1994ApJ...426L..39A

THE ASTROPHYSICAL JOURNAL, 426:L39–L41, 1994 May 1
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THE INFLUENCE OF H_2O LINE BLANKETING ON THE SPECTRA OF COOL DWARF STARS

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Received 1994 January 11; accepted 1994 February 10

ABSTRACT

We present our initial results of model atmosphere calculations for cool M dwarfs using an opacity sampling method and a new list of H_2O lines. We obtain significantly improved fits to the infrared spectrum of the M dwarf VB10 when compared to earlier models. H_2O is by far the dominant opacity source in cool stars. To illustrate this, we show the Rosseland mean of the total extinction under various assumptions. Our calculations demonstrate the importance of a good treatment of the water opacities in cool stars and the improvements possible by using up-to-date data for the water line absorption.

Subject headings: molecular data — stars: low-mass, brown dwarfs

1. INTRODUCTION

The quality and number of observations of M dwarfs has improved dramatically in the last few years. In parallel with this, the interest in detail model atmospheres for M dwarfs has increased. The problem of calculating realistic M dwarf atmospheres is very complex due to the large number of molecules that are expected to be present in the atmosphere and the many individual opacity sources that must be included in the model construction and the calculation of synthetic spectra. Saumon et al. (1994) have calculated a grid of zero-metallicity cool star atmospheres that is useful as a limiting case. Calculations of model atmosphere grids for M dwarfs with nonzero metallicity, which can be compared directly to observed spectra, have been performed by Mould (1976), Allard (1990), and Kui (1991). These calculations are able to reproduce many of the observed features found in the optical spectra but give comparatively poor fits in other spectral regions, particularly the infrared.

At IR wavelengths ($1 \leq \lambda \leq 20$ μm), water vapor is the most important opacity source in cool stars ($T_{\rm eff} < 3500$ K). Until recently, only relatively coarse data for the opacity of water vapor, due to Ludwig (1971), were available, and the fit to the IR spectra of M dwarfs was relatively poor. The Ludwig data suffered because the absorption was averaged in 25 cm^{-1} bins. As we show below, the spectral structure within these bins has a significant influence on the model atmosphere calculations.

In this *Letter* we report our initial results of an improved grid of model atmospheres and corresponding synthetic spectra calculated using a new list of H_2O lines. This new list contains about 6.2 million lines of H_2O in the range between 1 and 200 μm. Using the new list we have calculated plane-parallel, static, LTE, line-blanketed stellar atmospheres for a range of model parameters.

2. MODEL ATMOSPHERES

We use the model atmosphere code PHOENIX, version 4.4, to compute model atmospheres and synthetic spectra for cool dwarf stars. PHOENIX is described in some detail in Hauschildt et al. (1994) and Baron, Hauschildt, & Branch (1994), so we describe here only the most important features. PHOENIX solves the (special relativistic) equation of radiative transfer (RTE) in the Lagrangian frame self-consistently with the multilevel, non-LTE rate equations and the (special relativistic) radiative equilibrium (RE) equation in the Lagrangian frame. Recent improvements to PHOENIX include the following: (1) the numerical solution of the RTE is done using the Accelerated Lambda Iteration (ALI) method described by Hauschildt (1992), (2) the RE equation is solved by a modified Unsöld-Lucy method (Allard 1990), (3) the multi-level non-LTE continuum and line transfer problem is treated using the ALI method described by Hauschildt (1993), and (4) convection is included using the mixing length formalism (Allard 1990).

Some aspects of cool dwarf stars allow us to adopt a number of significant simplifications that lead to a substantial saving in CPU time per model calculation. In addition, since we are here mostly concerned with the formation and the effects of the water lines, this allows some further simplifications. First, the atmospheres of M dwarfs can be treated in the plane-parallel and static approximation since the gravities are $\log(g) \approx 5$, leading to a compact atmosphere with a relative extension of less than 1%. We neglect the effects of convective motion on line formation, since the velocities of the convection cells are too small to be detected in low-resolution spectra and will have a negligible influence on the transfer of line radiation. Second, we neglect NLTE effects for simplicity. This may be not a good assumption for modeling individual metal lines because the collisional rates may be very small due to the lack of free electrons and the relatively small collisional cross-sections for collisions with, for example, H and H_2.

Although PHOENIX can treat the effects of external radiation fields on the model atmosphere and the synthetic spectrum (cf. Baron et al. 1994), we assume here a negligible external radiation field for simplicity. It is clear, however, that UV radiation impinging on the M dwarf, from, say, a hotter companion, may change the structure of the atmosphere and the corresponding

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spectra. We plan to investigate these effects in subsequent work.

The equation of state used in PHOENIX includes up to 26 ionization stages of 39 elements (H, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, P, S, Cl, Ar, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Kr, Rb, Sr, Y, Zr, Nb, Ba, and La) as well as more than 100 molecules (Allard 1990, 1993). In the calculations reported in this *Letter*, we have considered only the first two ionization stages of each element and the full list of molecules. Molecular bands are included in the Just Overlapping Line Approximation (JOLA) for the most important bands of CN, TiO, OH, CH, CO, VO, MgH, SiH, CaH, and FeH. In addition, the Collision-Induced Absorption for H_2-H_2, H_2-H and H_2-He (Allard 1993) as well as the b-f and f-f atomic processes (Hauschildt et al. 1992; Allard 1993) are included in the continuous opacity.

