Session II

MODELS AND ABUNDANCE DETERMINATIONS

Exterior view of part of the Talya Hotel, the site of the symposium, looking West across the harbor.

Pool area of the Talya Hotel.

MODEL ATMOSPHERES FOR NORMAL AND PECULIAR RED GIANT STARS

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Abstract. I review the current status of model atmospheres for red giants, with special emphasis on recent progress and newer grids. I draw attention to some specific problems regarding opacity sources and present current and forthcoming efforts in cool-star atmospheric modeling.

1. Background

This paper follows up the excellent review articles of Johnson (1986), Gustafsson & Jørgensen (1994), and Gustafsson (1995). I will emphasize specific problems, recent achievements in producing and using newer grids, and upcoming models.

I shall review models for all types of red giants, the O-rich K and M stars, the C-rich R, N, and J–type stars, the intermediate MS, S and SC stars, as well as hydrogen-deficient (HdC) carbon stars and R CrB stars. At this point it is useful to recall that the chemistry in the atmosphere of these stars is dominated mostly by the C/O ratio. In O-rich objects, with C/O < 1, most C goes into CO, the most stable molecule, and the remaining O binds into oxides like TiO, VO, and H_2O. In a C-rich mixture, most O is bound in CO, and the remaining C forms CN, C_2, CH, HCN, C_2H_2, etc. When C/O ≈ 1, most C and O is in CO, most N in N_2, and metals with lower abundances start building compounds in significant amounts: ZrO, LaO, YO, and so on. This effect is often enhanced in S stars by the overabundance of *s*-elements dredged up on the AGB. Note also that at lower metallicity, molecules like CH are privileged over species such as C_2, the abundance of which drops faster with decreasing C abundance. This explains the dominant spectral features of CH stars.

R.F. Wing (ed.), The Carbon Star Phenomenon, 71-80.

2. Model Atmospheres: What For?

Model atmospheres are a crucial ingredient in our study of stars. Most observations lack any sense or cannot be fully exploited without the help of a model atmosphere. Obvious examples include the interpretation of spectra and the derivation of elemental abundances, and the understanding of interferometric observations in terms of stellar diameters or center-to-limb variations. To close the discussion of interferometric observations, let us mention that synthetic visibilities from static or hydrodynamic models are so far unsuccessful in matching high-quality observations of even normal red giants (see Quirrenbach et al. 1993). A general feature is that the amplitude of variation of the radius with wavelength is too small in the models. This is certainly a very strong constraint for the models, although not yet exploited.

Models are necessary for the generation of synthetic spectra at high (for abundance analysis) or low resolution (for example, for population synthesis or construction of color–$T_{\rm eff}$ diagrams).

The use of (good) model atmospheres has proved to be of particular importance in the modeling of red and brown dwarf evolution (Chabrier, Baraffe & Plez 1996). The outer boundary condition influences the calculated internal structure to a point which cannot be neglected. There are speculations that the atmospheric boundary condition is also of significance in red giants, especially for hot-bottom burning. The inclusion of model atmospheres is however more difficult in giant stars, mostly because of the lack of an easily defined radius.

Finally, the construction of model atmospheres might help us to understand the physics of real stars' outer layers. It is worth stressing again that this is not the primary purpose of models. Rather we want models that are good enough to understand and interpret our observations, yet still simple enough that we can easily use them and assess their behavior.

In short, model atmospheres are a link between our theories and observations, and a key to our understanding of observations.

3. Ingredients for a Good Model Atmosphere

In the following I will mostly discuss standard or classical models which are static, one-dimensional (i.e. consisting of homogeneous plane-parallel (PP) or spherically-symmetric (Sph) layers), in LTE, and in radiative and convective equilibrium (the convection treated with the mixing-length formalism). All these hypotheses are of course masking a much more complex reality with pulsation, 3–D convective motions, shock waves, and non-equilibrium chemistry and radiative processes. Some of these assumptions have been relaxed in more ambitious modeling (see §9). A great advantage of standard models is that they are relatively easy and inexpensive to compute. Great effort has thus been invested in including very detailed and complete line opacity in these models. In contrast, hydrodynamical models of pulsating red giants include only very crude radiative transfer (see §9). Only classical models are currently used in routine analysis of, e.g., chemical composition.

