Cool Stellar Atmospheres

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Abstract. We give an overview about the state-of-the-art in cool stellar (and sub-stellar) atmosphere simulations. Recent developments in numerical methods and parallel supercomputers, as well as in the quality of input data such as atomic and molecular line lists have led to substantial improvements in the quality of synthetic spectra when compared to multi-wavelength observations. A wide range of objects from M dwarfs and giants down to substellar objects is considered. We discuss effects such as atomic and molecular NLTE (and) line blanketing, external irradiation, and formation and opacities of dust particles and clouds; each of which affects the structure of the atmospheres and their spectra. Current models can simultaneously fit many of the observed features of a given star with a single model atmosphere, however, a number of problems remain unsolved and will have to be addressed in the future, in particular for very low mass stars and substellar objects.

1. Introduction

Stellar atmosphere modeling has experienced a renaissance in the past decade with the advent of better algorithms and faster computers. This has allowed research groups to remove or relax many of the “standard” assumptions that were made in the 70s and 80s and that had become accepted wisdom over the
Figure 1.  Best fit of Allard & Hauschildt (1995b) to the spectrum of the dM8e star VB 10 (Allard & Hauschildt, 1995a).  The corresponding H\textsuperscript{-} continuum obtained by neglecting molecular opacities only in the radiative transfer (long dot-dashed) reveals the magnitude of these opacities in a typical late-type M dwarf.  The Planck distribution of the same $T_{\text{eff}}$ is also shown for comparison.  From Allard et al. (1997).

years. Surprisingly (or not) the new calculations show that many of these assumptions are actually quite bad and can lead to spurious results or incorrect interpretations of observed spectra. The intricate connection between geometry (plane parallel or spherical), line blanketing (atomic and/or molecular) and non-LTE effects (using small to extremely large model atoms and molecules) began to emerge slowly as crucial ingredients for physically correct and meaningful interpretations and analyses of stellar spectra. Unfortunately, easy and simple solutions do not really work for stellar atmospheres (although everybody likes the easy way out and some of them are useful for teaching purposes) and have actually hindered progress and reduced the reliability of results.

New observational techniques opened and continue to open up new areas of stellar atmosphere research. The most important advance has been detailed observations of very low mass stars and after decades of searching, brown dwarfs and extrasolar giant planets. Modeling these objects requires sophisticated stellar atmosphere type modeling with complex equations of state and 100's of millions of molecular spectral lines in order to even approximately reproduce the observed spectra. These new observations have prompted further evolution of stellar atmosphere modeling and helped rejuvenate the field in general.

In the following we will briefly introduce the numerical methods that modern stellar atmosphere research employs (there are also plenty of legacy appli-
Figure 2. Spectral distributions of emerging fluxes at the stellar surface for 3,000 K models with metallicities corresponding roughly to the solar neighborhood ([M/H] = 0.0), halo ([M/H] = −2.0), and Population III ([M/H] = −4.0) stars. A black-body of the same effective temperature (smooth curve) is shown for comparison. From Allard et al. (1997).

cations and codes that are still widely used) and then discuss some results that are of interest in the context of this meeting.

2. Methods and Models

For our model calculations, we use our multi-purpose stellar atmosphere code PHOENIX (version 10.9 Hauschildt, Baron, & Allard, 1997; Baron & Hauschildt, 1998; Hauschildt, Allard, & Baron, 1999; Hauschildt et al., 1999; Hauschildt & Baron, 1999). Details of the numerical methods are given in the above references, so we do not repeat the description here.

2.1. Line opacities

One of the most important recent improvements of cool stellar atmosphere models is the treatment of molecular line opacity. Our combined molecular line list includes about 550 million molecular lines. The lines are selected for every model
Figure 3. Overview over selected departure coefficients for a NLTE model with $T_{\text{eff}} = 4000 \, \text{K}$, $\log(g) = 0.0$, and solar abundances.

