Towards a Satisfactory Understanding of AGB-Star Atmospheres?

Bengt Gustafsson

Department of Astronomy and Space Physics, Uppsala University
Uppsala, Sweden

Abstract. The understanding and the modelling of the atmospheres of AGB stars are discussed and found to be unsatisfactory for most purposes. A number of developments and possible actions to improve this situation are considered.

1. Introduction

Traditionally, model atmospheres are constructed with some simplifying assumptions as a basis: those of one-dimensional (plane-parallel or spherically symmetric) structures, hydrostatic equilibrium, convection according to the mixing-length “theory,” and local thermodynamical equilibrium. Moreover, effects of magnetic fields are totally neglected. Then, the fundamental equations are easily derived, and adequate algorithms for solving them are applied. Great amounts of physical data have next to be supplied for the calculation, in particular for describing the radiative transfer at different wavelengths. This results in a model atmosphere, with a model spectrum, which is then compared with the observed one. As a result of varying the physical parameters of the model, such as its effective temperature, surface gravity (or mass and radius) and chemical composition, until a satisfactory fit to the observations is obtained, these parameters may be estimated.

The mismatch that almost always remains after adjusting the parameters may often be ascribed to lacking or erroneous physical data. This is the case not the least for the AGB spectra which are affected by numerous molecules and dust. However, some discrepancies may still remain after allowance for errors in the data. And even if such discrepancies do not show up, there is no guarantee that the model parameters are correct. Instead, the method might lead to excellent fits but systematic errors in the fundamental parameters, reflecting the lack of realism in the basic assumptions.

The usefulness of traditional model atmospheres is not possible to establish without specifying for what purpose we wish to use them. The classical use is the determination of those stellar parameters mentioned above but also of age, rotation speed, magnetic field strength, interstellar reddening, distance, mass-loss rate, etc. In addition to this, one may wish to use the models when setting boundary conditions for other stellar models, such as models of stellar interiors, or of stellar outer envelopes and winds. A third application area is the use of stellar atmosphere models for extrapolations to “new” types of stars, i.e. stars not seen individually in the solar neighborhood such as very metal-poor stars with masses above a solar mass, or stars with metallicities significantly in excess
Towards Understanding AGB-Star Atmospheres

of two times solar. Such atmospheric models may be necessary for analysing integrated spectra of distant galaxies, or, in the first case, for calculating the degree of re-ionization of the gas in pre-galactic eras.

Still another use of model-atmosphere comparisons with observed spectra should be noted: to check that the physics in stars is understood. This includes several intricate areas of physics, such as spectral-line formation, magneto-hydrodynamics, dust formation, and formation of structures, sometimes far from equilibrium. In the latter important area, stellar atmospheres and the solar atmosphere in particular offer interesting examples which may serve as inspiration and even, in some cases, as model systems for the study of complex dynamical systems in general.

After these general points I shall now comment on what has been achieved for AGB stars by comparison between traditional models and observations (§2). Progress towards significant improvements in our understanding is discussed next (§3). After that, some suggestions for empirical and theoretical studies of the structure of AGB star atmospheres will be given (§4) before an ending note (§5).

This review should be seen as a complement to the much more detailed review presented recently by Gustafsson & Höfner (2004).

