canuto and Mazzitelli 1992) the most significant present development towards a satisfactory modelling of convection in stellar atmospheres is due to numerical simulations of photospheric convection. Of key significance for this development was the understanding that solar convective motions were measurable in photospheric spectra from line shifts and asymmetries (Dravins et al. 1981; Dravins 1982), and the use of supercomputers for simulating convection under realistic conditions, e.g., with a reasonable treatment of radiative cooling in the upper layers of the models. An illuminating discussion of the significance of radiative transfer in the upper layers of a convective atmosphere is given by Nordlund and Stein (1991). This theoretical development, initiated by Nordlund (1982), led to very important papers with Dravins (Nordlund and Dravins 1990; Dravins and Nordlund 1990a,b), where ab initio models were constructed for Procyon (F5IV-V), Alpha Cen A (G2V), Beta Hyi (G2 IV) and Alpha Cen B (K1 V) and compared in detail with high resolution spectra with, in general, a good agreement between observed and computed line asymmetries.

These numerical simulations of convection were calculated in the anelastic approximation ($\mathrm{div}\,\mathbf{u} = 0$) and with horizontal velocities constrained to be subsonic. The dependent variables, such as the velocity components, the density and the enthalpy, were represented by Fourier series horizontally and by cubic splines in the vertical direction. The boundary conditions on vertical boundaries were thus periodic. The radiation field was calculated in three dimensions, thus allowing for inhomogeneities, and line blanketing was considered by a schematic ODF treatment. Non-LTE effects in the iron ionization were also taken into account schematically. The radiative transfer equation was solved in 8 different directions in a grid with 32 vertical points defining the splines and 32×32 horizontal Fourier components. With a resolution of about 90 km in the solar case, this limited the box size to about $3\,000 \times 3000$ km, which is enough to contain a few granules. With a typical time step of 2 s each simulation

was run for a number of turn-over times of the convective motions in order to ascertain representative averages. For the Sun this corresponded to about 2 h of solar time which took about 20 h of CPU time on a Cray 1 with a highly vectorized code.

These simulations for solar-type stars suggest that convection is qualitatively similar for the different stars, with disjunct regions of slowly rising hot gas at the stellar surface that are limited by downflows which tend to concentrate at greater depths (cf. Fig. 4). However, an important finding is that the effects of convection in the visible photospheres are rather different, from the rugged surface of the model of the F-type star to the less violent convection in the K dwarf model, with considerably smaller temperature contrasts in the latter case. Also, the diagnostics – the line asymmetries – behave differently, in good agreement with observations (cf. Fig. 5). An important conclusion from these simulations (and from the solar study by Dravins et al. 1981) is that at least a considerable contribution to "microturbulence", i.e. the non-thermal strengthening of spectral lines which is usually ascribed to small scale motions, is not due to those at all but rather to motions on large scales with velocity gradients along the light rays. The simulated velocity fields show nothing like a Gaussian amplitude distribution, as is assumed in the micro/macro turbulence picture. We note, however, that an extra microturbulence addition may nevertheless be needed to describe the observed absorption line equivalent widths; however, as long as the anelastic approximation is made one can not expect the full line widths to be reproduced since sound waves are filtered out.

As regards the temperature structures the simulations strongly question the adequacy of one-dimensional models. The distribution of T-Pe points in the 3D photospheres mainly shows two regions – one hot and one cool. In particular, temperatures around the effective temperature, which are of dominating significance as spectrum forming layers in classical models, are hardly ever attained in the F-star model (cf. Fig. 6). Another result of this work is that, at least for the solar type stars, the granular size seems to scale roughly as the photospheric density scale height. This may be used to argue for the existence of giant convection cells in red giants (Schwartzschild 1975), but it is uncertain how far one may extrapolate this result.

Some of the results of Nordlund and Dravins for F stars and the Sun were obtained independently in more primitive models by Nelson (1980) and Artroshchenko et al. (1989), and also by Steffen and collaborators (Steffen et al. 1989; Steffen 1991; Steffen and Freytag 1991). The models by Steffen et al. were two-dimensional but avoided the inelastic approximation. Early models gave relatively stationary flows and smaller temperature fluctuations than Nordlund's models but later models with larger sizes and more degrees of freedom tend to be consistent with Nordlund's models.

In later work Nordlund, Stein and collaborators found it possible to relax the anelastic approximation in full 3D models (Stein et al. 1989). The equations were preconditioned by adopting logarithmic density as a dependent variable (instead of the density itself which varies by many orders of magnitude through the photosphere). Other dependent variables were the flow velocity and the internal energy per unit mass. The code was stabilized by applying artificial diffusion to the fluid equations. The boundary conditions were again periodic, and the properties of the gas and the radiation field were treated in considerable detail. With these methods a reasonable, though not perfect, agreement between statistical observed and calculated properties of solar granulation was found (Lites et al. 1989; see also the review by Spruit et al. 1990; Chan et al. 1991). Stein and Nordlund (1989) studied the topology of solar convection beneath the surface and found the downdrafts to concentrate into filaments, i.e. the topology shifts from disjunct upflow regions and connected downdrafts to the

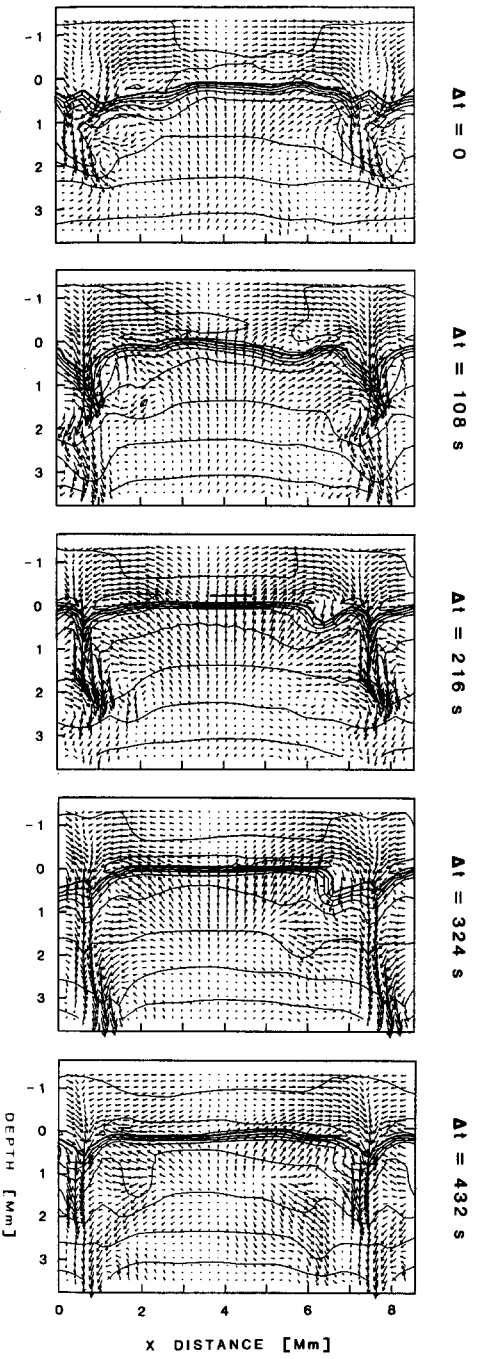

Fig. 4. Time evolution of granulation in a simulation for Procyon (F5IV-V) by Nordlund and Dravins (1990). The isothermals and the velocities are shown at five different times in a vertical plane. The cut goes across a large granule and its surrounding downflows. The bold temperature curve (the uppermost of the closely lying isothermals around a depth of about 0 Mm) is for $T = T_{\rm eff}$ =6 600 K, with others at 1 500 K intervals