The models include, self-consistently, line blanketing of the most important metal lines selected from the line list of Kurucz (1993) and the most important lines of the H_2O molecule. The combined lists contain close to 48.2 million ($\sim$42 million atomic and ionic and $\sim$6.2 million H_2O) lines; however, not all of them are important for the case at hand. Therefore, before every temperature iteration, a smaller list is formed from the original list. First, an optical depth point is chosen, usually at $\tau_{std} \approx 0.01$. Then, using the density and temperature for this point, the absorption coefficient in the line center, κ_l, is calculated for every line and compared to the corresponding continuum absorption coefficient, κ_c. A line is transferred to the "small list" if the ratio κ_l/κ_c is larger than a prespecified value of Γ (usually 10^{-4}). In the subsequent radiative transfer calculations, all lines selected in this way are taken into account as individual lines; all others from the large line list are neglected. This selection procedure is repeated at every iteration in order to include always the most important lines, even if the temperature stratification changes significantly. Using this selection process, we find that, typically, $\sim$50,000 metal lines and $\sim 2.1 \times 10^6$ H_2O lines are stronger than about 1% of the local (b-f and f-f) continuum absorption. In the model calculations we then use a direct opacity sampling method on a very fine wavelength grid with about 20,000 wavelength points. For each wavelength, we solve the radiative transfer equation using the absorption and scattering coefficients calculated at the particular wavelength.

The model atmospheres are characterized by the following parameters: (1) the surface gravity, log (g); (2) the effective temperature, T_{eff}; (3) the mixing length to scale height ratio, l, here taken to be unity; (4) the line threshold ratio, Γ; and (5) the element abundances.

3. WATER LINE LIST

A water linelist has been generated by direct calculation of rotation-vibration energy levels, wavefunctions, and associated transitions. These calculations were performed with the TRIATOM program suite (Tennyson, Miller, & Le Sueur 1993) using the best available (Fernley, Miller, & Tennyson 1991) H_2O potential due to Jensen (1989) and the recent dipole surface of Wattson & Rothman (1993). The present line list extends that reported by Miller et al. (1993), where details of the calculations can be found.

Calculations were performed for rotational levels up to $J = 30$. Although convergence is very good for states with $J \leq 20$ it deteriorates to about 10 cm^{-1} for states with $J = 30$. All levels up to 11,000 cm^{-1} above the ground state are included as well as many, but not all, higher ones. This energy cutoff is probably too low for a complete treatment of the water opacity problem and may have some effect on the opacity for wavelengths shorter than 1.8 μm.

Transitions were calculated using only rigorous selection rules concerning angular momentum ($\Delta J = 0, \pm 1$) and parity. Here 8.4×10^6 transitions were calculated, and 6.2×10^6, with line strengths greater than 10^{-10} D^2, were retained in the initial list.

4. RESULTS

Using the methods described above, we have computed a small grid of model atmospheres with solar abundances, log (g) = 5, and effective temperatures from 2200 to 3200 K. Each model was iterated until energy conservation was better than 0.1% in the radiative layers and the temperature changes in the convective layers were smaller than 1 K; see Allard (1990) for a description of the model calculation. The effects of line blanketing due to atomic, ionic, and H_2O lines are included self-consistently in the models. These atmospheres were then used to compute high-resolution synthetic spectra from the UV to the far-IR spectral regions.

In Figure 1 we compare the observed spectrum of the M8 star VB10 (solid curve): 0.6–1.5 μm (Kirkpatrick et al. 1993), and 0.9–2.5 μm (Jones et al. 1994) with our synthetic spectra calculated for $T_{eff} = 2800$ K. The dash-dotted curve gives the synthetic spectrum obtained using the water opacity given by Ludwig (1971), whereas the dotted curve is the synthetic spectrum obtained using the H_2O line list. The new model fits the region below 1.5 μm and above 2 μm significantly better than the old model using the Ludwig opacity.

Both models fail to fit the region around 1.6 μm. The Ludwig opacity is too large in this region, while our present water line