### 2. What Can Contemporary Models Do for You?

Spectral fits of high-resolution spectra presented in recent AGB work at the state of the art give in general a rather convincing impression. A few examples will be given here. Thus, García-Hernández et al. (2006, their Fig. 2), and de Laverny et al. (2006, their Figs. 2 and 4), demonstrate beautiful spectral fits and interesting results. A number of problems should, however, be noted. One is the absence of continuum regions, in particular in visual spectra. Another problem is the relatively great strength of many spectral diagnostics used, leading to weak abundance sensitivity and severe dependence on other factors such as velocity fields (“microturbulence”) and temperature in the upper atmosphere. This results in considerable errors in derived abundances. When great abundance effects are explored, as in the study by de Laverny et al. (2006) on the ratio of heavy s-elements to light ones in carbon stars in nearby dwarf galaxies, expected to vary by one order of magnitude, an error on the order of a factor of 3 in relative abundances may be tolerated. However, there are many interesting effects smaller than that, which one would wish to trace. For infrared spectra continuum problems may be smaller. Thus Wahlin et al. (2006) have recently derived CNO abundances for carbon stars in the Local Group from spectra in the $H$ (1.6 $\mu$m) and $K$ (2.3 $\mu$m) bands and find results consistent with theoretical predictions. However, due to other systematic uncertainties, e.g. in the model atmospheres, these abundances may also have considerable errors. An example of the significance of mastering the errors was recently offered by Gustafsson & Wahlin (2006) who suggested that $^{12}\text{C}/^{13}\text{C}$ ratios for nearby carbon stars as derived from high-resolution IR spectra in the $H$ and $K$ bands are not compatible with results from spectra in the 0.7–1.1 $\mu$m region, nor fully consistent with results from mm observations of the stellar envelopes or from PNe. In order to
draw potentially interesting conclusions from these results as regards, e.g., the origin of PNe, one has to be fully convinced that the IR results are correct.

One may ask the general question, what accuracy is required in analyses of AGB-star spectra. For abundance analyses to an accuracy of about 25% (i.e. 0.1 dex) which is needed for many purposes related to Galactic evolution, we need effective temperatures to 5% and surface gravities to within a factor of 2. For the temperatures this is often possible to achieve, but the gravity errors for Galactic field stars (with unknown distances and masses) are often larger. Still more severe, however, are probably errors due to systematic errors in the model atmospheres and synthetic spectra, the LTE assumption, and thermal surface inhomogeneities and dust emission. Each of these effects may well lead to abundance errors typically ranging from 0.2 to 0.5 dex.

As regards estimating other parameters by spectrum comparison with models, the inaccuracies are even more severe. Attempts to obtain radii and masses from spectra are not very successful, one problem being the calculated extension of the atmosphere itself which may be in error by an order of magnitude or more, due to the neglect of pulsations and other dynamical effects or errors in polyatomic molecular opacities. This, and the overlap of evolutionary tracks in the HR diagram, also make attempts to estimate stellar ages very problematic. When measuring rotation speeds from line profiles one would wish an accuracy of about 0.1 km/s or better in order to explore the possible connection between rotation and mixing. Pulsations, convection and blends, however, make it difficult to reduce the errors below 2 km/s. In estimating stellar magnetic fields it is hard to reach an accuracy better than $10^2$ gauss, due to departures from LTE, geometrical aspects and blends, while an accuracy ten times better seems needed for exploring the expected photospheric fields systematically.

Referring back to §1 we find that contemporary model atmospheres may be used to derive effective temperatures and abundances with some accuracy, but in general with much lower accuracy than the quality of state-of-the-art observations admits if the models were perfect. The models may be used to set boundary conditions for models of stellar interiors and evolution, but they are of little value for setting boundary conditions for models of winds and external envelopes. Model atmospheres may be used for extrapolations to types of stars that are not represented in the solar neighborhood. However, one should be aware of the risks involved: these models may be severely and systematically in error, making the extrapolations truly dangerous. This also applies to, say, models of carbon stars in metal-poor dwarf galaxies for which detailed checks by comparison of spectra at high resolution are difficult to carry out. Finally, contemporary models seem to be of little use for testing the understanding of the interesting physical processes in AGB star atmospheres.