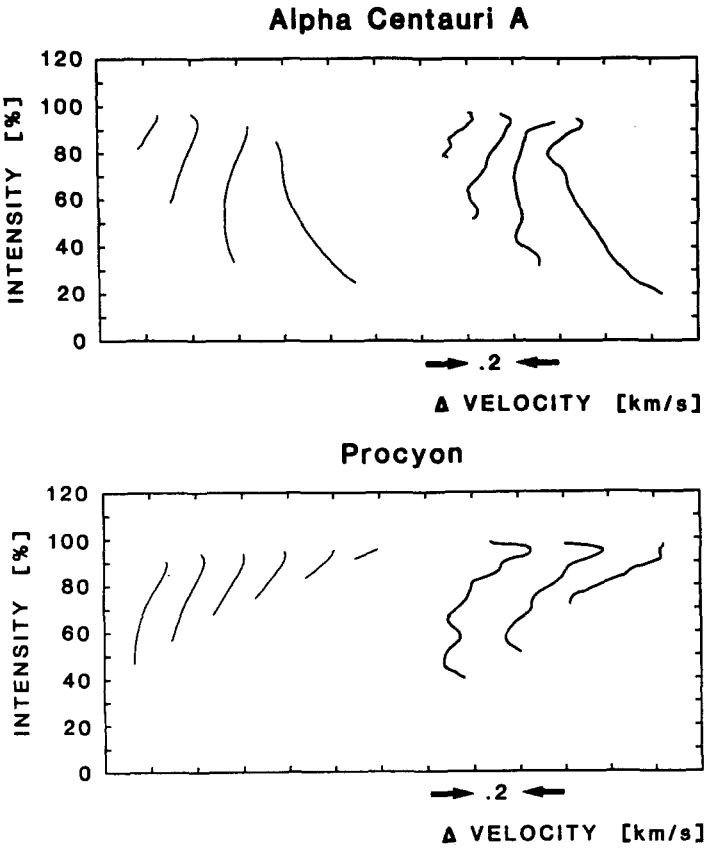

Fig. 5. Comparison between synthetic (left) and observed spectral-line bisectors for α Cen A (G2V) and Procyon (F5IV-V). Bisectors for synthetic Fe I lines of different strengths are shown and compared with corresponding observations. Obviously, the simulations are successful in reproducing the trends with line depth and the differences between the two stars. The bisectors have been given arbitrary wavelength shifts. From Dravins and Nordlund (1990b)

converse, and these filaments tend to merge at greater depths, with upflows occurring in successively larger regions. Stein et al. (1989), Stein and Nordlund (1991a,b) and Nordlund and Stein (1994) also explored various aspects of interaction between convection and waves. In a series of papers Nordlund, Stein and collaborators (e.g., Nordlund and Stein 1990; Stein et al. 1992; Nordlund et al. 1994) have also applied their methods to magnetoconvection and dynamos. In parallel with this progress, the computer development with efficient parallel computers has enabled a steady increase in the spatial resolution.

For other fundamental work on numerical stellar convection (however, with less direct application to stellar photospheres) see, e.g., the review by Cattaneo and Malagoli (1992).

It is important to note that the current improvement in our understanding of convection in late-type stars is strongly confined to solar-type Pop. I dwarfs. It may well be that convection in red giants occurs on different scales and is qualitatively different, and that convection in metal-poor dwarfs or M dwarfs severely affects temperature

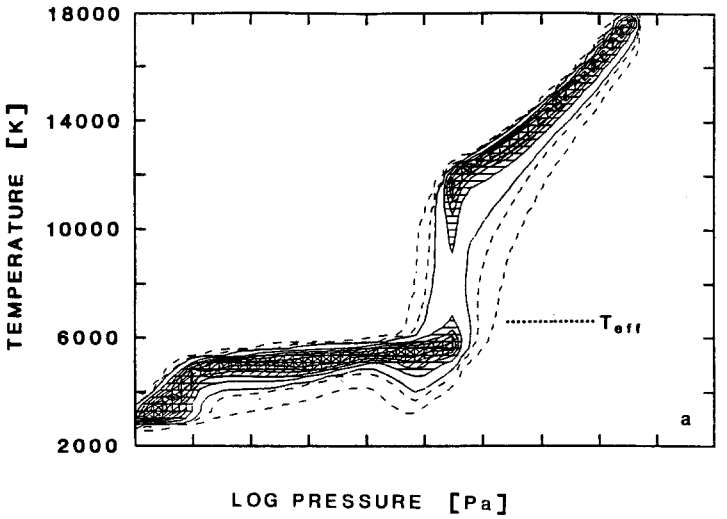

Fig. 6. Statistical properties of the hydrodynamic model of Procyon (cf. Fig. 4) during a representative sequence, showing the distribution of temperatures at different gas pressures. The outermost dashed contour contains 99% of the T-P points in the simulation, the next 95%, while the solid ones correspond to 90, 70, 50, 30 and 10%, respectively. The effective temperature ($T_{\rm eff}$ =6 600 K) is marked and is obviously not very representative for the gas in the model. From Nordlund and Dravins (1990)

structures and spectra. Also, the interaction between convection and magnetic fields may be very important, in particular for dKe and dMe stars. Similarly, the interaction between convection and pulsations may be very significant for the understanding of cool giant atmospheres. Further work, observational as well as theoretical, is obviously necessary.

4.3 Other dynamical processes

It is not possible here to review the very rich world of dynamical phenomena in stellar photospheres, on different scales in space and time, and all the interesting results that have been reached in the study of these phenomena in recent years. We shall instead confine this discussion to a few situations where the photospheric structures are directly and significantly perturbed, and where the interpretation of spectral diagnostics of the photospheres is affected.