from the master line list at the beginning of each model iteration to account for changes in the model structure (see below). Both atomic and molecular lines are treated with a direct opacity sampling method (dOS). We do not use pre-computed opacity sampling tables, but instead dynamically select the relevant LTE background lines from master line lists at the beginning of each iteration for every model and sum the contribution of every line within a search window to compute the total line opacity at arbitrary wavelength points. The latter feature is crucial in NLTE calculations in which the wavelength grid is both irregular and variable from iteration to iteration due to changes in the physical conditions. This approach also allows detailed and depth dependent line profiles to be used during the iterations. Although the direct line treatment seems at first glance computationally prohibitive, it leads to more accurate models. This is due to the fact that the line forming regions in cool stars and planets span a huge range in pressure and temperature so that the line wings form in very different layers than the line cores. Therefore, the physics of the line formation is best modeled by an approach that treats the variation of the line profile and the level excitation as accurately as possible. To make this method computationally more efficient, we employ modern numerical techniques, e.g., vectorized and parallelized block algorithms with high data locality (Hauschildt, Baron, &
Figure 4. Example of limb darkening for a subgiant model (calculated using spherical geometry and spherically symmetric radiative transfer) with $T_{\text{eff}} = 5000$ K, $\log(g) = 2.5$ and solar abundances. The computed (normalized to the center of the stellar disk) mono-chromatic intensities at $\approx 5000$ Å are shown (+ symbols) and compared to linear (dotted line) and square root (dashed line) limb darkening laws.

Allard, 1997), and we use high-end workstations or parallel supercomputers for the model calculations.

In the calculations presented in this contribution, we have included a constant statistical velocity field, $\xi = 2$ km s$^{-1}$, which is treated like a microturbulence. The choice of lines is dictated by whether they are stronger than a threshold $\Gamma \equiv \chi_l/\kappa_c = 10^{-4}$, where $\chi_l$ is the extinction coefficient of the line at the line center and $\kappa_c$ is the local b-f absorption coefficient (see Hauschildt, Allard, & Baron, 1999, for details of the line selection process). This typically leads to about 10 – 250 million lines which are selected from master line lists, depending on model parameters. The profiles of these lines are assumed to be depth-dependent Voigt or Doppler profiles (for very weak lines). Details of the computation of the damping constants and the line profiles are given in Schweitzer et al. (1996). We have determined by test calculations that the details of the line profiles and the threshold $\Gamma$ do not have a significant effect on either the model structure or the synthetic spectra. In addition, we include
Figure 5. This plot shows the difference between synthetic spectra calculated for a model atmospheres assuming complete settling of all formed dust particles below the layers where spectrum forms ("cond" model) and for a model that assumes that the dust particles remain close to the layer in which they formed ("dusty" model) for $T_{\text{eff}} = 1700$ K, $\log(g) = 4.5$ and solar abundances.

about 2000 photo-ionization cross sections for atoms and ions (Mathisen, 1984; Verner & Yakovlev, 1995).

The effects of water lines on the M dwarfs SED was discussed in Allard et al. (1994). For the work presented here, we have replaced the UCL water vapor line-list (Miller et al., 1994; Schryber, Miller, & Tennyson, 1995, hereafter: MT-H$_2$O) used in Hauschildt, Allard, & Baron (1999) with the AMES water line-list (Partridge & Schwenke, 1997, hereafter: AMES-H$_2$O). This list includes about 307 million lines of water vapor. For the calculations shown in this paper we have used H$_2$O and neglected other, much less abundant, isotopes of this molecule. More details can be found in Allard, Hauschildt, & Schwenke (2000) and Allard et al. (2001). We have compared the AMES-H$_2$O results to results obtained with the new SCAN water vapor line list (Jørgensen et al., 2001) and found only small differences for our modeling purposes.

The water vapor opacity is governed by the completeness of the line list used, but also by the adopted atomization energy. The partition function of
Figure 6. The optical Cousins broad-band synthetic photometry of solar metallicity and fixed gravity (log(g) = 5.0) models of the NextGen grid (dotted line), AMES-MT grid (long-dash line), and AMES grid (full line) are compared to the photometric sample of Leggett (1992). This sample contains mostly M dwarfs and metal-depleted M subdwarfs of the solar neighborhood, and becomes scarce in the late-type dwarf regime.

the molecule cancels out in the final absorption coefficient, after we have multiplied cross-sections by number densities. But since water is an important chemical equilibrium species, errors in the partition function can indirectly affect the model structure and spectra. The Allard & Hauschildt (1995b) models were based on the Ludwig (1971) hot flames water cross-sections in the form of straight means, and used the JANAF partition function for water vapor (Irwin, 1988). The NextGen models were, on the other hand, computed with the MT-H_2O line list and a partition function computed from the MT-H_2O levels. We note that the AMES-H_2O partition function is practically identical to JANAF values, while the MT-H_2O value is smaller than JANAF for temperatures above 3000K, possibly due to the energy levels missing in the MT-H_2O data. We have therefore adopted for this and later work the JANAF partition function. We use an atomization energy of 9.5119 eV from Irwin (1988) for all models calculated after Allard & Hauschildt (1995b).
Figure 7. Same as Fig. 6 for near-infrared broad-band colors covering the water opacity range. Please note that the hot star tail of the sample, near H-K=0.1, is reproduced by the NextGen and AMES-MT models for the lower gravities predicted by evolution models for 5 to 10 Gyrs isochrones. Of the models shown, only the NextGen are grain-less, which explains their curling up at the low temperature end compared to AMES-MT models.

