Abstract

In this review presented at the Symposium *A Stellar Journey* in Uppsala, June 2008, I give an account of the historical development of the MARCS code, and its premises from the first version published in 1975 to the 2008 grid. The primary driver for the development team who constantly strive to include the best possible physical data, is the science that can be done with the models. A few preliminary comparisons of M star model spectra to spectrophotometric observations are presented. Particular results related to opacity effects are discussed. The size of errors in spectral energy distribution (SED) and model thermal stratification is estimated for different densities of wavelength sampling. The number of points used in the MARCS 2008 grid (108 000) is large enough to ensure errors of only a few K in all models of the grid, except the optically very thin layers of metal-poor stars. Errors in SEDs may reach about 10% locally in the UV. The published sampled SEDs are thus adequate to compute synthetic broadband photometry, but higher resolution spectra will be computed in the near future and published as well on the MARCS site (marcs.astro.uu.se). Test model calculations with TiO line opacity accounted for in scattering show significant cooling of the upper atmospheric layers of red giants. Rough estimates of radiative and collisional time scales for electronic transitions of TiO indicate that scattering may well be the dominant mechanism in these lines. However, models constructed with this hypothesis are incompatible with optical observations of TiO (Arcturus) or IR observations of OH (Betelgeuse), although they may succeed in explaining H₂O line observations. More work is needed in that direction.

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(Some figures in this article are in colour only in the electronic version.)

1. MARCS: a little history

The MARCS model atmosphere code has been in use since the mid-1970s. It has its roots in Bengt Gustafsson’s early work on a Feautrier-type method for a model atmosphere including convection (Gustafsson 1971). A number of features, including detailed continuous opacities, had already been incorporated in that pre-MARCS version. And typically for Gustafsson, it was directly applied to an astrophysical problem: determining the metallicity of F type stars (Gustafsson and Nissen 1972). A few years later, Gustafsson’s collaboration with Eriksson, Nordlund, and Bell gave birth to MARCS: a code for Model Atmospheres in Radiative and Convective Scheme (Bell et al 1976, Gustafsson et al 1975). It allowed the computation of hydrostatic, plane-parallel (PP), line-blanketed atmospheres, with convection included, following Henyey et al’s (1965) formulation of the Mixing Length Theory (MLT). Line opacity was included in the form of Opacity Distribution Functions (ODF), and metal-poor FGK-type stars were modelled. The 1975 paper is highly recommended in the field, as it discusses in great detail the underlying assumptions, the algorithm, its implementation and the resulting model structures of varying stellar parameters. The grid was also used right away in astrophysical applications: abundance determinations, colour calibrations etc. This version of the MARCS model has been used for almost two decades by its creators and collaborators, and probably longer by others.

Simultaneously, however, there was great interest in (i) updating the code and its input data, and (ii) extending...
its applicability to other spectral types. The latter became effective with Eriksson et al.’s (1984) efforts which, less than a decade later, delivered a model of cool carbon stars with polyatomic opacities included (HCN and C$_2$H$_3$), and applied them to determine abundances in carbon stars (Lambert et al. 1986). This development of MARCS was made possible because the expertise necessary to compute these new opacities was available in the team. Eriksson et al. (1984) demonstrated the strong effect of polyatomic opacities on atmospheric structures and emergent spectra, and pointed out the necessity to refine these opacities$^2$. Two years later carbon star models were computed using the Opacity Sampling (OS) method by Ekber et al. (1986). They demonstrated that the ODF hypothesis does not work well when opacities from different sources and not correlated in wavelength (e.g., diatomics and polyatomics) dominate at various atmospheric depths. The OS method is then more reliable provided a large enough number of sampling points are used (see section 4.1). At that time computer limitations hampered the wide use of OS, but the trend had been launched: the next MARCS would use OS.