A marginal example of this category of phenomena is chromospheric heating – the uppermost layers of the photosphere are affected by this as the temperature minimum is defined by heating mechanisms, and the depths of strong photospheric lines may be affected. Leaving the empirical results in this respect to the following section we shall here note that there is still no quantitative comprehensive theory of chromospheric heating: In the solar case it is highly questionable whether the acoustic flux is able to heat the low and middle chromosphere (see, e.g., Jordan 1991) and it is excluded for the upper chromosphere and the corona. Acoustic shocks have, however, been suggested to be of significance as a heating mechanism for the internet regions (cf. Kalkofen 1991; Carlsson and Stein 1992). The latter work is based on the first fully self-consistent time-dependent non-LTE radiation hydrodynamics calculations, with

both lines and continua, and it demonstrates clearly the significance of non-LTE for the heating and the temperature profile of the shock (as well as the power of the ALI method, cf. Fig. 7). Another demonstration of the complexity of this problem is the study of the non-linear interaction between hydrodynamic shock waves by Fleck and Schmitz (1993), which shows that the behaviour of an atmosphere excited by a broad spectrum of acoustic waves differs strongly from that disturbed by a train of monochromatic waves, since the high-frequency shocks merge and form strong long-period shock waves.

Instead of (or in addition to) acoustic waves, magnetic fields probably play a key role for the heating of the chromospheres of late-type stars, at least of the dwarfs. This makes the theoretical modelling of chromospheres a very difficult problem. However, the magnetic activity declines as the star evolves up the giant branch, and it has been proposed that at least the chromospheres of slowly rotating red giants could be controlled by non-magnetic processes such as acoustic shocks providing the observed minimal, so-called basal mechanical flux (cf. Schrijver 1987; Rutten et al. 1991). However, the recent comparison by Judge and Cuntz (1993) between predictions for an *ab initio* time-dependent chromospheric model for Aldebaran (K5 III) and observations of the C I] 2325 Å line profile shows severe discrepancies and casts doubts on whether acoustic shocks are mainly responsible even in this case.

When strong molecular lines (such as the CO rotation-vibration lines) in the infrared compete with a continuum opacity like H^-, instabilities can occur in the cooling of an optically thin gas, as was first pointed out by Ayres (1981) and Kneer (1983). This phenomenon can be of large significance for the structure of the layers around the temperature minimum of the atmospheres, as well as for the layers further out in cool stars (for the role of CO in the solar atmosphere see also Sect. 5 below). The classical model-photosphere problem may get two or more separate solutions in this case at the surface if the formation of the molecules is temperature dependent (Muchmore 1986; cf. also Scholz 1985), and domains in the temperature-density plane around at least one of these solutions may get highly unstable to perturbations. Stimulated by the discovery that the upper atmosphere of the Sun and Arcturus show a "bifurcated" structure (see Sect. 5, below) Cuntz and Muchmore (1989) calculated the propagation of acoustic waves in the outer atmosphere of Arcturus, with consideration of radiative damping through CO and SiO. They found that for weak shocks a cool molecular-dominated outer atmosphere resulted, while for strong shocks a hot chromosphere, similar to that of semi-empirical models based on Ca II and Mg II emission, was obtained. It was also proposed that these radiative instabilities, occurring when $\frac{\delta \Phi}{\delta T} > 0$ (with Φ defined in Eq. (1)) could be significant not only for solar-type chromospheres but also, with other molecules like SiO and CS, for a number of different astrophysical situations (e.g., Muchmore et al. 1987). Recently, Cuntz and Muchmore (1994) found that SiO plays a less important role than previously thought, and that a thermal "runaway" leading to very strong cooling with dust formation is not a probable result of this instability in itself. It should also be noted that the estimates of the effect as such are dependent on the assumption that the molecular lines are optically thin and that the studies of it until now do not take the detailed absorption with contribution from various molecules, including H_2O, and strong metal lines into consideration. Our own experience from work on static carbon-star model photospheres has shown that multiple solutions are sometimes obtained when a small number of strong opacity sources are considered, but that they tend to vanish when all relevant absorption mechanisms are taken into consideration. This should, however, not be confused with the dynamical effects described above, and observations of carbon star spectra do give a hint that

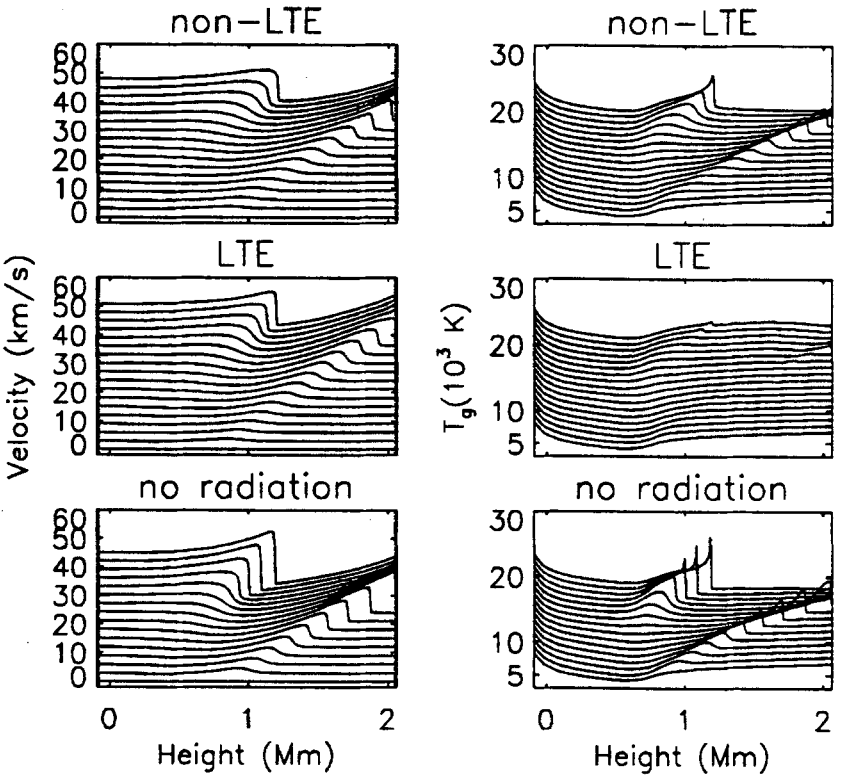

Fig. 7. Velocity (left) and temperature (right) as functions of height and time for calculations of shock propagation with time-dependent non-LTE in the solar atmosphere by Carlsson and Stein (1992). Three different cases are shown: non-LTE populations and radiation, LTE populations and radiation, and only collisional rates and no radiation, respectively. The time interval between the curves is 10 s, and the displacement is 3 km/s and 1000 K per time step. The significance of time-dependent non-LTE for the heating is clearly seen. From Carlsson and Stein (1992)

the chromosphere of also the coolest stars consist of cool and hot patches weaved into one another (Jørgensen and Johnson 1991). One should also consider the effects that departures from LTE and velocity fields may have on this phenomenon. Since many of the strong lines are decoupled from the local thermal gas, while the ro-vibration lines of e.g. CO are not, this probably increases the possibilities for instabilities.