I will consider only two specific aspects of good modeling. Other, more detailed discussions can be found in e.g. Gustafsson & Jørgensen (1994). Atomic and molecular data are the main ingredient of any realistic models. Partition functions and dissociation energies are of course needed for the computation of partial pressures of species and the equation of state. Continuous and line opacities have a strong effect on the spectrum and thermal structure (see Carbon 1979 for an excellent discussion of blanketing). In O-rich objects TiO and H_2O dominate the spectrum, while CN, HCN and other species characterize the spectra of C-rich objects. Some molecules affect both the spectrum and the thermal structure (TiO, H_2O, HCN), while others affect mainly the spectrum (LaO, ...). This involves a large quantity of factors like the position of the absorption band in the spectrum, the depth in the atmosphere where it occurs, with what strength, how many lines, etc. Note also that if lines mostly scatter instead of absorbing (as suggested for electronic transitions of diatomic molecules by Hinkle & Lambert 1975), their effect on the thermal structure is much weaker. A huge effort has therefore been put into collecting and evaluating molecular line lists for a variety of species supposed to dominate the blanketing in cool stars. Gustafsson (1995) discusses current knowledge (or absence thereof) on opacities in detail.

The computation of models involves a discretization on frequencies. Various methods have been devised, dictated by the then-available computer resources. The line opacities are sampled or averaged in various ways. Jørgensen (1992) provides a review of these approximations. Let us just say that with current computer facilities only the best method should be used: namely, opacity sampling (OS). It consists, in a Monte Carlo spirit, of selecting a number of frequencies (in most cases 1000 to 10 000 seems to be enough) in the spectrum. The opacity is then calculated exactly at these particular points by summing up contributions from all lines and continua. The solution of the radiative transfer at all these frequencies then allows the evaluation of the integrals on the radiative field (specific intensity, flux, etc) needed for the solution of the model-atmosphere problem. All other methods — straight mean (SM), opacity distribution function (ODF), etc — perform some average of the opacity prior to any solution of the radiative transfer. This is of course not equivalent to the OS approximation, but in some cases is not so bad (ODF only). The ODF method offers an alternative to OS (but with less flexibility and no extremely significant gain in computing time), with the notable exception of carbon stars with $T_{\rm eff}$ lower than about 3000 K (Ekberg, Eriksson & Gustafsson 1986). It will therefore most likely be abandoned in the near future.

4. Problems

We need line positions (not so critical for the calculation of model structure or photometry), line strengths, and broadening parameters. The data is too often of low-quality, incomplete or non-existent. Even such basic data as dissociation constants are sometimes not accurate enough (see the debate around D_0°(CN)). The situation is now considerably better than at the end of the last decade. I will here only review recent progress for a few specific species.

The electronic transition systems of TiO give rise to most of the features in the optical spectra of M giants. The situation has been unsatisfactory for many years, especially regarding the transition probabilities of the bands. The lifetimes of most states have recently been measured accurately by Hedgecock, Naulin & Costes (1995). This should provide good line-strengths when combined with the extensive line lists of Plez, Brett & Nordlund (1992) or Jørgensen (1994). One persistent problem, however, is the lack of a definite lifetime for the $E^3\Pi$ state which gives rise to the ϵ band system, of importance around 1 μm. Laboratory measurements only provide a lower limit. Also the ϕ and δ system strengths still rely on the absorption measurements by Davis, Littleton & Phillips (1986). Before better laboratory determinations become available, there is the possibility of semi-empirically calibrating these bands by careful use of narrow-band colors (see §5).