The extension towards cool oxygen-rich stars is where it all started for me. I had started my PhD in France on empirical modelling of Mira stars based on speckle interferometric observations. As I was getting about nowhere, my supervisor wisely sent me to Uppsala, to spend about a year with Bengt Gustafsson and learn as much as possible about cool star atmospheres. The challenge became quickly to produce cool star atmospheres for oxygen-rich stars, as only a carbon star setup was available$^1$. Opacities for TiO and H$_2$O were missing: the chemical equilibrium did not include important species like TiO, and sphericity was included in a trial version but did not work properly. Thanks to Mats Larsson, Bosse Lindgren, and Lars Pettersson at Stockholm University, I was introduced to the arcane ideas of quantum chemistry, and could produce a first line list for TiO. Together with John Brett we computed VO and CaH line lists. We could not compute H$_2$O in the same manner, as our limited quantum chemistry skills stopped at 2-atom species, but used a trick to produce a pseudo line list from NASA observations of rocket exhausts (mean opacities and line density, together with a distribution of strengths). We knew this was in need of improvement, together with some other opacities, but it would allow, just as for carbon stars, a first assessment of the impact of these species on the atmospheric structure. The inclusion of spherical symmetry was made with the help of Åke Nordlund using his algorithm (Nordlund 1984). Finally, the MARCS code was made cool oxygen-rich-capable by modifying the chemical equilibrium routine, and OS was substituted for ODF with 11 000 points, keeping, however, ODF as an option. The extensive Kurucz atomic line data was included by Bengt Edvardsson (see Edvardsson et al. 1993). In Plez et al. (1992), the improved code, as well as the impact of molecular opacities and sphericity on models is described. Low resolution spectra are compared to observations of M giants and the models (Plez 1992) are compared to other grids. These models too were used with success in many applications in the following years.

Using the same code skeleton, Jørgensen et al. (1992) published a grid of carbon stars, with 5400 OS points, sphericity and C$_3$ opacity, although the latter would prove to be overestimated by a large factor later on. They also discuss in detail the effect of sphericity.

With the same code as Plez (1992), Edvardsson et al. (1993) computed a grid of metal-poor solar-type stars with a combination of 4100 OS points in the UV ($\lambda < 4500\,\text{Å}$) spectrum and 1400 ODF points in the red and, in a milestone paper, applied it to the chemical analysis of Galactic disc stars.

The evolution continued towards more exotic spectral types, with the first grid of line Blanketed H-deficient models by Asplund et al. (1997b) (see also Asplund et al. 1997a), Bound–free opacities were updated using data from the opacity project, and free–free opacities were added for carbon and helium ions. These were of course used to analyse RCB and related stars (e.g. Asplund et al. 1997).

There are a number of other papers summarizing add-ons and updates: Brett (1995) published a grid of M dwarfs; Bessell et al. (1998b) (see also Bessell et al. 1998a), in their work on the calibration of Johnson–Cousins photometry used an updated MARCS grid of cool star models, both giants and dwarfs, including updated molecular opacities, a much more extensive chemical equilibrium and more OS points; Plez et al. (2003) added ZrO opacities and computed the first S-type star atmosphere grid with detailed blanketeting (100 000 OS points) and made a first attempt at classifying S stars using the synthetic spectra and colours; and Gustafsson et al. (2003) published the web an extensive updated grid of FGK-type stars down to very low metallicities. The two latter grids used a completely revised chemical equilibrium with 92 elements and their ions as well as over 500 molecules, with updated partition functions and dissociation energies.

2. MARCS 2008

The papers above, starting around 1998, were all paving the way, and announcing the much awaited new MARCS$^4$. The idea of a large grid of updated MARCS models covering the cool part of the HR diagram dates back to a suggestion Bengt made to me in the park on Rackarberget at Dan Kiselman’s PhD party in 1993. Updates were constantly added, but had culminated two to three years before 1998, while I was on the payroll of Uppsala Observatory again. Citations of Gustafsson et al. in preparation date back to 1998. At some point we had a single version of the code, and a single set of physical input data, but I got my job in Montpellier and the entropy started increasing again. This is without mentioning the Copenhagen branch that already

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$^2$ Thanks to the hard work of our colleagues in quantum chemistry this problem has been solved for HCN (Harris et al. 2002, 2006), but is a solution still awaited for C$_2$H$_3$. I gain strongly encourage molecular physicists and quantum chemists to assemble a line list for that species. There is a great reward: analysis of carbon AGB stars in the local group and the history of carbon, understanding of cool carbon dwarfs, etc.