A global effect on the photospheres is certainly caused by stellar pulsations. Although detailed observations of line splitting, photospheric velocity fields and emission lines have been performed since long (for a recent example, see the study of cepheids by Breitfellner and Gillet 1994) the modelling of these phenomena is relatively recent and still far from fully realistic. The pioneering photospheric models for cepheids by Karp (1975, and references cited therin) and for Miras by Hill and Willson (1979) were highly schematic.The hydrodynamics of Mira atmospheres and its interaction with dust formation has been treated since then with increasing technical sophistication by Bowen (1988), Fleischer et al. (1992) and Feuchtinger et al. (1993). These models show very interesting and complicated extended structures with considerable mass loss when dust-formation is allowed for. However, the radiative transfer was not considered in detail, and the photospheric spectra were not predicted. Interesting attempts to consider the radiative transfer more in detail have recently been made by Luttermoser and Bowen (1990, 1992). Bessell et al. (1989a) have constructed a grid of exploratory Mira model photospheres, assuming radiative and local thermodynamic equilibrium as well as that the shock-heated region emitting emission lines is confined to a very narrow layer, and found them to reproduce observed colours, monochromatic radii and doubled line profiles fairly well, although the observed strong emission lines are not reproduced (Bessell et al. 1994). In the early Bowen models the shocked material relaxes much more slowly towards equilibrium (cf. Beach et al. 1988) but these were found to produce spectra different from those observed according to Bessell et al. (1989a). Bowen's current models have a more sophisticated cooling mechanisms and do not seem to show this defect. Bessell et al. (1994) have more recently calculated self-consistent hydrodynamic models for Mira where molecular line blanketing was included. The formation of photospheric lines in these models was discussed by Scholz (1992) who found that the matter outflow below, and the downfall above, the shockfront may seriously affect the curve of growth, such that considerable errors in abundances may result from standard interpretation with a microturbulence parameter. In many cases, according to Scholz, the use of static models may be possible in the analysis of Miras – however, there are exceptions to this, in particular when analyzing lines of molecules dissociating at greater depths; these lines, as well as their effects on the thermal structure of the upper atmospheric layers, may be severely affected by changes in the stratification and the velocity broadening in the upper Mira photospheres.

As regards the structural effects of less regular pulsations for semi-regular or irregular variables among the cool giants the knowledge is as yet very limited; no detailed photospheric models exist where these effects have been considered or analysed. Presumably, however, these effects correspond to smaller departures from the static case than for Miras.

In spite of the absence of significant molecular absorption and dust, the hydrodynamical modelling of cepheid photospheres is not much more advanced than that of Miras. One reason for this is that the shocks are larger in amplitude and thus produce much higher temperatures, so that the cooling must be described over a large range in T and contain a number of specific processes of significance for the radiation in different spectral lines. In order to model cepheid photospheres, Sasselov and Raga

(1992) have developed a hydrodynamic code (based on the Godunov method) with a multi-level non-LTE radiative transfer treatment of H, He, and ionized Mg and Ca. The program should be applicable as long as the resulting shock waves do not dominate the energy balance. This code was recently used by Sasselov and Lester (1994) to generate time-dependent pulsating models. The resulting atmospheric structures depart significantly from static models. They, as well as the light curves, depend in a complex way on the amplitude of the piston, driving the pulsations in the bottom. The models of Sasselov and Lester (1994) do not generate the observed chromospheres which instead are added semi-empirically by the authors. It is not clear to which extent this failure may be due to remaining imperfections in the description of the complex time-dependent radiative transfer.

5 Semi-empirical models

The difficulties in calculating physically satisfactory and selfconsistent ("theoretical") models of stellar atmospheres have stimulated various attempts to derive the atmospheric structures from observations, or sooner from a combination of observations and theory. Many of these attempts were primarily aimed at finding the structure of the upper atmospheres, which cannot be modelled by theoretical models in radiative equilibrium. However, also semi-empirical models of the photospheres have been tried. Mainly following the order of the historical development, we shall start our discussion of semi-empirical model photospheres with solar models, then continue to Pop. I stars of spectral types F to K, next discuss Pop. II subdwarfs and end with the use of CO lines in studies of red giant atmospheres.

Semi-empirical models of the solar photosphere have been constructed for a long time (e.g., Lundblad 1923), and preferred to flux-constant theoretical ones, except in differential studies of solar-type stars relative to the Sun, where systematic errors in the stellar-photosphere models could be assumed to cancel to the zeroth order if solar models from the same theoretical grid were used. The semi-empirical solar model photospheres, such as those of Vernazza et al. (1976) or Holweger and Müller (1974) – the latter of which is still often used and found successful (cf. Gehren 1979; cf. also Rutten 1990) – are based on a wide range of criteria such as continuum fluxes and centre-to-limb variation at different wavelengths, and spectral line strengths. The observational information is more meagre for stars, and so one has traditionally used theoretical flux-constant models for them instead. An exception to this is the use of scaled solar models (where the $T(\tau)$ relation is just adopted from a semi-empirical model photosphere and scaled to the stellar effective temperature).

With the possibility of obtaining high-quality data for extended regions in stellar spectra, and the findings that the theoretical models are not always successful in describing these observations, the interest in semi-empirical modelling of stellar photospheres has increased. Pioneering work in this direction was based on the wing profiles of strong spectral lines. If the damping constant and the abundance of the relevant element are well known (the former, e.g. from solar observations), and if the line formation is properly understood, one may relatively easily invert the observed profile to a temperature-depth relation. Thus, Holweger and his collaborators modelled the photospheres of the red giants Arcturus (K2 III, Mäckle et al. 1975) and Pollux (K0 III, Ruland et al. 1980). These red giant models were essentially based on the profiles of the Mg b lines, Na D lines, the Ca II H and K and IR triplet lines, the Ca I 4226 Å line and the Fe I 4383 Å line. The models were some hundred de-

grees cooler in the optical-depth interval $0.001 < \tau(\text{cont}) < 0.01$ than corresponding flux-constant models from the MARCS program (Gustafsson et al. 1975; Bell et al. 1976). A similar attempt, though based only on the K line, was made by Desikachary and Gray (1978) who found opposite tendencies for red giants when comparisons with flux-constant MARCS models were made. Drake and Smith (1991) rediscussed strong Ca I and Ca II lines in the photosphere of Pollux, allowing for departures from LTE. They found the MARCS model more successful in reproducing the line wings than the semi-empirical model by Ruland et al. (1980), but also constructed an empirical model of their own for the star, in rather close agreement with the flux-constant model.