We conclude that contemporary models are unable to meet reasonable demands from the scientific community. This is not only a scientific problem but also a political dilemma. By consulting members of the Observing Programme Committees of various major telescopes, I have estimated the annual telescope cost for RG and AGB studies to be on the order of 20 million Euro or more. Some simple arguments, matching the cost/gain for improving/degrading the S/N to the improvement one could hope for in analysing spectra by increasing the number of theorists in the modelling endeavor, suggest that it would be very worthwhile to strengthen these theoretical efforts considerably also in econom-
ical terms. If we do not do that, it seems that the RG/AGB community will not have a very good case when arguing for more telescope time, or for bigger telescopes.

3. How Could We Improve the Models?

In discussing how to model AGB stars it is important to take a number of trivial facts into serious consideration. Thus, stars are dynamical systems (1), and this fact is of great significance for their structures. Moreover, they have three spatial dimensions (2). Electromagnetism exists, also, in stars (3). The stars are not in thermal equilibrium (4) and they have free outer boundaries (5). Finally, dust forms, also, in AGB star outer atmospheres (6). The path towards improved models passes these various steps, one at a time. The self-consistent model with all aspects considered simultaneously still remains to be made.

3.1. Dynamics: Convection

Long ago, Nordlund (1982) and Nordlund & Dravins (1990) – see also Stein & Nordlund (2000) – did pioneering work in calculating successful 3D models with consistent hydrodynamics and radiative transfer for solar-type stars. In general, they successfully reproduced the stellar spectra with no free dynamical parameters like turbulence parameters, which was a remarkable achievement. This work was refined and extended to Pop II stars by Asplund et al. (1999). The methods have recently been applied to giant stars of different metallicity by Collet et al. (2006). Kucinskas et al. (2006) have used a similar approach (“a box in a star”) to construct models for M giants. Freytag (2003) has used his “star in a box” approach, suitable for stars where sphericity effects are important and the pressure scale height $H_p$ is a significant fraction of the stellar radius, to simulate the dynamics of atmospheres of red supergiants, and Höfner et al. (2005) have also tried these methods for an AGB star model. A general finding from these simulations is that the models show granulation patterns with characteristic scales proportional to $H_p$, which means that they represent a considerable fraction of the stellar radius for the lowest gravity objects. The giant convection cells also prevail if the numerical spatial resolution is increased, although more fine structure then appears Chiavassa et al. (2006). The effects on abundance determinations, which are on the order of 0.1–0.2 dex for solar-type stars, were found to be much greater for the metal-poor stars. In particular, the almost adiabatic cooling of the up-streaming gas in the surface layers of the giant models by Collet et al. (2006) strongly affects the formation of molecules, changing the CNO abundances by typically 1 dex for the most metal-poor stars or even more. At present, it is unclear how great the abundance effects will be for AGB stars, but in particular when strong and temperature-sensitive abundance criteria are used one may expect serious errors.

In the near future, the radiative transfer in the 3D models will be improved. For the “star-in-a-box” models, non-gray radiative transfer needs to be implemented, and detailed molecular opacities included. Further ahead lies relaxing the LTE assumption. Full-star models will eventually be developed where the stellar inner core regions and the outer layers are handled in detail with dust formation and mass loss allowed.
3.2. Magnetic Fields,

There is some indirect evidence for magnetic fields in the atmospheres of AGB stars. For example, Vlemmings et al. (2006, and references therein) have studied H$_2$O masers around supergiants and miras and deduce fields at the stellar surface on the order of $10^2$ gauss. X-ray emission from AGB stars has been explored, e.g. in the case of Mira Kastner & Soker (2004), but the origin may sooner be due to the companion of the M giant. The bipolarity of PNe has been interpreted by Blackman et al. (2001) as being due to $\alpha\omega$-dynamos of the PPNe, which then requires fields on the order of 400 gauss. Also, star spots on AGB stars have been found with the IOTA imaging interferometer at 1.6 $\mu$m for 12 of the 16 stars explored Ragland et al. (2006).