$^1$ This turned out to demand much more time, and I stayed in Uppsala for a total of 3.5 years: first for 16 more months as a French civil servant, teaching French conversation part-time to students and personnel of Uppsala university, then on a Swedish PhD fellowship. I met my wife during that time, and since then Sweden has become a second home country to me.

$^4$ It was dubbed MARCS$^35$ (guess why!) in 1998, and was supposed to be the final version for the new generation MARCS grid, while we were sketching the first draft of a series of papers, the first of which appeared only ten years later.
had diverged in 1991. We had a number of small workshops along the years to try to (i) get a single version of the code, (ii) update input data, (iii) find tricks to avoid crashes of extreme models, such as high luminosity, low gravity and cool supergiant models and (iv) draft a series of papers and decide what to discuss in what paper. Then, of course, in between these meetings, other exciting projects, teaching and administration took over. From September 2007 to May 2008, my sabbatical in Uppsala allowed us to once more, and this time for good, get a single more debugged, more updated (especially of continuous and line opacities) code from the Montpellier and Uppsala ones. The first paper in a presumably long series appeared recently (Gustafsson et al 2008) and the grid is (partly) on the web at http://marcs.astro.uu.se. MARCS 2008 is characterized by new opacities for H₂O, the atomic collisional line broadening included using the description of Anstee and O'Mara (1995), and the hydrogen lines modelled using a code by Barklem, described in Barklem and Piskunov (2003). About 108,000 OS points are used. Full details are provided in the paper which also relates some of the historical background and discusses in depth the physical assumptions, numerical methods and physical data used. About 10,000 models were computed.

3. Comparisons to observations

One decisive test to be passed by the models is a comparison to observed high-resolution spectra and spectral energy distributions (SEDs). High-resolution spectra allow us to check in detail if individual lines are well accounted for in the model, whereas low-resolution SED comparisons permit us to assess more easily problems in continuous opacity, thermal gradients and missing opacities. These comparisons must be carried out using stars with well determined stellar parameters spanning the grid of the models. In this volume, Bengt Edvardsson presents the first comparisons of the MARCS models to the SEDs of the Sun and solar-type stars. I have made a small number of comparisons for M-type dwarfs and giants. The results I present here are very preliminary. The model SEDs are the fluxes sampled at the 108,000 OS points and as such are not like an observed spectrum (see figure 1). When averaging on a wavelength interval including many OS points, the mean average level of the spectrum is recovered because, statistically, the OS points hit the continuum and lines of all strengths. Therefore, the sampled fluxes are a good representation of the SED only when binned to a much lower resolution. Our OS scheme has a constant wavelength resolution of \( \lambda / \Delta \lambda = 20,000 \) between 900 Å and 20 μm.

Comparisons were made with spectra from the MILES (Sánchez-Blázquez et al 2006) and STELIB (Le Borgne et al 2003) libraries, with both observations and synthetic SEDs binned to 50 Å intervals. For the giants (M1 to M6 III, i.e., 3800 K to 3250 K), the fit is generally good, except for excess absorption in the models around 5100 Å, most probably due to MgH, and ups and downs short of 4200 Å reminiscent of what Edvardsson (this volume) finds for the Sun (see section 4.1 for a possible explanation of one part of this). At M6 III, there is a hint of a missing opacity around 7500 Å (LaO?). The dwarfs are more difficult. Using a \( T_{\text{eff}} = 3950 \) K allows a fit of the TiO bands of an M0.5V template, but the computed spectrum is then too blue. A lower temperature of 3750 K gives a better shape for the continuum at the expense of, however, too deep TiO bands. In all cases there is excess blue flux in the model. At M6V, TiO bands are fitted but there is also excess flux in the blue. Work with Mike Bessell in the few days after the conference, using his own higher resolution spectrophotometry, allowed us to tie the blue flux problem to CaOH absorption, and maybe the AlH in metal-deficient stars, while providing better global fits. Detailed spectral comparisons need to be done, especially for dwarfs, missing opacities should be assessed and, if possible, the problem cured, and a temperature scale based on the models should be derived, as has been done for red supergiants (Levesque et al 2005, 2006). A paper in the MARCS 2008 series will be devoted to M stars and will detail these comparisons.