Another early attempt in empirical modelling of red giant stars was made by Peterson (1976), who used excitation equilibria of metal atoms to construct empirical models of two K2 III stars, κ Oph and μ Leo, in a study of the so-called super-metal-rich stars – μ Leo is the prototype of this phenomenon. She found indications that μ Leo has a surface temperature about 200 K cooler than that of κ Oph, and ascribed the SMR phenomenon entirely to the steeper temperature gradient – an interpretation that is in conflict with more recent abundance determinations from weak metal lines that actually confirm the star to be metal rich (cf. Branch et al. 1978; Gratton and Sneden 1990).

Semi-empirical models of upper photospheres of giants and dwarfs were also constructed by Linsky and collaborators already in the 1970s (cf. Linsky 1980 and references quoted therein) on the basis of Ca II H and K and Mg II h and k lines, but the main emphasis was then on the chromospheres and the temperature minimum region. One example of this impressive work is the models by Kelch (1978) for the active chromosphere dwarfs 70 Oph (K0V) and ϵ Eri (K2V). Kelch had to increase the temperature in the upper photosphere, relative to contemporary Kurucz models, in order to fit the wings. More recently, Thatcher et al. (1991) modeled the ϵ Eri photosphere, matching flux profiles of the Ca IR triplet, Hα and Hβ, the Na D lines and the Ca II H and K lines with non-LTE calculations. They found that the Kelch photosphere does not fit the Na D lines very well and constructed a rather different model, which, e.g., departs from a MARCS model with corresponding fundamental parameters by several hundred K at $\tau_{5000} = 0.1$. Drake and Smith (1993) tested different models for ϵ Eri in attempts to reproduce the Ca II 8542 Å triplet line and found the MARCS model, and even more so a scaled solar model, to reproduce the line better than the Thatcher et al. model. In particular, they found no indication of a temperature increase in the upper photosphere, related to the enhanced chromospheric activity. One should also note that Steenbock (1983), from studying the spectra of 4 G5-K2 dwarfs in the Mg b 5172 Å region, found that scaled solar models give a better fit than flux-constant ATLAS6 models (Kurucz 1979). For the hotter Procyon (F5IV-V), however, Steffen (1985) concluded that a flux-constant ATLAS6 model with appropriate convection parameter reproduced the K and H line wings better than a scaled solar model, while the ATLAS6 model for the Sun was not very successful.

Summing up the results for Pop. I stars of spectral types F – K we conclude that there are indications from strong line profiles that the flux-constant models are not always optimal. However, the empirical models that have been constructed until now have not been entirely successful; they are rather dependent on what lines are used and on the quality of the observations. It seems that forthcoming efforts in this area should be based on more comprehensive data sets of very high quality.

Other stars that are sufficiently different from the Sun, and sufficiently important from an application point of view to warrant attempts of semi-empirical modelling, are

the Pop II subdwarfs. Magain (1985) found that the continuum fluxes of the prototype subdwarf HD 19445 and of the somewhat more evolved HD 140283 were not matched very well by MARCS models – the models seemed to be too faint in the blue, and the effective temperature as estimated from the blue-visual flux was significantly higher than that judged from the infrared flux. (A possible but smaller effect of this type was also traced and discussed by Gustafsson and Bell (1979) for Extreme Pop II giants.) Also the ionization equilibrium of iron was found by Magain (1985) to be not well reproduced by the MARCS models. Magain adjusted the temperature structure of the models to match the observations, and obtained models with much greater temperature gradients. However, Bell and Oke (1986) did not verify the mismatch in UV flux for HD 19445, nor did they trace any similar effects for 3 other subdwarfs. It is also not certain that Magain's model adjustment is valid in principle. Temperature inhomogeneities may be the cause for the continuum flux discrepancy, thus "broadening" the flux distribution as compared with plane-parallel homogenous model photospheres. Although the high densities make these inhomogeneities less pronounced for dwarfs than for giant stars, the transparency of the photospheres in the blue and ultraviolet in low metallicity stars makes it more probable that one should see effects of convective inhomogeneities in Pop.II sub-dwarfs than for more metal-rich dwarfs. Departures from LTE most probably affect the excitation equilibrium. Magain (1985) found his revised models to reproduce the line wings of Hβ and the Ca II K line. We note in passing that Smith et al. (1992) found the Ca II triplet 8542 Å line of the subdwarf Groombridge 1830 to be very well reproduced by a standard MARCS model, while e.g. a scaled solar model has a temperature gradient which is far too steep.

Recently Fuhrmann et al. (1993) showed that the Balmer Hα and Hβ lines together form a powerful tool for studying the deeper photospheric structure of the subdwarfs. Within the standard model framework, strong restrictions are given by these line profiles on the parameters of the mixing-length theory (cf. Fig. 8). (E.g., the choice of these parameters of Kurucz (1979) is shown to lead to discrepancies while the choice made for the MARCS dwarfs models seems to lead to hydrogen line profiles more consistent with observations.) Note, however, that it is very questionable whether this "theory" and the assumption of plane-parallel stratification may at all be trusted enough to motivate detailed fits of quantities with little and unclear real physical meaning.

In this connection it is also worth pointing out the long standing discussion on the discrepancy between ratios of oxygen to iron abundances for metal-poor stars, when estimated from the high excitation O I triplet lines at 7774 Å, as compared with other lines ([O I] 6300 Å or OH lines). The high abundances determined from the triplet lines are not easy to explain as a non-LTE effect (Kiselman 1993). Although a revision of the temperature scale for the subdwarfs may be one explanation for the discrepancy (King 1993) it may also contain new information on the deep temperature structure of these stars (cf. Bessell et al. 1991) or on temperature inhomogeneities in the atmospheres (Kiselman 1993). Similarly, other high excitation lines, as well as pronounced low-temperature lines such as molecular bands, contain diagnostic power for these stars which has hardly been exploited as yet. In general, systematic work with many spectral criteria modelled in non-LTE is to be recommended in further efforts to construct semi-empirical models of these stars. One opportunity for cooler metal-poor stars which has not been used is offered by the increasing free-free absorption towards longer infrared wavelengths. Accurate IR fluxes could thus be measured and used for modelling the temperature structures of these stars.

