Opacity Problems in Cool Low Mass Stars

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1 Introduction

In this contribution we want to discuss M star atmospheres and their dependence on molecular opacities. A star belongs to the spectral class M if its optical and infrared spectrum shows strong bands of TiO and numerous strong metal lines so that for wavelengths < 4000 Å there is "hardly any flux left" (Jaschek & Jaschek 1987). M stars cover a very large range in luminosity: M dwarfs are the intrinsically faintest stars, whereas M giants and supergiants reach luminosities that are among the highest known. General properties of these objects are given in Table 1 (after Schmidt-Kaler 1982).

A good knowledge of M star spectra is of crucial importance for the understanding of the properties of the Milky Way (and other galaxies as well) for the following reasons (see also Lambert, this volume, and Liebert, this volume):

- M dwarfs have a space density of about 0.1 pc^{-3} and therefore constitute about 80 % of the total number of stars in the solar neighborhood. Although their individual masses are very low, their large number even let them dominate the mass distribution.
- Since the luminosity of stars varies approximately with mass $\propto M^{-3.2}$, M dwarfs evolve very slowly. Therefore, M dwarfs of very different ages can be found and the abundances of metals in their atmospheres reflect in most cases (possible exceptions may be the carbon dwarfs, see Green et al. 1992, and Liebert, this volume) the abundance distribution of the Galaxy at the time of their birth. In other words: from the understanding of the M dwarfs we can get a full account of the chemical evolution of the Milky Way.
- M giants return large amounts of heavy elements to the interstellar medium where the enriched gas is used for a subsequent generation of stars.
- Due to their high luminosity M giants often dominate the integrated (infra)red light of galaxies.

Unfortunately, spectrum formation is extremely complicated in these stars so that we are only now starting to obtain models that can be used for spectral analysis. Up to very recently, understanding was also hampered by the fact that reliable and reasonably high resolution spectra in the region of maximum flux were not available. The progress in infrared detector technology in the last years made it possible that now even for extremely faint stars digital spectra with resolutions sufficient for detailed analysis are available (G. Rieke, private communication). Another jump is expected with the ISO satellite to be launched 1995.

In the next section we describe in some detail the temperature and pressure stratifications in these stars and comment on the geometrical extension of the giants. Section 3 is devoted to a discussion of consequences of errors in the opacities, in particular we address the run-aways in giant atmospheres that may occur when water vapor forms and we point to the fact that the convection in the dwarfs extends from very shallow layers to the center so that errors in the outermost parts propagate through all parts of the object. In Section 4 we review the present agreements and disagreements between synthetic and observed spectra. Based on this discussion, in Section 5 a list of most urgently needed molecular data for future improvements of M star models is presented.

Table 1. Approximate physical parameters of M stars (after Schmidt-Kaler 1982); note that the luminosities of dwarfs are lower by a factor ≈ 2 after Kirkpatrick et al. (1993)

	dwarfs	giants/supergiants
luminosities $/L_\odot$	10^{-3}—8×10^{-2}	3×10^2—3×10^5
radii $/R_\odot$	2×10^{-1} —6×10^{-1}	4×10^1—2×10^3
masses / $M_\odot$	0.06—0.5	1—24
eff. temperatures (K)	2600 —3800	2600—3800
log gravity (cgs units)	4.6 —4.9	−1—1

2 Structure of M star atmospheres

In Fig. 1 we show the pressure distributions in some giants and in dwarfs as a function of the radial coordinate r: giant atmospheres are in many cases geometrically extended (both in relative and absolute terms) and their pressures are relatively high in spite of the low gravity; in fact, the pressures are comparable to those in the solar photosphere (see Vernazza et al. 1981). This is a consequence of the fact that the absorption coefficients are very small (e.g. H^- absorption is very weak due to the lack of electrons) and therefore photons can traverse large column densities. In contrast, the atmospheres of dwarfs are extremely thin (typically a few hundred kilometers compared to a radius of 1 to 4×10^5 kilometers) so that a comparison of different cases is hardly possible in this representation.