Absorption bands of H_2O fully dominate the infrared spectra of the coolest O-rich stars. Real *ab initio* line lists (Jørgensen & Jensen 1994, Miller et al. 1994) are now starting to be used instead of the mean opacities of Auman (1967) and Ludwig et al. (1973) or the statistically generated lists of Alexander, Augason & Johnson (1989) and Plez, Brett & Nordlund (1992). The new lists are being tested in M dwarf models and seem to provide better models. They should be applied to giants very soon.

VO appears in the near IR spectra of the coolest M giants. There is unfortunately no laboratory measurement of the strength of the A–X or B–X bands. Brett (1990) performed an astrophysical calibration of these bands by comparing model spectra with observations. This is a delicate exercise, as errors in the model thermal structures or spectra, caused by missing or poorly calibrated opacities, may induce systematic errors in the calibration. We hope to perform a better calibration of these bands with newer models and better data (see §5).

5. Illustration of Progress

The computation of synthetic spectra, especially at high resolution, requires more complete and higher quality line data than model construction. Despite the problems mentioned above, and other missing species such as LaO and YO, progress has been steady over the past few years. Plez, Smith & Lambert (1993) carried out an abundance analysis of bright AGB stars in the SMC (Li, ^{12}C, ^{13}C, metals, *s*-elements) using extensive line lists for TiO. The simultaneous fit of various spectral regions was possible in a self-consistent way, without the need for invoking any extra "fudge" opacity as in previous studies. Fluks et al. (1994) derived a new $T_{\rm eff}$ scale for M giants by fitting synthetic spectra with carefully calibrated observations in the optical region. This scale is in excellent agreement with the Ridgway et al. (1980) scale, based on angular diameter measurements. We are reaching good agreement over most of the spectrum. Comparisons of synthetic spectra and colors with observations yield consistent values of $T_{\rm eff}$. There seem to remain some problems for stars cooler than about 3100 K (later than M6–M7), probably due to a mismatch in H_2O opacity. It is not fully clear yet if the new *ab initio* line lists will resolve this discrepancy.

For carbon stars, the extensive chemical analysis of Lambert et al. (1986), using ODF models with polyatomic opacities, was able to explain the H_2 line strength as a natural consequence of the blanketing effect of the polyatomic molecules. Earlier attempts had predicted H_2 lines that were too strong. However, the CH and HCN bands appear too strong in the models. This situation is still unresolved and awaits further work in the modeling of carbon-rich atmospheres (OS with newer opacities, in progress; see §8). There may be a need for inclusion of more opacity-contributing molecules as well as dust in the cooler models. It is also worth mentioning that Ohnaka & Tsuji (1996) find carbon isotope ratios much lower than Lambert et al. and that the reasons for this difference still need to be explained.

Alvarez & Plez (1998) are carrying out a study of Mira variables using the observations of Lockwood (1972) with 5 narrow-band filters in the near-infrared. These filters, based on the Wing system (see Wing 2000), isolate (more or less, the region is crowded!) specific TiO and VO absorption bands. The synthetic colors match pretty well the observations of reference non-variable M giants, thanks to the use of high-quality model atmospheres and very extensive line lists. It is possible to tune the strength of some of these bands (the ones which have no accurate lifetime measurement) to obtain a better fit in color-color diagrams. This is only allowed because the models are of high quality (they have been well tested in other respects: $T_{\rm eff}$–color relations, spectroscopy, ...) and they are not so much affected by these particular changes. Narrow-band colors appear quite powerful in assessing the quality of, or even for calibrating, model spectra.