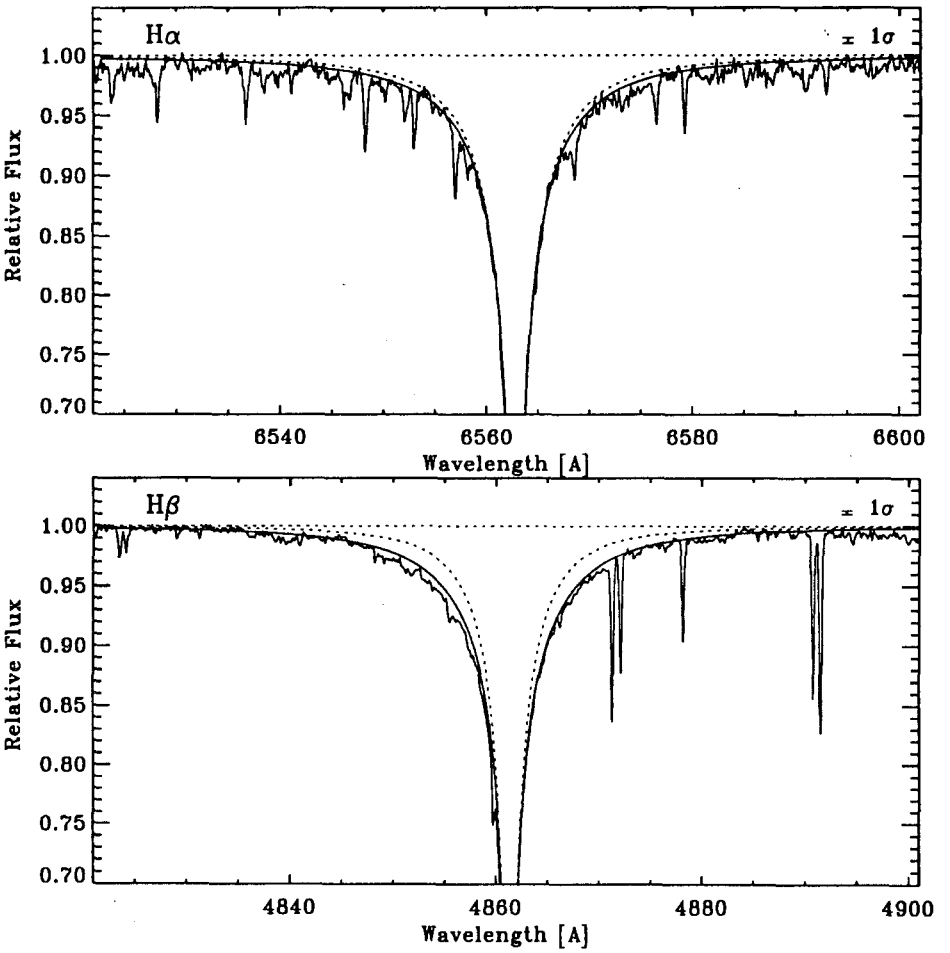

Fig. 8. Profile fits for Balmer lines in the spectrum of the Extreme Pop. II subdwarf HD 140283. In addition to the observed profiles models with mixing length $l = 0.5\,H_p$ (full line) and $l = 1.5\,H_p$ (dotted line) are shown. Obviously, the effects of mixing length convection on the spectra are considerable in this case. From Fuhrmann et al. (1993)

For the coolest stars suitable criteria for modelling the temperature structures are not only, or primarily, the wings of strong lines and continuum fluxes (even if the last remark above for the metal-poor stars may also be relevant here) but in particular the molecular bands. The rotation-vibration lines (of the ground electronic state) may be used for mapping the temperature structure assumed to be essentially formed in LTE (Hinkle and Lambert 1975) and have different (and known) relative strengths and thus formation depths. A demonstration of this potential is the work of Sauval et al. (1984) on the pure rotation spectra of OH in the Sun, where a consistency in abundances for different lines puts strong constraints on models of the solar photosphere (favouring the Holweger-Müller (1974) model). Much of the contemporary use of the possibilities of the ro-vibration lines has, however, been concentrated on comparatively strong CO lines.

Heasley et al. (1978) observed the CO fundamental ($\Delta v = 1$) bands at 4.6 μm in the spectrum of Arcturus (K2 III) and found the lines to be so strong and deep that they could not be matched with models with a relatively high temperature minimum, needed to fit the wings of the Ca II H and K lines. The authors ascribed this to the existence of temperature inhomogeneities in the upper photosphere, the hotter regions being visible in the Ca II wings, the cooler ones in the CO lines. Ayres and Testerman (1981) observed the same bands in the solar spectrum and demonstrated the existence of large amounts of cool material at high altitudes in the solar photosphere, suggesting a dichotomy in the temperature structure with differences at an optical depth τ_{5000} of about 10^{-5} of more than 1000 K (cf. also Noyes and Hall 1972!). This idea was further explored and elaborated in a study of solar CO $\Delta v = 1$ and 2 bands and Ca II K lines by Ayres et al. (1986). Kneer (1983) suggested that the dichotomy is due to an instability caused by radiative CO cooling; however, the first simulations of such instabilities overestimated the cooling since optical-depth effects were not considered, and the study by Mauas et al. (1990) suggest that CO cooling may not fully account for the cooling of the gas at the temperature minimum of the solar atmosphere.

In a new series of papers Ayres, Wiedemann and collaborators have further explored the CO lines as diagnostics for upper photospheres. Ayres and Wiedemann (1989) reinvestigated the non-LTE effects for the fundamental bands and found them to be negligible for solar models, and of minor importance for the spectrum of an Arcturus model. They applied their procedures to a grid of model atmospheres of late-type stars (Wiedemann and Ayres 1991) and compared the resulting spectra to high resolution spectra of a number of stars, primarily giants, from spectral type F5 to K5 (Wiedemann et al. 1994). They found a decrease in temperature with increasing height in layers where the chromospheric models show a temperature increase. The upper layers of MARCS model photospheres for these stars are in radiative equilibrium. Wiedemann et al. (1994) found that these models, extrapolated out into the CO forming layers, reproduce the CO line profiles well for the cool stars (later than K0) while the earlier ones have higher surface temperatures, as judged from the CO line cores, than the models. The authors ascribe this phenomenon to a larger areal filling factor of the chromosphere among the earlier spectral types.

Also for the coolest red giant stars the strong CO lines reveal complex atmospheric structures. Analyzing the first overtone ($\Delta v = 2$) CO spectra of M giants, Tsuji (1988) traced the presence of a cool extra molecular layer, presumably distinct from the photosphere and at low velocity relative to it. For the second overtone ($\Delta v = 3$) bands, formed deeper in the photosphere, he found excitation equilibria in good agreement with flux-constant model photospheres (Tsuji 1991). In a traditional model-photosphere analysis, however, the resulting microturbulence parameters and

the abundances were found to be systematically different for the different overtones, and the author interpreted this, together with the line shifts, as an indication that systematic velocities and velocity gradients from granular motions affect the line widths in complicated ways.