There also exist impressive simulations of dynamo action in supergiants like $\alpha$ Ori. Dorch (2004) has thus found that the dynamo driven by convection (called the “local small-scale dynamo” in the solar case) in “star-in-a-box” models forms large-scale magnetic fields in a supergiant. This is just a natural result of the large spatial scales of convection in those stars. For a simulation starting from zero fields, there is a rapid growth of field strength for about 100 years, after which a slower-mode rate takes over. The typical field saturates at about 120 gauss, while local maxima occur at 500 gauss. The filling factor is considerable – more than half the stellar surface is covered with fields stronger than 50 gauss.

It seems clear that fields of these strengths and coverage could seriously affect the motions in the upper atmospheres and winds. Further MHD modelling, applied to AGB stars directly, seems very important.

3.3. Pulsations.

As is shown in Susanne Höfner’s review in the present volume, stellar pulsations couple together with dust formation in a profound way, making the upper stellar atmosphere depart very significantly from static models. For the mean structures the exponential decrease of density with height, typical of hydrostatic equilibrium, is replaced by a much slower density decrease. Although not perfect, the quantitative agreement between observed and calculated fluxes, line shapes and radial velocity variations for pulsating stars is impressive. Particularly important is that the dynamical models also lead to much improved predictions of mass loss. Further advances in dynamical modelling are eagerly awaited.

3.4. NLTE

Although solving the full NLTE problem for a late-type 1D stellar model is still a non-trivial problem, the work of Hauschildt and collaborators demonstrates that it is within reach, methodologically. A direct treatment of a great multitude ($\sim 10^5$) of individual spectral transitions for calculating a solar model Short & Hauschildt (2005) shows that the structural NLTE effects are relatively limited, amounting to at most about $+200$ K in $T(\tau_{5000})$ around $\tau_{5000} = 10^{-4}$ and a more shallow temperature gradient in the interval $10^{-4} \leq \tau_{5000} \leq 10^{-2}$. There is no guarantee, however, that the effects are as small for the AGB stars, with their lower atmospheric densities. In particular, the risk should be noted that the excited electronic states of molecules, such as TiO or C$_2$, could be partly decoupled from the local kinetic temperature, which might then severely affect the atmospheric structures. The dominating continuous H$^-$ opacity is also crit-
ically dependent on electron donors like Ca, Al and Mg atoms, the ionization equilibria of which should be studied in detail. The notorious lack of accurate cross sections for collisions between hydrogen atoms and opacity-contributing atoms and molecules is a severe problem for attempts to estimate these effects. Atomic and molecular physicists who undertake the hard work to provide cross sections are not always fully appreciated in their own circles. They should be supported vigorously by stellar astronomers.

3.5. ... and Dust.

For the cooler AGB stars (which may in fact include the majority of them) dust formation is important not only for the outer envelopes and the dynamics of their winds, but also for their spectra and flux distribution, as well as for their photospheric structures and dynamics, which are affected by back-scattering of radiation from the outer layers. So, a self-consistent treatment of dust formation is needed for sound modelling. As is clear from Anja Andersen’s and Peter Woitke’s reviews in the present volume, we are relatively far from such treatments as yet, especially for oxygen-rich chemistries. Again, we have to do our best to promote the further study of the physics and chemistry of dust formation.

3.6. Are Current Methods Able to Handle the Full Problem?

It should be noted that even if the (magneto)hydrodynamics of the stellar atmospheres complicates the modelling, as compared with static models, the direct complications due to the dynamics are not the main problem. The indirect effects, leading to inhomogeneities which require a 3D treatment of radiative transfer, are much more important. In general, the non-locality of radiative transfer – affecting the energy balance in the gas as well as the momentum transfer – remains the major challenge in stellar-atmosphere modelling, provided that the physical data (such as collision cross sections) are given.