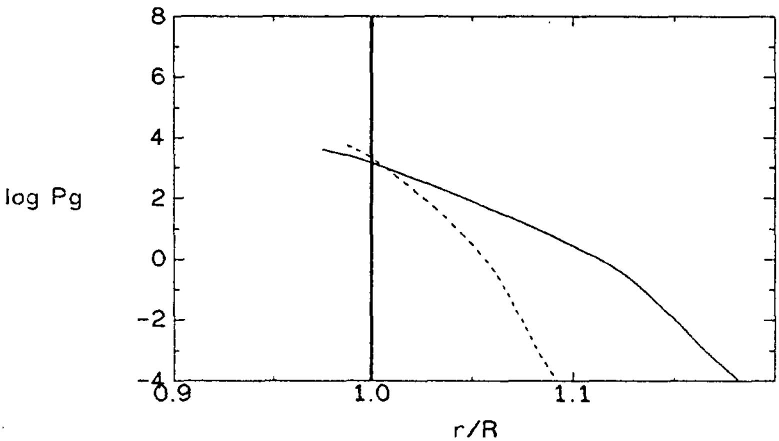

Fig. 1. Gas pressure distributions in M stars plotted as function of the normalized radial coordinate. The thick vertical line indicates the pressures in dwarfs, the broken curve refers to a giant model with parameters: M=1 $M_\odot$, L = 500 $L_\odot$, R= 83 $R_\odot$, the full curve to a giant model with M=1 $M_\odot$, L = 2000 $L_\odot$, R = 166 $R_\odot$. All models have solar composition. Note the compactness of the dwarf atmospheres compared to the large geometrical extension of giant models, in particular if they have high luminosity.

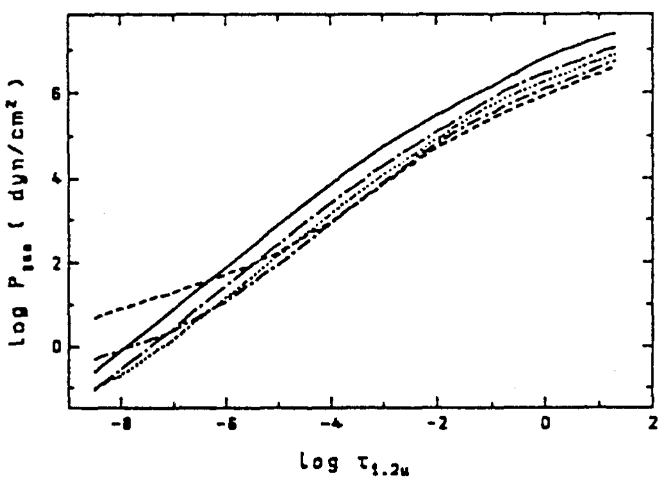

Fig. 2. Typical gas pressure distributions in M dwarfs (after Allard 1990) plotted as a function of the optical depth at 1.2 μm. The curves refer to models with effective temperatures of 2000 (—), 2500 (-.-), 2750 (...), 3000 (-.-.) and 3250 (- - -) K, solar metallicity, and $\log g = 5$.

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Table 2. Parameters of giant models (see Bessell et al. 1989). The models X350H and X350C represent two solutions of the structure equations with the same parameter set (see text).

model	luminosity/$L_\odot$	mass/$M_\odot$	radius/$R_\odot$	T_{eff}	log g	chem. comp.
ZZ300	2×10^3	1	166	3000	-0.00	3× solar
Z300	2×10^3	1	166	3000	-0.00	solar
WW300	2×10^3	1	166	3000	-0.00	0.1× solar
X350C	10^4	1	273	3500	-0.44	solar
X350H	10^4	1	273	3500	-0.44	solar

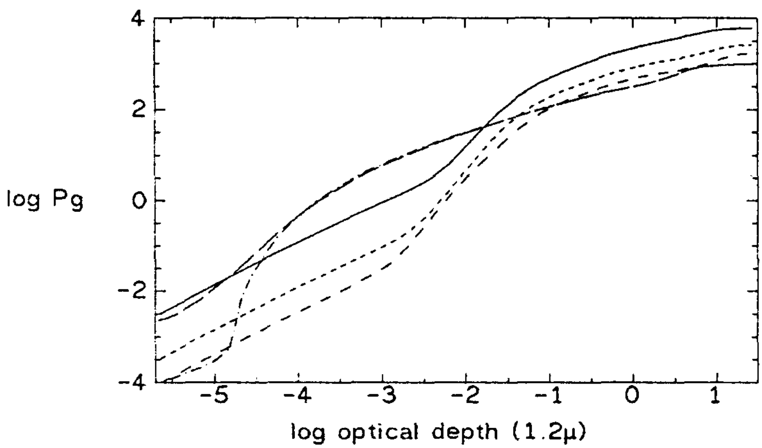

Fig. 3. Same as Fig. 2 but for the giant models ZZ300 (- - -), Z300 (– – –), WW300 (—), X350C (– . –) and X350H (— —). The model parameters are given in Table 1.