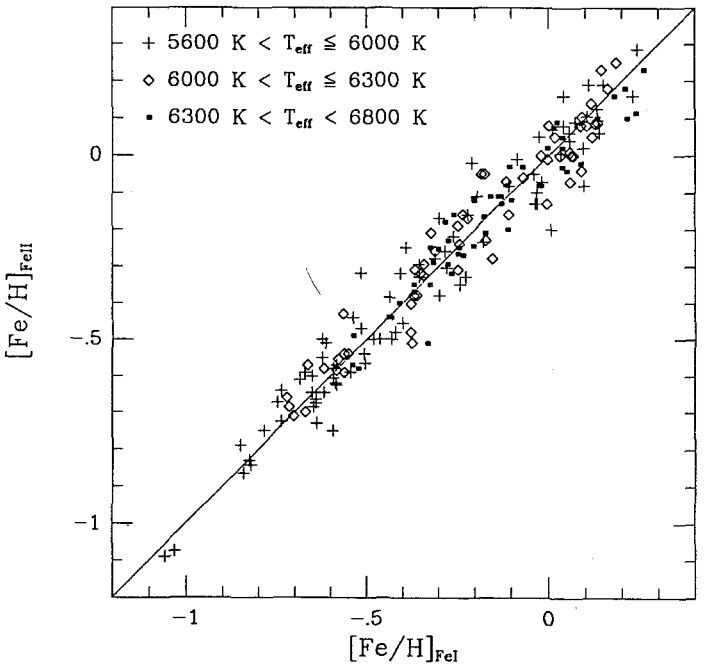

Fig. 9. Iron abundances derived for almost 200 solar-type disk dwarfs by Edvardsson et al. (1993) from Fe I and Fe II lines, respectively. The symbol for each star depends on the stellar effective temperature. The line in a line with a slope of 1.0. The fundamental parameters of the stars were determined from uvbyβ photometry, and the consistency between lines from Fe I and Fe II is therefore an independent check on the procedure and the model photospheres, a check that in this case gave a quite satisfactory result

Johnson (1991) and Jørgensen and Johnson (1991) discussed the outer atmosphere of the N0 star TX Psc, for which a semi-empirical model chromosphere has been constructed to match the observed Mg II h and k lines (Eriksson et al. 1986; Luttermoser et al. 1989). The point is now that this model chromosphere does not match the deep CO line cores observed for the star, nor does it match any stationary wind model, constructed to produce the observed mass loss. The conclusion that the upper atmosphere of this star also is inhomogeneous seems hard to escape.

The current development in stellar spectroscopy, of crossed echelle spectrometers and large two-dimensional detectors guarantees that major portions of the stellar spectra will often be attainable at high S/N and high resolution for many stars under relatively detailed study. Thus, information on the state of the photosphere will often be overdetermined in spectral analyses, containing far more than only information on the classical fundamental parameters of the star. It will be possible to check the model atmosphere and its temperature structure and, if necessary, to improve it. This may often be recommended in studies of single stars, but may also introduce unnecessary inhomogeneities when stars or results from different studies are to be intercompared. A notable strength in, for example, survey studies of the type performed by Edvards-

son et al. (1993) for 189 solar-type disk stars, and which certainly brought down the spurious errors, was the use of one homogeneous grid of model photospheres (cf. Fig. 9). As is indicated by the results presented above, existing empirical models are not unambiguous but depend on the observational criteria selected, on spurious errors in these criteria, and on other circumstances. However, there is also a more fundamental argument against too much fitting with $T(\tau)$ relations.

The basic shortcomings of standard late-type model photospheres lie not only in their $T(\tau)$ (i.e., essentially in the uncertainty in the mechanical (convective etc.) flux as a function of depth), but at least as much in the assumption of homogenous, plane-parallel stratification. One may therefore ask whether it would be possible to attempt systematic semi-empirical modelling with inhomogeneous spherical models. Observable criteria should then also include velocity shift and bisectors of spectral lines, and intensities of spectral lines most sensitive to the effects of temperature inhomogeneities. Simple schemes of this sort have been discussed, e.g., by Gray and Toner (1985), Gray (1989) and by Dravins (1990). It may even be conceivable that the dynamic simulation of compressible convection could be tried in such models; then in analogy with the semi-empirical modelling discussed for plane-parallel models one would relax the condition that the depth derivative of the mean of the total energy flux over satisfactorily large horizontal surfaces is zero. Such a scheme, replacing the simple hydrostatic equilibrium equation with the full dynamical treatment, would then be complemented with a calculation of the 3D radiative transfer in non-LTE for the criteria used for modelling – as a result the corrections to the flux derivative at each depth could be estimated. However, it is not at all clear that such detailed semi-empirical models will be needed – it remains as yet to be seen whether 3D hydrodynamical *theoretical* models suffice to describe the stellar spectra satisfactorily. This theoretical route should, in fact, in our opinion be systematically explored before too extensive efforts are made in semi-empirical modelling of photospheres.

6 Conclusions

It should be clear from the discussion above that considerable improvements have been made in recent years in the modelling of late-type stellar photospheres. This is true concerning "classical modelling", where the step from assuming plane-parallel stratification to spherical symmetry has been taken, and found to be significant for supergiants and cool giants. Most important is the very impressive improvement in the quality and volume of atomic and molecular data, in particular data for line blanketing. Significant improvement has also occurred with new methods for studying "non-classical" aspects of the photospheres, such as new numerical methods for non-LTE calculations and convection and other hydrodynamical processes, which have enabled simulations that bring new fundamental insights into the physical intricacy of these systems. At least as important are new observational developments, which enable systematical studies of the non-thermal properties and dynamics of the photospheres. The very impressive improvement of high-resolution spectroscopy is most significant among these developments; this also includes the widening of the spectral range into the vacuum ultraviolet and the infrared with high spectral resolution and high S/N for apparently faint stars. Other significant new observational results include studies of photospheric radii and structures by means of interferometry of giant stars, mapping of surface structures by Doppler-imaging, and measurements of magnetic fields on

late-type stars. Recent studies of the spatial and dynamical structure of the solar photosphere are also very important contributions.

One may ask, with this background: What major further improvements in the photospheric models are possible today, and which are likely to occur in the next few years to come? And *how important* would it be to get this done?

For solar-type stars of different metallicity a detailed survey with synthetic spectroscopy should be pursued to find out to what extent the missing-opacity problems are now solved, as a result of the new atomic and molecular data. Since there are indications, discussed above, that problems still remain in this respect, it is very important that this work precedes further extensive calculations of detailed photospheric models and spectra. It should be possible to carry out studies of non-LTE effects, and their effects on the temperature structure as a function of metallicity (in particular for subdwarfs), although the result will be dependent on the uncertain collision cross sections. Also, 3D convection models should be calculated for these stars and compared to observed line bisectors, and the effects of using these models, e.g. on the calibration of colours and in abundance analysis, should be explored. Furthermore, the coupling between the thermal inhomogeneities and the non-LTE effects should be investigated in these cases. (This coupling probably strengthens the non-LTE effects.) Finally, empirical models, based on accurate and comprehensive spectroscopic and spectrophotometric data should be attempted for the subdwarfs.

In view of the great significance accurate abundance analysis of these stars has for the study of the early evolution of the Galaxy, and the importance of that field for other areas of astronomy and cosmology, it seems very worthwhile to carry out the projects listed above.