Available methods for handling this problem today are finite-difference methods, finite-element methods and Monte Carlo methods. Of these, the finite-difference methods dominate in stellar-atmosphere applications; for reviews see e.g. Carlsson (2003) and Hauschildt & Baron (2006). Utilizing operator splitting (ALI) with multigrid techniques and obtaining the formal solution from long- or short-characteristics one finds for the total time \( t(3D) \) for solving the 3D problem: \( t(3D) \geq N_x \times N_y \times t(1D) \), where \( t(1D) \) is the corresponding time for the 1D problem. Since the number of points in the horizontal directions, \( N_x \) and \( N_y \), each must be on the order of \( 10^2 \) or more, we find that at least about 15 years of further computer development is needed, adopting the well-known Moore’s law Moore (1965), before the full problem can be solved with realistic efforts. However, the potential of parallelizing the problem may still not have been fully exploited; on the other hand the memory needed even for small model atoms in 3D problems is very considerable and the convergence rate of the ALI methods in 3D cases is usually slower than in the 1D case.

It is, however, probably not necessary to solve the full NLTE problem for all atoms and molecules affecting the energy balance in the stellar atmosphere. Statistical approaches may be used, provided that the radiative losses and gains are calculated to the precision needed. Attempts to devise such approaches have been made and are presently being further developed – we need to ascertain that
such methods work well enough without solving the full problem, at least for checking purposes, for each new type of stars for which they are applied.

4. And What Can We Do While Physicists and Moore’s Law Work?

A proper scientific attitude in the present situation is certainly not to sit down waiting for the next generations of computers. Nor is it reasonable to just go on using traditional models for interpreting spectra. Instead, the present situation calls for different approaches, at least as a complement. Although I shall here schematically divide the discussion into one empirical and one theoretical subsection, I wish to stress that each approach needs a close collaboration with “the other side.” In particular in a situation when fully self-consistent models cannot be produced, one needs to blend both aspects and essentially base the work on semi-empirical modelling.

4.1. Some Challenges for Observers

At least for accurate observations of Galactic AGB stars the quality of observed spectra is generally considerably greater than that of the calculated spectra – i.e. after the fitting of traditional models to high-resolution spectra by varying the model parameters it is realistic to assume that most of the discrepancies remaining are due to modelling problems. In this situation, it is reasonable to use the information excess of the data to attempt deriving further properties of the real atmospheres. Even if this may be difficult to achieve unambiguously with normal spectra only, there is a wide arsenal of instrumental methods available to us, including spectropolarimetry and angular interferometry which may put additional constraints on important atmospheric properties outside the scope of traditional modelling. Very schematically, only a characteristic temperature, a pressure, and velocity fluctuations at different scales, $T_{ch}$, $P_{ch}$, and $V_{ch}$ (macro) and $V_{ch}$ (micro) used to result from traditional analyses. One could argue that also vertical gradients, like $dT/d\tau$, $dP/d\tau$ and $dV/d\tau$ could be accessible via accurate spectroscopic observations. Further quantities, like pressure scale height, magnitudes and length-scales of horizontal temperature fluctuations, and length-scales of fluctuations in flow velocity, may be possible to measure interferometrically. Also, photospheric magnetic field strengths, and their fluctuations, may be possible to map in the future using spectropolarimetric interferometry. Finally, the measurement of mass loss, and its fluctuation with time and across the stellar surface, can be developed, although the interpretation of such measurements will most certainly be severely model-dependent.

4.2. and Some for Theorists

A very general and urgent need is for a better physical understanding of the results that model simulations generate. For example, the spatial scales and time scales that show up in 3D simulations should be understood from basic theory. Similarly, the scaling laws of characteristic scales and amplitudes with fundamental stellar parameters that one finds empirically from simulations should be further analysed. One example is given here: It is found from the numerical simulations of convection cited above that the size of convection granulae, $\Gamma$, scales in proportion to $H_p$ for different stars over many orders of magnitude in
Towards Understanding AGB-Star Atmospheres

Figure 1. The base-10 logarithm of characteristic granular sizes, $\log G$, plotted versus $\log H_p$ for simulations of convection in stellar atmospheres ranging from solar-type stars (Nordlund & Dravins 1990; Dravins et al. 1993), to giants of different metallicities (Collet et al. 2006; Kucinskas et al. 2006) and supergiants Freytag (2003). The line corresponds to the linear relation: $G = 10 \cdot H_p$. A similar simple scaling was noted by Freytag et al. (1997) in simulations for stars in the range from white dwarfs to stars somewhat above the main sequence.