Therefore, we give in Figs. 2 and 3 the run of the pressures as a function of the optical depth at 1.2μ (which in most cases is similar to the Rosseland depth). From this representation it is obvious that the gas pressures in the dwarfs are 2 to 5 orders of magnitude higher than in the giants and therefore are comparable to those in cool white dwarfs. A reduction in the metallicity can further dramatically increase the pressures. This ensues from the fact that molecules make up the opacity and that their abundance depends usually quadratically on the metallicity.

The corresponding temperature distributions (Figs. 4 and 5) also show significant differences between dwarfs and giants: in the outer (optically thin) parts the dwarfs have to a very good approximation a constant temperature whereas for the giants it drops $\propto 1/\sqrt{r}$ as a consequence of the geometrical extensions

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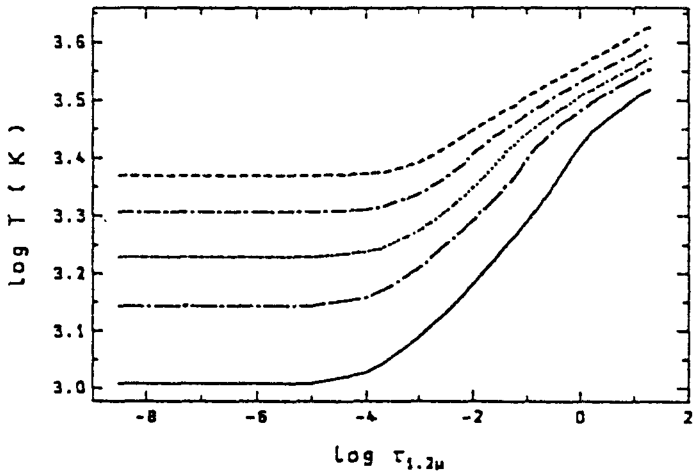

Fig. 4. Same as Fig. 2 but for the temperature distribution

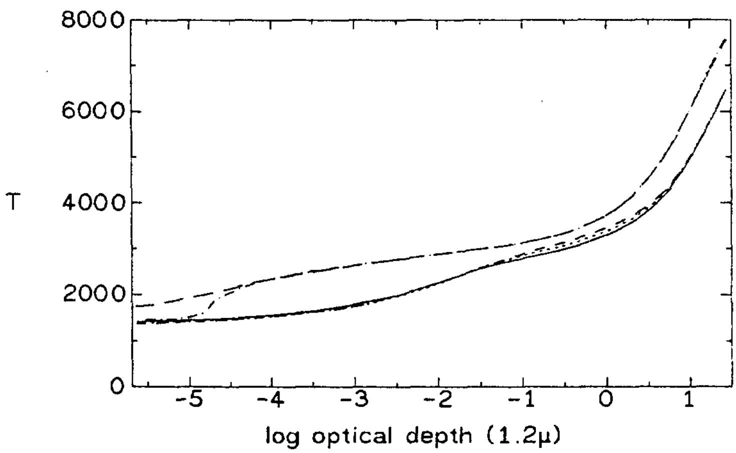

Fig. 5. Same as Fig. 3 but for the temperature distribution

of the atmospheres (in principle, the same is true for dwarfs; however, here the density decrease is so rapid at practically constant r that this effect is not seen in the spectra). On the other hand, in the inner parts, the temperatures of giants rise very fast since all energy is transported by radiation, whereas for the dwarfs convection reduces the temperature gradient strongly. Therefore, for identical effective temperature the giants' temperatures are lower in the outer atmospheric layers and much higher in the deeper layers than the temperatures for dwarfs.

These pressures and temperatures imply that the photospheric extinction in M stars is essentially determined by molecular absorption (whereas in so-called

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infrared stars significant amounts of dust seem to form inside the photosphere). Figs. 6 - 11 give the runs of the partial pressures (normalized to the total gas pressure) of some molecules that play an important role for the atmospheric structure.