2.2. Equation of State

The equation of state (EOS) is an enlarged and enhanced version of the EOS used in Allard et al. (1997). We include about 500 species (atoms, ions and molecules) in the EOS. This set of EOS species was determined in test calculations. The EOS calculations themselves follow the method discussed in Allard & Hauschildt (1995b). For effective temperatures, $T_{\text{eff}} < 2500\,\text{K}$, the formation of dust particles has to be considered in the EOS. In our models we allow for the formation (and dissolution) of a variety of grain species.

2.3. Non-LTE

The NLTE treatment of large model atoms or molecules such as H$_2$O and TiO which have several million transitions is a formidable problem which requires an efficient method for the numerical solution of the multi-level NLTE radiative transfer problem. Classical techniques, such as the complete linearization or the
Figure 8. Same as Fig. 6 and 7 for broad-band colors sampling side-to-side of the SED’s flux peak.

Equivalent Two Level Atom method, are computationally prohibitive for large model atoms and molecules. Currently, the operator splitting or approximate λ-operator iteration (ALI) method (e.g., Cannon, 1973; Rybicki, 1972, 1984; Scharmer, 1984) seems to be the most effective way of treating complex NLTE radiative transfer and rate equation problems. Variants of the ALI method have been developed to handle complex model atoms, e.g., Anderson’s multi-group scheme (Anderson, 1987, 1989) or extensions of the opacity distribution function method (Hubeny & Lanz, 1995). However, these methods have problems if line overlaps are complex or if the line opacity changes rapidly with optical depth, a situation which occurs in cool stellar atmospheres. The ALI rate operator formalism (Hauschildt, 1993; Hauschildt & Baron, 1999), on the other hand, has been used successfully to treat very large model atoms such as Fe directly and efficiently (cf. Hauschildt & Baron, 1995; Hauschildt et al., 1996; Baron et al., 1996; Hauschildt & Baron, 1999).

3. Results

In the following sections we will give a few representative results that highlight important new developments in stellar atmospheres.
3.1. Line blanketing

The number of molecular lines that are important in M dwarf (and later) atmospheres is quite large. About 215 million molecular lines are selected (see above) for a typical giant model with $T_{\text{eff}} \approx 3000$ K whereas about 130 million molecular lines have to be considered for a dwarf model with the same effective temperature. The large “density” (in wavelength space) of molecular lines causes large line blanketing effects as illustrated in Fig. 1 for a very simple case. The nearly complete coverage of the optical spectrum by TiO lines and of the near IR spectrum by H$_2$O lines effectively locks the peak of the spectral energy distribution in place at around $1.1\mu$m even for substantially different $T_{\text{eff}}$, in stark contrast to the behavior expected for blackbodies. Line blanketing also produces a strong metallicity effect on the spectra as illustrated in Fig. 2. Lowering the metal abundances reduces both the TiO and H$_2$O opacities by roughly the same amount. However, the H$_2$O opacity in the near IR is replaced by increasingly (with lower metallicity) stronger collision induced opacities (due to the larger pressures in the spectrum forming regions). Therefore, the spectrum gets bluer with lower metallicities, even for comparatively low effective temperatures.

3.2. NLTE effects

Due to their very low electron temperatures, the electron density is extremely low in M stars; absolute electron densities are even lower than found in low density atmospheres, such as those of novae and SNe. Collisional rates due to collisions with electrons, which tend to restore LTE, are thus very small in cool stars. This in turn could significantly increase the importance of NLTE effects in M stars when compared to, e.g., solar type stars with much higher electron densities and temperatures. Collisions with molecular hydrogen and helium will at least partly compensate for the diminished electron collisions, but cross-sections for these processes are not very well known. Therefore, the assumption of LTE for atoms and molecules in cool stars is by no means certain and needs to be verified for each species individually. We have performed test calculations to place an upper limit for the importance of atomic NLTE effects in cool stars by only considering electron collisions.