4. Opacity effects

A thorough discussion of the general effects of blanketing, of the impact of different opacity sources and of the effect of abundance and microturbulence changes on blanketing in various temperature regimes of the MARCS models is presented in Gustafsson et al (2008). Here, I will only complete this discussion with two items: the impact of wavelength sampling and some trial calculations on scattering in molecular lines.

4.1. Wavelength sampling

I have already stressed the fact that a large number of OS points are necessary in order to statistically well represent
the opacity, i.e., to sample equally well the continuum and lines of all strengths. But what is large enough? There are two issues: (i) how many points are needed to give a good representation of blanketing effects, and therefore provide a converged temperature stratification, in the sense that more points will not lead to changes in the model stratification larger than a prescribed value (say 1 K), (ii) how many points are needed to give a good representation of the SED, with a given model stratification (figure 1). These two numbers may well be different. I computed a series of models with subsets of our 108 000 OS points: three models with about 36 000 points, ten with 11 000 points and 30 with 3600 points. This was done for (i) a model of the Sun, (ii) a 5300 K M giant, and (iii) a 5500 K metal-poor dwarf ([Fe/H] = −2). For each set of models, the average spectrum and standard deviations were computed, and the same was done with the thermal structure (T − T\text{Ross}).

In the case of the Sun, with 36 000 OS points, temperature fluctuations are less than 10 K above T\text{Ross} = −2.0, and less than 1 or 2 K below. With 11 000 points (up to 100 K for the most deviant model), they are of the order of 30–50 K above T\text{Ross} = −3.5. Fluctuations stay below 15 K in all cases for T\text{Ross} > −2. The situation is much better for the cool giant, with temperature errors less than 20 K everywhere (−6 < T\text{Ross} < +2), down to 3600 sampling points. Errors decrease to less than 4 K everywhere with 36 000 points. In contrast, the situation is worse in optically thin regions for the metal-poor dwarf: temperature errors increase from 15 K at T\text{Ross} = −4 to 120 K at T\text{Ross} = −6, even with 36 000 points. The situation is better in the line-forming region: less than 10 K fluctuations below T\text{Ross} < −2.0, at all samplings. Therefore, errors in the T-structure due to sampling are only a few Kelvins in all cases for sampling densities in excess of 36 000 points. At smaller optical depths, errors may be large for metal-poor stars, and are small for cool giants (<10 K). Errors in the temperature stratification occur only if the line opacity is not well sampled, i.e. if the line and the OS-point densities are both too low.

When using 36 000 points, errors in the fluxes are below a few per cent wherever the flux matters, with the notable exceptions of the UV flux of solar-type stars and the IR CO bands of red giants. The case of the Sun is illustrated in figure 2. The errors around 3000 Å are of the order of 5–20%, and around 5% at 4000 Å. The trend at all wavelengths when increasing from 3600 to 36 000 points indicates that the new MARCS grid with 108 000 sampling points should provide SEDs with systematic errors \(\sqrt{3}\) smaller. With 36 000 OS points, the SED for the cool giant model shows errors of 5–10% in the IR CO bands at 1.6 and 2.5 \(\mu\)m. This is due to the intense CO lines that are sparsely distributed and sampled at a resolution of about 6500. Not surprisingly, the flux of the metal-poor dwarf is very well modelled even with low sampling (there are almost no lines), except where there are lines, i.e., in the UV band. When sampling at 36 000 points, errors reach much more than 10% only below about 1600 Å and are less than 2–5% between 3000 and 4000 Å.

In conclusion, the 108 000 OS points used in the computation of the MARCS 2008 models are sufficient for getting the thermal stratification errors down to a few Kelvins for all model parameters of the grid. An exception is the optically very thin layers of metal-poor stars, due to the fact that only a few lines dictate the thermal equilibrium in these layers. This is, however, a region where NLTE or 3D effects mostly probably play a greater role. The situation is worse for the sampled SEDs that may still be off by over 10%, especially in the blue UV band, as many lines act on the spectrum without greatly affecting the temperature structure, e.g., atomic lines in cool giants (see figure 5 in Gustafsson et al. 2008), MgH or CH in the Sun. Of course, better SEDs can be computed afterwards at very high resolution, and this will be done for the MARCS models. The sampled SEDs can nevertheless be used, e.g., to compute broadband colours.