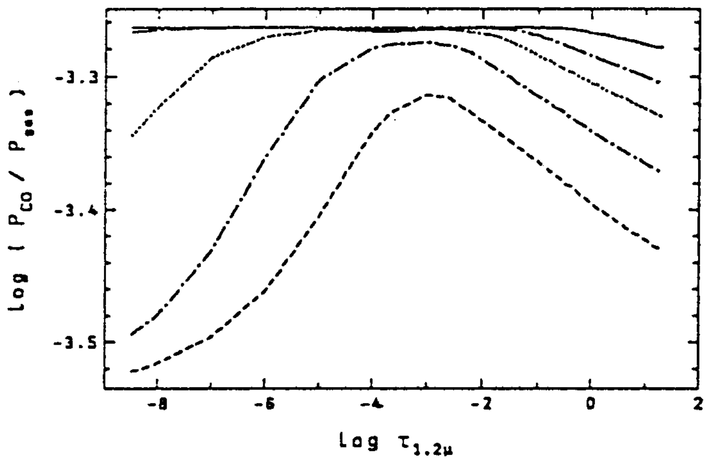

Fig. 6. Partial pressure of the CO molecule (normalized to the total gas pressure) as a function of the optical depth at 1.2 μ in dwarf atmospheres (from Allard 1990).

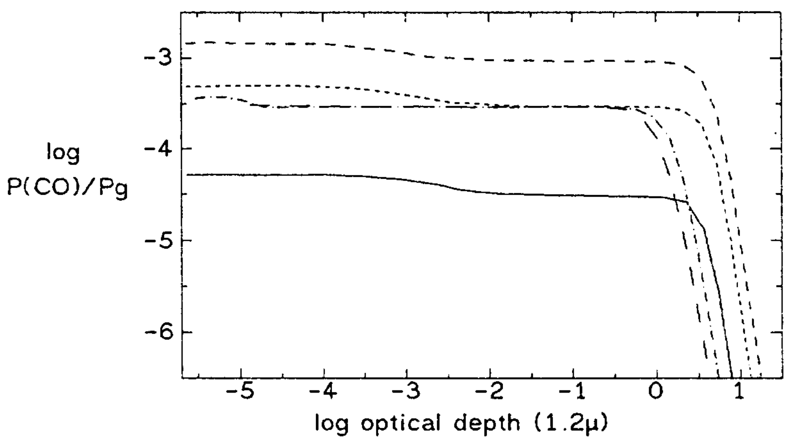

Fig. 7. Same as Fig. 6 but for the giants of Fig. 3

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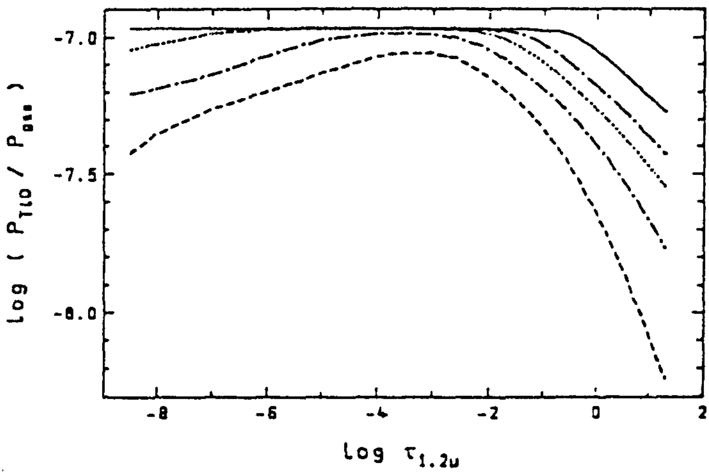

Fig. 8. Same as Fig. 6 but for TiO.