6. Existing Grids

It is now time to describe the existing models and to discuss them briefly. The following table is largely inspired by Table 1 in Gustafsson & Jørgensen (1994). In general, models using the OS approximation (or possibly ODF for O-rich atmospheres) should be preferred. For carbon stars, the most reliable models are the ones that include opacities from polyatomic molecules in the OS approximation. The uncertainties in opacity sources and strengths are larger for C-rich mixtures. This is made more critical by the generally low $T_{\rm eff}$ of carbon stars. In M–type star models, there is still the uncertainty

TABLE 1. Grids of model atmospheres for red giant stars

Sp. Type	$T_{\rm eff}$	log g	[M/H], C/O	Notes	Ref.
O–K	3500 –50000	0.0 – 5.0	-5.0 – 1.0	OS	(1)
G–K III	3750 – 6000	0.75 – 3.0	-3.0 – 0.0	ODF, no TiO	(2)
M I–III	2600 – 4200	-2.0 – 2.5	0.0	VAEBM	(3)
M III	2500 – 4000	0.0 – 2.0	0.0	OS+SM	(4)
M III	3000 – 4000	0.0 – 2.0	0.0	OS	(5)
M I–III	3000 – 4000	-0.5 – 1.5	0.0	OS, Sph	(6)
N, R	2600 – 4500	-1.0 – 1.0	C/O=3.2 etc	ODF	(7,8)
N, S	2500 – 3500	0.0	C/O=0.6 – 2.0	OS+SM	(9)
N	2500 – 3500	-1.0 – 0.0	-1.0 – 0.0 C/O=1.01 – 1.5	ODF, poly	(10, 11)
N	2500 – 3400	-1.0 – 0.5	-1.0 – 0.0 C/O=1.02 – 2.0	OS, poly, Sph	(12)
R	3800 – 4800	2.0 – 3.0	0.0 C/O=1.02 – 3.5	ODF	(13)
R	4200 – 5400	2.0 – 3.0	0.0 C/O=1.74	OS	(14)
Miras	2300 – 3350	$L \approx 10^4 L_\odot$	0.0	SM, Sph, dyn	(15)
R CrB, HdC	5500 – 9500	-0.5 – 2.0	C/He=0.1 – 10%	OS+ODF	(16)

Notes: OS: opacity sampling, ODF: opacity distribution function, VAEBM: Voigt-analog Elsasser band-model, SM: straight mean, Sph: spherical, poly: including polyatomic opacity sources, dyn: hydrodynamical models

References: (1) Kurucz (1992); (2) Bell et al. (1976); (3) Tsuji (1978); (4) Johnson et al. (1980); (5) Brown et al. (1989); (6) Plez et al. (1992); (7) Querci et al. (1974); (8) Querci & Querci (1975); (9) Johnson (1982); (10) Eriksson et al. (1986); (11) Lambert et al. (1986); (12) Jørgensen et al. (1992); (13) Olander (1981); (14) Johnson & Yorka (1986); (15) Bessell et al. (1989, 1996); (16) Asplund et al. (1996)

due to H_2O at $T_{\rm eff} < 3100\,{\rm K}$.

7. Latest News

A new grid of models for R CrB and HdC stars has just been completed by Asplund et al. (1997). Previous grids by Schönberner (1975) and Jones (1991) included older continuous opacities and no line-blanketing in the former case. The Asplund et al. models are based on the MARCS code (Gustafsson et al. 1975), with improved and expanded continuous opacities (dominated by C I) and line-blanketing in a mixture of OS and ODF. The grid covers $5000\,{\rm K} \leq T_{\rm eff} \leq 9500\,{\rm K}$, $-0.5 \leq \log g \leq 2.0$, $0.001 \leq {\rm C/He} \leq 0.1$. The inclusion of blanketing steepens the temperature gradient and provides an explanation for the presence of C_2 and CO lines up to $T_{\rm eff} = 7000\,{\rm K}$, and for C II and He I lines down to the same temperature. The model for R CrB itself matches the observed spectrum very well from the UV to the IR. The authors also discuss the density inversion present in their models in the He ionization region and its possible link with an instability and episodic mass-loss. They conclude that non-LTE effects on C are not very large, and they announce upcoming models including spherical symmetry.