From Euler’s equation for an anelastic flow it follows directly that $\Gamma \approx g^{-1}$, with $g$ denoting the surface gravity, which then leads to the scaling found with scale height (cf. Figure 1). Stellar flows are, however, not anelastic. Moreover, the magnitude of the temperature fluctuations varies mildly with fundamental parameters of the stars. This variation as well as the very size of the temperature fluctuations are still to be understood from physical principles.

The question of what is driving a particular phenomenon, and which are only secondary effects, is often not answered properly today, even though satisfactory simulations exist. Examples are found among the calculations of atoms and molecules in statistical equilibrium, where the analyses of the resulting departures from LTE often make us confused in the search for hens among the eggs. In fact, a better understanding would also lead to an adequate theory for how optimal model atoms, with a given restriction on the number of affordable levels and transitions, should be designed.

5. Ending Note

Figure 2 shows Nils Dunér, Professor of Astronomy at Uppsala University from 1888 to 1903, observing with the then new 36-cm double refractor at Uppsala Astronomical Observatory. Dunér was a pioneer in carbon-star research, and discovered several of the bright carbon stars, viz. stars of Type IIIb (or Secchi Type IV), by visual observations with the Uppsala refractor and, earlier in his career, with the smaller refractor at Lund Observatory. He expressed his enthusiasm with these objects; e.g. in a late paper Dunér (1899) he characterizes the spectrum of Y CVn as “Remarkably beautiful, with 3 very bright and one rather faint ultra-blue zone.” He ends this paper: “I shall make no [further] investigations ... since Professor Hale is engaged on this very problem, and neither the refractor nor the atmospheric conditions at Uppsala can be compared with those at the Yerkes Observatory.” The observation methods have advanced very considerably since those days. Also the theoretical understanding of the AGB stars is much more advanced — however, it is far from what should be possible, what is wanted as a basis for other stellar work, and what is needed to match
Figure 2. Professor Nils Dunér, observing with the 36-cm double refractor at Uppsala Astronomical Observatory in the late 19th century.
the impressive observations. If we continue our analysis of the observations with the present level of ambition some critics might rightly conclude that we are not as foresighted as Professor Dunér.

References

Chiavassa, A., Plez, B., Josselin, E., & Freytag, B. 2006, EAS, 18, 177
Moore, G. 1965, Electronic Magazine, April 19, 1965
Stein, R.F. & Nordlund, Å. 2000, Solar Physics, 192, 91

Discussion

Busso: Maybe one should ask atomic physicists, aeronautics people, etc. to make measurements for us in the fancy conditions of stellar atmospheres. We discovered for example that you need the turbulent drag coefficient $C_D$ for any turbulent simulation, at Reynolds numbers never covered by present/past experiments.

Gustafsson: Yes, I agree very much. However, as regards physics supporting astrophysics, this is often not very highly appreciated within the physics com-
munity since it is not regarded as fundamental. Therefore, we astronomers should actively support helpful physicists.

Gallino: The expected $^{12}\text{C}/^{13}\text{C}$ ratio in C-rich AGB stars may strongly depend on the metallicity. (The $^{12}\text{C}$ dredged up is primary, and no $^{13}\text{C}$ is dredged up).

Gustafsson: Yes, but the bright N-type stars in our sample all have metallicities in the interval $-0.3 \leq [\text{Fe/H}] \leq 0.0$. The PNe in the comparison may include some more metal-poor ones.