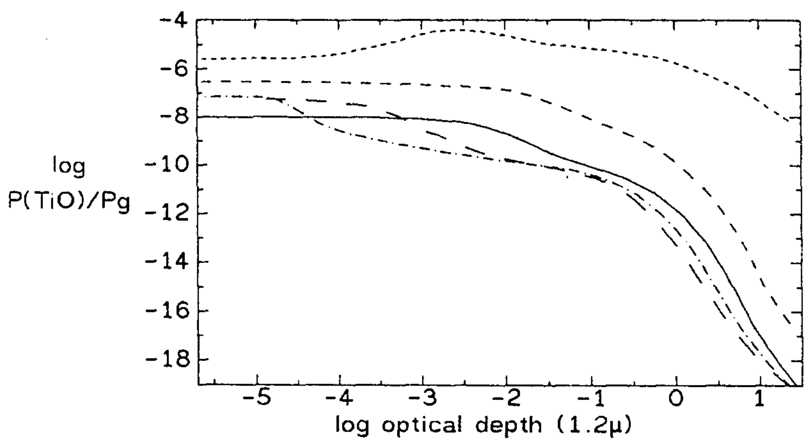

Fig. 9. Same as Fig. 7 but for TiO

3 Effects of incomplete and incorrect opacities

3.1 First order estimates of direct and indirect effects

Due to the low temperatures (and high pressures in dwarfs) in the atmospheres of M stars errors in the dissociation energies and/or temperature fluctuations lead to serious changes in the equilibrium constants and therefore often in the particle concentrations. For example, uncertainties of 0.5 eV for a dissociation energy of 5 eV and of 50 K for a temperature of 1600 K imply a change in

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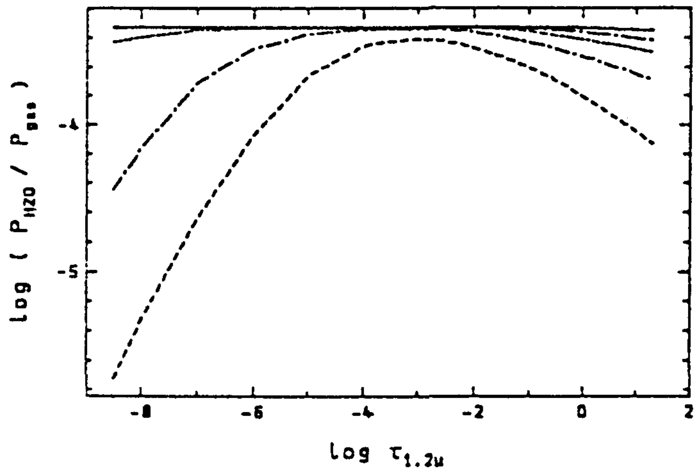

Fig. 10. Same as Fig. 6 but for H_2O

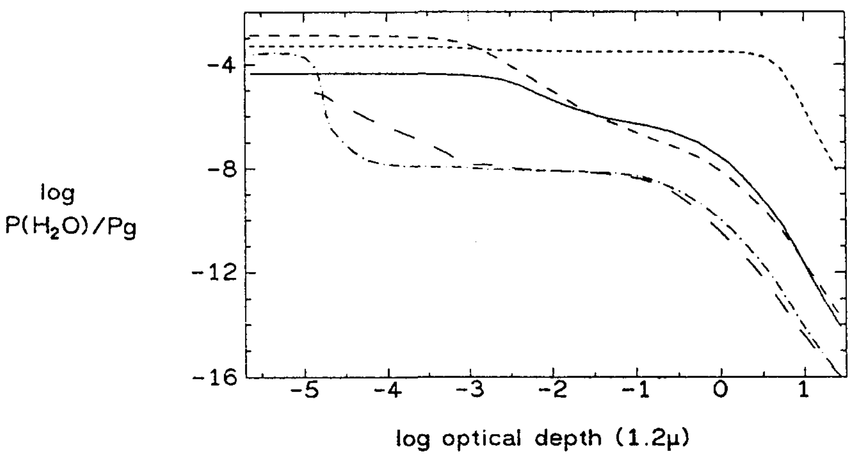

Fig. 11. Same as Fig. 7 but for H_2O

the equilibrium constant of a factor 20 (!) corresponding to an uncertainty in the density of a given species up to the same factor (see Costes & Naulin, this volume, Eq. (2)). Note, however, that in a spectral analysis the molecular data are considered to be fixed laboratory quantities and the temperatures are to be adjusted to such values that the band strengths and therefore the molecular concentrations are fitted.