4.2. Scattering versus absorption

Molecular lines have a large effect on the thermal structure of cool stars, through heating or cooling of the outer layers and backwarming of deeper layers. TiO-numerous electronic transition lines in the optical are known to lead to an important heating of the outer layers of cool stars. This is due to this strong opacity appearing on the blue side of the local source function and affecting thermal heating: \[
q = \int_0^\infty \kappa_\lambda (J_\lambda - B_\lambda) \, d\lambda, \quad (\text{with } q = 0 \text{ in local thermodynamic equilibrium (LTE)}),
\]
hot radiation from below, \(J_\lambda\), and the large \(\kappa_\lambda\) in the blue impose an increase of \(B_\lambda\) in the surface layers). Surface heating or cooling only happens if the opacity is in absorption, and a scattering term has no effect. It is quite possible that some molecular lines do indeed form closer to scattering than pure absorption in the tenuous outer layers of red giants. Hinkle and Lambert (1975) have already suggested, based on the meagre available collisional excitation data, that electronic transition of molecules in cool star atmospheres may be dominated by radiative processes and not by collisions with electrons or hydrogen. In the following, we examine again the particular situation of TiO.

Radiative transitions occur with \(t_{\text{rad}} = 40–100\ \text{ns}\) in most TiO electronic transitions. This means that collisional rates of excitation between these levels must be at least \(2.5 \times 10^7 \text{ s}^{-1}\) in order to compete and ensure LTE populations. For collisions with electrons, if we use the—most probably
inappropriate but the only one available—approximations of van Regemorter (1962) and Jeffries (1968) (see also Rutten 2003), an electron density of at least $3 \times 10^{14}\text{cm}^{-3}$ is needed. In typical MARCS cool supergiant models, $2 \times 10^6 < N_e < 2 \times 10^{10}\text{cm}^{-3}$, well below the limit. Lambert (1993) proposed a modification of Drawin’s (1969) formula, for hydrogen collisions with atoms that we may use—for lack of better estimates—to derive a critical hydrogen density of about $2 \times 10^{12}\text{m}^{-2}$. In the same MARCS models as above, we find $2 \times 10^{17} < N_e < 2 \times 10^{24}\text{m}^{-3}$. Alternatively, using measured quenching rates in oxides, e.g. the measurements of Badie et al (2008) in YO, for Ar, He and O$_2$, we find a critical density of perturbers of about $10^{23}\text{m}^{-3}$ in order to reach collisional excitation rates of $2.5 \times 10^7\text{s}^{-1}$. The efficiency of H collisions would have to be at least five orders of magnitude larger than that of He for hydrogen to be of significance in the excitation of YO electronic levels, and similarly of TiO. It seems thus very likely that radiative processes indeed dominate over collisional processes in the population of electronic levels of TiO and in transitions between them.

I therefore conducted a test calculation to study the impact of red giant models on the thermal structure if TiO lines were formed in scattering. The first set of models had $T_{\text{eff}} = 4300\text{K}$, $\log g = 1.75$, [Fe/H] = $-0.5$, and $M = 1\ M_{\odot}$ representing Arcturus. The model with TiO in scattering has a temperature about 250 K lower at $\tau_{5000} = 10^{-5}$, decreasing to about 130 K at $\tau_{5000} = 10^{-4}$ and vanishing at $\tau_{5000} = 10^{-3}$, the pressure stratification remaining unchanged. This cooling is what Ryde et al (2002) propose to explain the appearance of H$_2$O lines at $12\ \mu\text{m}$ in the Arcturus spectrum. However, when using the cooled MARCS model to generate a synthetic spectrum in the optical spectrum, TiO band heads (e.g. $\gamma(0,0)$ at 7054 Å) become visible, whereas they remain undetected in Hinkle et al’s (2000) FTS spectrum of Arcturus.