We have calculated a small number of NLTE models in order to investigate the importance of NLTE effects on the structure of the model atmospheres. The results for cooler models were discussed in Hauschildt et al. (1997) and are not repeated here. Figure 3 shows an overview of selected NLTE species for models with $T_{\text{eff}} = 4000$ K, $\log(g) = 0.0$ and solar abundances. The total number of NLTE levels in each model is 4532 with a total of 47993 primary NLTE lines (see Hauschildt & Baron, 1999; Hauschildt et al., 1999, and references therein for details). For most of the species, the departure coefficients are always close to unity, in particular for species with resonance lines and photoionization edges in the UV part of the spectrum. The species shown in Figure 3 are species with the most pronounced departures from LTE. The departures are generally too small to significantly affect the structure of the atmospheres. Results for NLTE calculations for the CO molecule show that the high cross-sections of H$_2$ and He collisions restore LTE very successfully in the case of dwarf stars (Schweitzer, Hauschildt, & Baron, 2000).
3.3. Dust and cloud formation

The effects of dust formation on the atmosphere are mainly (a) the removal of important opacity sources (e.g., TiO, VO) from the gas phase and a corresponding weakening of their spectral lines; and (b) the presence of additional opacities produced by the grains themselves, cf. Fig. 5. The latter depends on the behavior of the macroscopic dust particles:

a) They might remain as dust clouds in the layers where the dust originally formed and thus cause strong optical and IR opacities due to these clouds ("Dusty" models).

b) They could rain out and settle below the line and continuum forming regions, resulting in no grain opacities detectable in the spectrum ("Cond" models).

c) They can form depleted clouds in the atmosphere so that dust opacities would only be present in the cloud layers but not necessarily in all the layers where the dust had originally formed ("Settle" models).

Observational evidence (see below) suggests that case (a) is realized for $T_{\text{eff}} > 1800$ K (late M dwarfs to early L dwarfs) whereas for giant planets and extreme T dwarfs case (b) appears to be more appropriate. In the intermediate regime, partial clouds appear to form and case (c) must be investigated. At the present time, this sequence is still very tentative and the physical models of dust and cloud formation have to be refined to obtain a truly physical picture of brown dwarfs and extrasolar giant planets.

3.4. Importance of Spherical Symmetry

Limb darkening is an important tool for the investigation of the structure of stellar atmospheres, in particular for subgiants and giants. It is now possible to use fortuitous microlensing events to study the detailed spectral variations of a microlensed giant, allowing us to more strictly test model atmospheres. In Fig. 4 we show the limb darkening in the optical ($\sim 5000$ Å) for a cool giant with $T_{\text{eff}} = 5000$ K and $\log(g) = 2.5$ (solar abundances). For comparison, linear and square-root limb darkening laws are also shown. The form of the limb darkening and the deviations of the computed intensities from the simple limb darkening laws changes substantially with wavelength and model parameters (see also Orosz & Hauschildt, 2000). This is caused by the effects of spherical radiation transport, which tends to concentrate the emitted intensities closer to the center of the stellar disk than the plane parallel approximation does. Curvature close to the rim of the stellar disk reduces the total emissivity and optical depth and thus produces less emitted radiation than plane parallel models in which the pathlength and optical depth close to the rim actually approaches infinity. In order to obtain reliable and useful stellar atmosphere information from microlensing observations we need to use rather sophisticated modeling, simple approximations will in most cases not work. Using detailed limb darkening models as shown here has helped Orosz & Hauschildt (2000) to address a number of problems regarding lightcurves of eclipsing binaries.
3.5. Colors

To better judge of the impact of opacity changes on the overall SED of M dwarfs in general, we have computed synthetic photometry as described in Allard & Hauschildt (1995b) for three sets of models: (1) the NextGen grid based on Jorgensen (1994) TiO lines and MT-H$_2$O (2) the AMES grid based on (Schwenke, 1998, hereafter, AMES-TiO) TiO lines and AMES-H$_2$O opacities, and (3) the AMES-MT grid based on AMES-TiO and MT-H$_2$O opacities. The results are compared to a photometric sample of M dwarfs (Leggett, 1992) in Figs. 6, 7, and 8. Since M dwarfs form a tight sequence in optical VRI two-colors diagram despite the age and metallicity scatter of the sample (see Allard & Hauschildt, 1995b) this diagram imposes a strong constraint on model atmospheres. We find that models based on AMES-TiO opacities are systematically redder in $V - R$ and $V - I$ than models based on the Jorgensen (1994) line list. The new models agree much better with observations and the new TiO data removes most of the discrepancy shown by the NextGen models in the lower main-sequence. Small remaining discrepancies may be attributed to the JOLA handling of VO and CaH which tends to slightly overestimate their opacities in the present models. Leinert et al. (1999) studied the low resolution HST/FOS spectra of an M6 dwarf (LHS1070A) and found the AMES-MT models indeed agree quite well both with the observed SED and absolute fluxes within errors on the parallax of the system. They however noticed that some “continuum” flux excess remains important in the visual part of the SED (0.45 to 0.65 $\mu$m). However, there is no a priori reason to assume that the a-f oscillator strengths are inaccurate, and these remaining problems could be related to other effects of the model structure.