The consequences of incorrect and/or incomplete opacities can easily be estimated if we consider the radiative transfer equation (or radiative transport

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equation) which reads in its conventional form for spherical media (Mihalas 1978)

$$\cos\theta \frac{\partial I_\lambda}{\partial r} + \frac{\sin^2\theta}{r} \frac{\partial I_\lambda}{\partial \cos\theta} = (\kappa_\lambda + \sigma_\lambda)(S_\lambda - I_\lambda) \quad (1)$$

(r = radial coordinate, θ = polar angle, S_λ = source function = ratio of emission to extinction). After discretization in space and angle it reduces to a linear system of algebraic equations that can be written in matrix notation for wavelength λ

$$\mathbf{A}_\lambda \mathbf{I}_\lambda = \mathbf{B}_\lambda, \quad (2)$$

or

$$\mathbf{I}_\lambda = \mathbf{A}_\lambda{}^{-1} \mathbf{B}_\lambda \quad (3)$$

where the intensity vector $\mathbf{I}_\lambda$ contains as components the specific intensities for all depths and angles, $\mathbf{A}_\lambda$ describes the spatial and angular couplings between the intensity components, and $\mathbf{B}_\lambda$ gives the photon sources. $\mathbf{A}_\lambda$ and $\mathbf{B}_\lambda$ depend linearly on the absorption and scattering coefficients per unit volume, κ_λ and σ_λ, resp. Therefore an uncertainty or modification of κ_λ or σ_λ implies that

$$\begin{aligned} \mathbf{A}_\lambda &\rightarrow \mathbf{A}_\lambda + \Delta\mathbf{A}_\lambda \\ \mathbf{B}_\lambda &\rightarrow \mathbf{B}_\lambda + \Delta\mathbf{B}_\lambda. \end{aligned} \quad (4)$$

As a consequence, the intensity vector is changed to first order by

$$\Delta\mathbf{I}_\lambda = \Delta\mathbf{A}_\lambda{}^{-1} \Delta\mathbf{B}_\lambda - \mathbf{A}_\lambda{}^{-1} \Delta\mathbf{A}_\lambda \mathbf{I}_\lambda \quad (5)$$

Equation (5) gives the direct effects that are maximal if the norm $||\mathbf{A}_\lambda||$ is minimal as is well known (see Unsöld 1958). They are relevant only at the considered wavelength. The indirect effects that concern the whole spectrum result from a change in the temperature distribution $\Delta\mathbf{T}$ induced by the opacity changes. For a static configuration in radiative equilibrium they can be estimated from the requirement that the total flux has to be the same at all depths. If we write the flux vector

$$\mathbf{F}_\lambda = \mathbf{g}\mathbf{A}_\lambda{}^{-1} \mathbf{B}_\lambda \quad (6)$$

(the matrix $\mathbf{g}$ contains the weights for the angle integration) the temperature modification due to the change in the opacity is

$$\begin{aligned} \Delta\mathbf{T} \approx \quad & \frac{\pi}{4\sigma_s} \Big(\mathbf{g} \int_0^\infty \Big[-\mathbf{A}_\lambda{}^{-1} \frac{\partial \mathbf{A}_\lambda}{\partial \mathbf{T}} \mathbf{A}_\lambda{}^{-1} \Delta\mathbf{B}_\lambda + \mathbf{A}_\lambda{}^{-1} \frac{\partial \Delta\mathbf{A}_\lambda}{\partial \mathbf{T}} \\ & - \mathbf{A}_\lambda{}^{-1} \frac{\partial \mathbf{A}_\lambda}{\partial \mathbf{T}} \mathbf{A}_\lambda{}^{-1} \Delta\mathbf{A}_\lambda \mathbf{I}_\lambda + \mathbf{A}_\lambda{}^{-1} \frac{\partial \Delta\mathbf{A}_\lambda}{\partial \mathbf{T}} \Big] d\lambda \Big)^{-1} \int_0^\infty \Delta\mathbf{F}_\lambda d\lambda \end{aligned} \quad (7)$$

(σ_s indicates the Stefan-Boltzmann constant). The expression shows that for the indirect changes the *temperature derivatives* of $\mathbf{A}_\lambda$ and $\mathbf{B}_\lambda$ as well as of $\Delta\mathbf{A}_\lambda$ and $\Delta\mathbf{B}_\lambda$ are of particular importance, i.e. that a species like H_2O with a strong temperature dependence of its concentration has a much stronger effect on the stratification than a molecule that hardly varies with $\mathbf{T}$.

Since the dwarfs have convection zones that extend to very close to the surface the radiative temperature gradient $\nabla_r = (d\ln T/d\ln P)_r$ plays a central role for the atmospheric structure. A similar calculation as above shows that an additional opacity changes ∇_r not only directly but also via its first and *second* temperature derivative.