I did the same experiment with a model appropriate for Betelgeuse ($T_{\text{eff}} = 3600\text{K}$, $\log g = 0$, [Fe/H] = $0$ and $M = 15\ M_{\odot}$). In this case the cooling amounts to about 250 K at $\tau_{5000} = 10^{-5}$, to about 130 K at $\tau_{5000} = 10^{-3}$, and vanishes around $\tau_{5000} = 2.5 \times 10^{-2}$. Ryde et al (2006) detected the 12 $\mu\text{m}$ water vapour lines in Betelgeuse as well but could not reproduce them with a standard atmosphere model at 3600 K, which is the temperature derived from the optical spectrum. They needed a much cooler (3250 K) atmosphere. Our cooled MARCS model does not, however, reproduce the water lines: they remain too faint. In addition, neighbouring OH lines become too strong, but that could be alleviated by a decrease of O. The 2.3 $\mu\text{m}$ CO bands (Wallace and Hinkle 1996) are marginally better reproduced with the cooled MARCS model, but not better than using a molsphere, i.e. a spherical shell of gas at 2000 K, on top of the photospheric model, as has been advocated by various authors to explain spectroscopic and high angular resolution observations of red supergiants in the IR (e.g. Perrin et al 2007, Tsuji 2000).

Despite collisional timescale estimates being too long compared to radiative timescales to ensure LTE in electronic transitions of TiO, the simple assumption of its transitions occurring in scattering is not compatible with existing observations of red giants and supergiants. In particular, it cannot solve the 12 $\mu\text{m}$ H$_2$O lines puzzle. A better assessment of collisional rates in TiO, as well as a full NLTE treatment of electronic transitions, taking into account optical depth effects, as the lines may become optically very thick, would be of great value. Coupling with hydrodynamics should also be studied in detail as the balance between expansion cooling and radiative heating may be shifted by large amounts in the upper atmospheric layers (see the contribution by Wolfgang Hayek in this volume).

5. Final thoughts

After over 30 years, MARCS is now as mature as it can be within its approximations (hydrostatic, LTE, MLT). A much updated grid covering the red part of the HR diagram is now being published on the web (http://marcs.astro.uu.se), and the first paper in a series that will detail the behaviour of all models, compare the synthetic spectra to observations for a selected sample of template stars, or discuss synthetic photometry, has just appeared (Gustafsson et al 2008). Although we are increasingly turning our development activities towards relaxing some of the simplifying hypotheses upon which MARCS rests, it is likely that updates of the MARCS grid will be made available in the future, especially when better or additional opacities can be included. The drive behind the development of MARCS has always been the science that can be done with it, and that is unlikely to change. It is a tool that despite eluding dynamical effects, includes very detailed accounts of opacities and is flexible and light enough that it can be used to test many ideas (effects of line scattering on atmospheric stratification, impact of NLTE over-ionization on H$^-$ opacity, etc). In that respect, it will remain irreplaceable for many years to come.

Acknowledgments

The MARCS code and its package of tools, e.g. detailed spectrum calculation is the result of many years (decades!) of collaborative, and mostly enjoyable, work within the MARCS team: Bengt Edvardsson, Kjell Eriksson, Bengt Gustafsson, Åke Nordlund, Uffe-Graae Jørgensen, as well as a number of others whose names appear above. I am especially happy to thank Bengt, Kjell and Bengt for inviting me during this year I have spent on sabbatical in Uppsala. It has been an exciting time, although of course I did not get done one-third of what I hoped to do ... but the first MARCS 2008 paper is out! I thank Nils Ryde for discussions on molspheres and for helping me to get the best out of TEXES observations kindly provided by Mats Richter. Most of all I wish to express my gratitude to Bengt, who, in addition to being a constant source of inspiration, showed me how to never be satisfied with a result before I fully understood it. This may sometimes be very irritating, when projects or papers get stuck for months or years because of such a difficulty, but the reward is greater in the end. Tack! Och grattis till födelsedagen!

Appendix. Discussion

Q: (T Lynas-Gray) I note with interest the difficulty in matching energy distributions for M dwarfs. Did you use the water line list by Schwenke and Partridge, or the one by Barber and Tennyson?

A: The one by Barber and Tennyson.
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