8. Coming Soon

The above grid is a step toward a more ambitious project in progress in the Uppsala group. The goal is the completion of an "ultimate" grid of standard models for stars of spectral types later than about F. After all the progress of the past years, especially in opacity quality and completeness, the time is now ripe for the production of a consistent grid of models including all the best data and covering a large area of the HR diagram, extending Kurucz' work to cooler temperatures and more exotic chemical compositions. This involves the careful (and painful) compilation, computation and evaluation of line and continuous opacity data. Only the best possible data will be included, with the least possible ad-hoc or astrophysical calibration, and with laboratory data whenever possible. Partition functions and molecular equilibrium constants will also be reviewed. The models will be PP or Sph, in LTE, static, with a range of [Fe/H], CNO, α–elements, ... covering all foreseeable needs. The emphasis will be placed on obtaining good synthetic spectra and colors.

9. ... And Later, beyond Classical Models

Some attempts have been made to relax some of the classical model hypotheses. Hydrodynamical models have been constructed, and a first attempt at including non-LTE (for Ti, Ti^+ and TiO) in the model calculation has recently been reported (Hauschildt et al. 1996).

Radially pulsating atmospheric models have been produced by Bowen (1988) and Bessell, Scholz & Wood (1996) for O-rich stars and by the Berlin (e.g. Winters et al. 1995) and Vienna (Höfner, Feuchtinger & Dorfi 1995) groups for C-rich objects, with various degree of sophistication in the description of dust formation, cooling/heating, etc. Many exciting and sometimes surprising results have come from these studies, but some aspects still need improvement. Most dynamical modeling has so far relied on very crude descriptions of the radiative field. A better treatment, with about 100 frequency points in LTE, will probably be included in the course of the next few years. The driving of the pulsation is included as a piston at the bottom of the envelope. The atmosphere acts as an active filter which results sometimes in multiple periodicity, or semi-periodic behavior (Winters et al. 1994). The inclusion of the driving zone in a self-consistent way will be necessary to understand why and which stars show multi-periodicity or only semi-periodicity. The coupling between convection and pulsation may play a role too, but cannot be studied before a more realistic description of convection is included in the models.

Another direction of research is offered by the extension to cool stars of the 3–D modeling of convection (as done by Nordlund and collaborators for solar type stars: see Nordlund & Dravins 1990, and references in Gustafsson & Jørgensen 1994).

Extensive non-LTE included at the modeling stage is the third development beyond standard models. Especially important is the coupling between electron donors, H^-, and molecules. The main, and very serious, problem is the lack of collisional cross-sections for most relevant species, and for virtually all molecules. Large model atoms are not sufficient. Good quality data are also needed here if meaningful results are to be expected.

I shall conclude here by saying that there is a strong motivation to construct better model atmospheres; many reasons may be found in this volume. We will soon access regions of the spectrum that are only poorly known (ISO). Large telescopes will allow us to extend our studies to other galaxies. With the advent of "modern" classical models and the systematic exploration of non-classical directions, the next decade should provide for a lot of excitement and a rich harvest of new results.

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Discussion

Luttermoser: A comment about the NLTE photospheric modeling that is currently underway: it is important to include the chromospheric radiation field flowing backward down onto the photosphere. It has an important impact on the excitation and ionization of neutral metals in the photosphere, especially in the upper photosphere (i.e. $\tau_{\rm Ross} < 1.0$).

Plez: Yes, you are perfectly right!

Steffen: What is your choice for the mixing length parameter of convection, and how sensitive are your models to the assumed convective efficiency? What about microturbulence?

Plez: We use $\alpha = 1.5$. This only affects the structure of the red giant models at large optical depth (> 10). The impact on spectra or colors is negligible. For microturbulence we use about 2 $\rm km\,s^{-1}$. This enters only in the broadening of spectral lines. It is not included in the turbulent pressure term, but could be.

Mowlavi: Could you comment on the importance of using good model atmospheres for the calculation of stellar structure evolution?

Plez: The atmospheric boundary condition most probably influences the Hot Bottom Burning. Good atmospheres are also of course necessary for relating the model parameters to observations ($T_{\rm eff}$, ...).