For G and K giants a most important effort is to explore the possibilities of 3D convection models. For these stars the relevant scales of convection are still unclear, and it is not obvious that the essentials of the phenomenon can be described within the limited spatial scales possible to consider today in detailed simulations. However, attempts are worthwhile and results should be compared with observed line profiles and also semi-periodic low-amplitude velocity variations observed for several of these stars. New detailed studies of non-LTE effects with differential comparisons between stars of different temperatures, pressures and metallicities should also be possible and rewarding.

Stars of this type dominate the light and appearance of elliptical galaxies and centres of spirals. Many of the most interesting ones may, however, have properties that are not common in the solar neighbourhood, such as very high metallicities. It seems very important to put the modelling of them on a more sound footing and this certainly requires the work suggested above.

For M, S and C giants a large amout of work remains before one has reached the applicability that already characterizes the classical models of solar-type stars. Further efforts on molecular line lists for blanketing and synthetic spectra are necessary. Dynamical processes in these photospheres, and their interaction (such as the interaction between convection and pulsation, or mass loss and molecular formation), need a number of more or less schematic model studies - we are certainly far from a "unified model atmosphere" of these utterly complex systems. Another area that motivates exploration is the effect of dust formation in the outer layers on the photospheres. In this situation, semi-empirical modelling, both of temperature structure and velocity fields, should be tried systematically, using in particular the ro-vibration molecular lines.

The role of these stars in nucleosynthesis and for the understanding of stellar evolution certainly motivates further exploration of their photospheres. Moreover, their role as distinguishable tracers of structure and evolution in nearby galaxies give further reasons to considerably improve the modelling of their spectra.

Similarly, the *supergiant stars* are of great significance; however, in these cases theoretical modelling beyond the "classical" spherically symmetric models is not very immediate. Non-LTE effects in the line calculations can be considered and are probably often important since the density in the gas is so low. Even non-LTE effects on the structure may be taken into consideration, but the effects of the more or less regular velocity fields on the structure and the departures from spherical symmetry connected with these fields and with the strong radiative pressures are still beyond realistic ab initio modelling. Here, semi-empirical models, based on monitoring of the stellar spectra, seem more promising.

Many *K and M dwarfs* are within reach of the new infrared spectrometers and this may motivate more ambitious modelling than the present classical models. It is not clear, however, how good these models are for the K dwarfs. The convection effects seem less significant there than for the solar-type stars. If the present lists of atomic and molecular lines are satisfactory for these stars – which is not known – and the damping treatment, which is important since the pressures are high, is realistic enough – which is not known either - then the K dwarfs may well be the type of stars for which the classical models are most successful! For the M dwarfs the comparisons between observed spectra and current models show, in spite of considerable progress in the modelling in recent years, that substantial improvements in the molecular data are needed before fully satisfactory models can be computed. Of immediate need are good f-values and line lists for VO, FeH and CaOH band systems, and more knowledge about pressure broadening (cf. Fig. 10, Kirkpatrick et al. 1993).

For the *brown dwarfs* and the *coolest white dwarfs* also more work on molecular line absorption, e.g. from CH_4, as well as collisionally induced absorption is very important before, e.g. the photometric properties of these objects can be accurately predicted.

With many recommendations here to do more profound and detailed work in the field of stellar photosphere modelling, one may finally ask whether the authors, themselves at least part-time occupied in efforts of this kind, are not mainly advocating their own business, in a perfectionism that actually is not needed in most applications of models in a science often, by tradition, happy with order-of-magnitude estimates. This is not so. The reasons are that

1. in comparison with investments in new stellar spectrometers and their feeding telescopes, the manpower necessary to *very substantially* improve the modelling of stellar photospheres, and thus of the analysis of the spectra obtained with these spectrometers, is *very limited*,
2. the major uncertainty in, e.g., abundance analysis with modern spectrometers is not due to the observational errors, nor to errors in the underlying laboratory data, but to the uncertainties in the models of the photospheres, and
3. we have very good reasons to believe that a higher accuracy in analysis of stellar spectra in general will reveal important new phenomena and structures, some of them of fundamental significance for the understanding of our universe, and many of them of great interest in themselves.

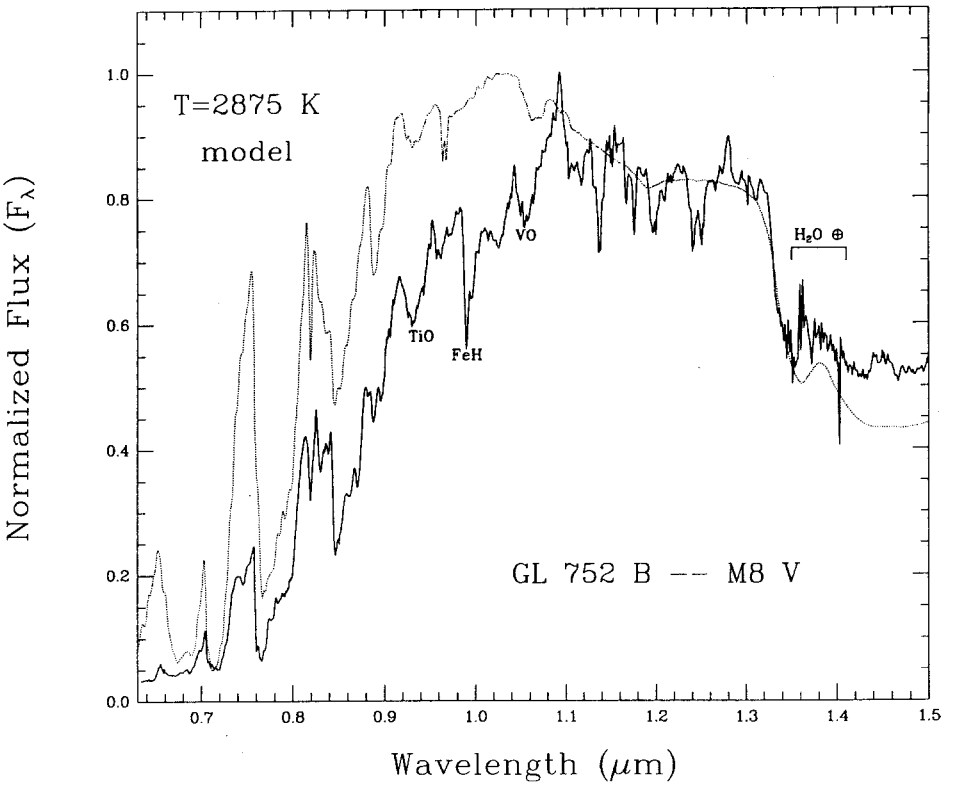

Fig. 10. The spectrum of the M8 dwarf GL 752 B as compared with that of a model photosphere by Allard (1990), chosen to give an optimal fit in the red. Recent experiments with improved f-values of the TiO systems gave considerably better agreement with the observed spectra (Allard 1994), but fully satsifactory model and spectrum computations will have to await detailed line lists and bettter estimates of f-values for VO and FeH. From Kirkpatrick et al. (1993)

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