3.2 Opacity induced temperature ambiguities in M giant atmospheres

The considerations so far have been completely general. However, we will discuss now two effects that are particular to M stars as far as we know:

If in giant atmospheres a molecule forms that can absorb effectively at infrared wavelengths carrying high fluxes (so that it cools via a picket-fence type cooling mechanism due to a near-surface absorber; see e.g. Mihalas 1978) and that has an increasing concentration with decreasing temperature, there may be a positive feedback: the molecule starts to form, it cools the upper atmosphere somewhat, the monochromatic absorption of the molecule increases, the layers of relevant monochromatic optical depth move outward resulting in an even lower temperature so that still more molecules form that in turn cool even further etc. The process only stops when equilibrium is reached and no more absorbing particles are formed. In actual calculations the feedback can be initialized by the iteration to radiative equilibrium and can lead for one given parameter set to two temperature distributions that fulfil all structure equations. An example is given by the models X350H (without H_2O cooling) and X350C (with H_2O cooling) in Fig. 3 (see also the results of detailed numerical experiments by Jørgensen, this volume).

3.3 The radiative layer and the structure of M dwarfs

The second effect occurs in the M dwarfs and is a consequence of the fact that these stars are fully convective except for a tiny layer very close to the surface (mean optical depth often smaller than 0.01): errors in the opacity lead to errors in the radiative gradient ∇_r and these in turn lead to errors in the optical depth, i.e. at the pressure and temperature, where convection starts. This implies that the "wrong adiabate" is entered. Since the real temperature gradient is very close to the adiabatic one for the high pressures of M dwarfs it means that such an error is hardly damped out and therefore the whole stellar structure may be erroneous. Note also that additional errors may be introduced by discretisation schemes for the radiative transfer equation (as e.g. the Feautrier scheme, see Mihalas 1978) that are of first order only close to the surface.

4 Comparison of synthetic and observed M star spectra

After the pioneering dwarf models of Mould (1976) progress has recently been made by the PhD theses of Kui (1991) and Allard (1990; see also Allard et al. 1992) that include both the relevant bands and proper radiative transfer. Allard also includes some metal line blanketing. For warmer objects quite satisfactory agreements with observations could be obtained (Leinert et al. 1990, Kirkpatrick et al. 1993) in most wavelength ranges; in particular, for Gl 866 also a very good fit for the NaI D lines could be obtained. By selecting better transition probabilities Allard (1994) was able to get in addition very good fits to infrared spectra of very cool objects (except for wavelength regions where water vapor dominates) and therefore eliminates the problem of too flat flux gradients found by Kui. However, it should be pointed out that these comparisons were – with the exception of line profiles for Gl 866 – all made for data of rather low resolution. When high resolution observations for dwarfs become available, new problems have to be expected.

For giants, comparisons between synthetic and observed spectra also show satisfactory agreement at most effective temperatures over wide portions of the spectrum, but various significant discrepancies remain. A comprehensive review of recent achievements in interpreting red giant spectra is given by Jørgensen 1991. For the Mira variables among the late M type giants, spectrum synthesis is still in a pioneer stage (see Bessell & Scholz 1989; Scholz 1992) since the structure of the atmospheres is determined by the propagation of shock fronts.

5 Data needed for future improvements of synthetic M star spectra

From the description given above it should be evident that still much work is needed for a full understanding of M star atmospheres. Regarding the opacities the main needs concern to TiO, H_2O, FeH, VO;

- complete line lists (so that the sum rules are well fulfilled) and corresponding transition probabilities that are accurate to better than 10%;
- accurate thermodynamical data, in particular partition functions; they should be in a form that the first and second temperature derivatives could be calculated accurately;
- data on line broadening.

In addition, it should be mentioned that for the modeling of very cool and luminous giants as Mira stars it is necessary to have highly accurate ($\lambda/\Delta\lambda \approx 3 \times 10^5$) relative line positions since the atmospheres of these objects are no longer in hydrostatic equilibrium but pulsate and therefore the correlation of line positions has a strong effect on the temperature distribution and the emitted spectrum (as can be seen from the $\partial I/\partial\lambda$ term in the transfer equation for the comoving frame, see Scholz 1992). Furthermore, all M dwarfs seem to possess coronae that radiate strongly in the X ray range (Th. Fleming, private communication). Thus it can be expected that quite a high X ray flux impinges on the matter of the photosphere and changes significantly its thermodynamical state. In particular, the level populations are very far from their LTE values (see Johnson, this volume). If we want to model this effect we need enormous amounts of photoionization, photoexcitation and collisional excitation cross-sections as well.

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