The use of AMES-H$_2$O seems also to bring some improvements to the modeling of near-infrared colors. Fig. 7 shows that the late-type dwarfs can be better reproduced by the new water opacities than by the MT-H$_2$O line list. However this diagram is sensitive to both gravity (lower gravity models loop lower) and metallicity, which makes it difficult to constrain the models on the adequacy of the water opacities used with them. However, Leggett, Allard, & Hauschildt (1998) and Leggett et al. (2000) have used the AMES models in their analysis of M dwarfs and brown dwarfs, and found excellent general agreement of the predicted near-infrared SED with observations. However these analyses used the models to derive the parameters of the studied stars and brown dwarfs based on fits to the near-infrared SED or photometry, and could not make an independent statement on the quality of the water line list.

M dwarfs again form a sequence in the mixed-colors IJK diagram (Fig. 8), although less tightly than in the VRI diagram. Unresolved binary stars produce K-band flux excess and lie below the sequence. H$_2$ pressure-induced opacities depress the K-band flux of metal-depleted dwarfs so that they systematically lie above the sequence. But, as opposed to the JHK diagram, this one is not particularly sensitive to gravity in M dwarfs which allows a sequence to be defined. Models should therefore pass through the bulk of early-type M dwarfs at $J - K = 0.8$, and follow a relatively $J - K$-insensitive sequence towards late-type dwarfs. We find that models based on the AMES-H$_2$O opacities lie, as did the Allard & Hauschildt (1995b) models before them, 0.2 magnitude in $J - K$ to the blue of the observed sequence! Our tests show that this result is independent
of the TiO opacities used. The NextGen models already reproduced perfectly the location of lower main-sequence stars in this diagram. AMES-MT models computed using the AMES-TiO and MT-H₂O line lists behave adequately both in the optical and infrared. Why? Perhaps the new water vapor line list is still not complete enough at high temperatures and lacks opacity in the J-bandpass i.e. around 1.3 μm? Or could it have too much opacity in the K-window i.e. around 2.2 μm? Until these questions can be answered, we hope that the two main sets grids of models we have computed (AMES and AMES-MT) will allow independent detailed confrontations to observations of cool stars that will more precisely locate the source of the problem.

4. Summary and Conclusions

In this paper we have discussed a few new results of stellar atmosphere modeling that have helped to resolve some outstanding problems understanding and interpreting observed stellar spectra. During the last decade, progress was made by breakthroughs in both methodology and computer technology, which has lead to substantially improved models and synthetic spectra. In many cases, even our currently “best effort” models cannot reproduce observed spectra satisfactorily, this is particularly the case for L and T dwarfs. However, this is due to physical effects that we “know,” but we cannot currently describe well enough (e.g., incomplete line lists for key molecules or dust and cloud formation processes). Another area that requires much more work is our detailed understanding of winds from both hot and cool stars. There is currently a lot of effort being put into the solution of these key problems, although it is clear that once they are solved, others will pop up in unexpected places.

Most of the model grids that are described in this contribution are available on the WWW at http://phoenix.physast.uga.edu and via FTP at ftp://calvin.physast.uga.edu/pub. The model grids are updated frequently and spectra, model structures and colors are all available at the above sites.

Acknowledgments. This work was supported in part by the CNRS, INSU and by NSF grants AST-0086246 and AST-9720704, NASA ATP grant NAG 5-8425, NASA ADP grant NAG5-9222, and LTSA grant NAG 5-3619, as well as NASA/JPL grant 961582, NASA grant AST-0086246, as well as grants GO-0-1013C & HST-GO-08671.09-A to the University of Georgia. PHH was supported in part by the Pôle Scientifique de Modélisation Numérique at ENS-Lyon. Some of the calculations presented in this paper were performed on the CNUSA IBM SP2, the IBM SP2 and SGI Origin 2000 of the UGA UCNS, on the IBM SP “Blue Horizon” of the San Diego Supercomputer Center (SDSC), with support from the National Science Foundation, and on the IBM SP and the Cray T3E of the NERSC with support from the DOE. We thank all these institutions for a generous allocation of computer time.
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