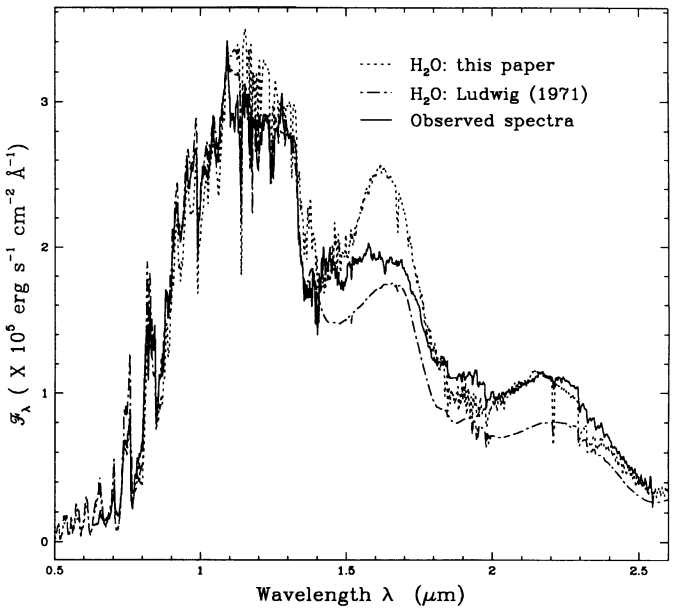

FIG. 1.—Observed spectrum of VB10 (*solid curve*) compared to synthetic spectra, plotted on a *linear flux* scale. The dash-dotted curves gives a synthetic spectrum computed using the Ludwig (1971) water opacities, whereas the dotted curve is a synthetic spectrum computed using the new H_2O line list. Model and observed spectra have been normalized at 1.1 μm. We did not change any model parameters in order to improve the fit; both models assume $T_{eff} = 2800$ K, log (g) = 5, and solar abundances.

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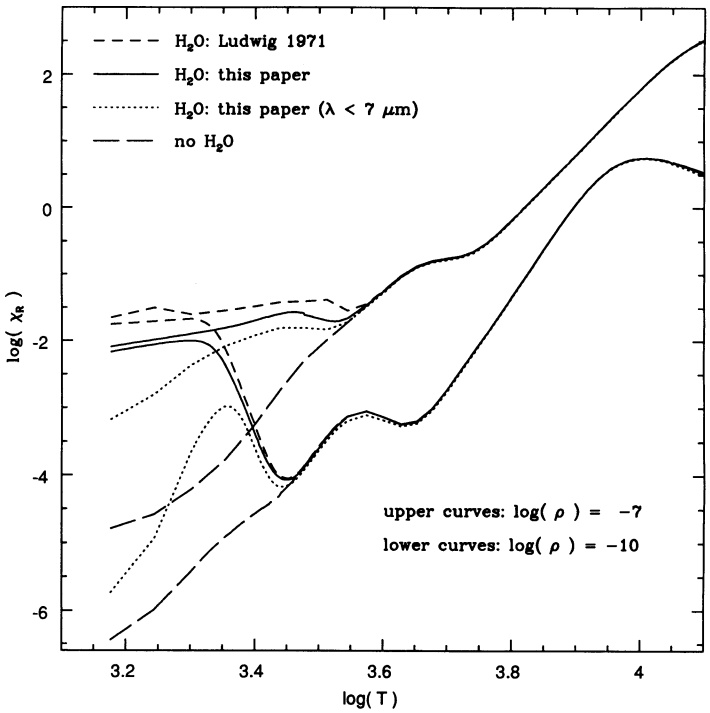

FIG. 2.—Rosseland mean opacity as a function of electron temperature for two densities. The solid curves give the results obtained using the H_2O line list, the long dashed curves are the results if the opacity of water vapor is neglected, the dotted curves indicate the result obtained if only H_2O lines with wavelengths smaller than 7 μm are considered, and the short dashed curves the result obtained using the Ludwig (1971) water vapor opacities.

list underestimates the opacity. In this region the opacity due to water vapor has a pronounced minimum both in the Ludwig data and the new H_2O line list. In addition, the opacity due to other absorbers is also relatively small so that photons can escape from deeper and hotter layers. While it is difficult to see how matters could be improved using the Ludwig data, since it overestimates the opacity, the present water vapor line list is especially incomplete *below* 1.8 μm. We expect, therefore, the fit to be further improved using future, more complete, line lists for water and other species.

In Figure 2 we demonstrate the importance of water vapor on the Rosseland mean opacity using various prescriptions for the absorption coefficient of H_2O. The solid curve gives the results obtained with the new H_2O line list, whereas the dashed line gives the results obtained using the Ludwig water opacities. We have also plotted the results obtained by neglecting H_2O completely as an opacity source (but including it in the equation of state) and by artificially neglecting water lines above 7 μm. In general, the Ludwig opacities are significantly larger than the opacities calculated using the line list directly (this can also be seen in Fig. 1), in particular for lower temperatures. For lower temperatures, the H_2O lines with wavelengths larger than 7 μm are very important; neglecting them changes the Rosseland mean by more than two orders of magnitude. The importance of water as an opacity source can be seen clearly by comparing the curves with the one obtained by neglecting water.

5. CONCLUSIONS

In this *Letter* we have reported our initial results for model atmospheres of cool M dwarfs calculated using a new list of water vapor lines. Our opacity sampling treatment of the water lines is sufficiently fast to calculate larger model atmosphere grids and can also be used to compute tables of Rosseland and Planck averages of the extinction and absorption coefficients. The new atmopheres lead to synthetic spectra that give a significantly better fit to infrared observations of VB 10 when compared to previous results obtained using the Ludwig (1971) water opacities. We demonstrated the huge effect of the new H_2O line list on the Rosseland mean opacity for lower temperatures. The differences between the Ludwig opacity and the new water opacities are very large, and, therefore, a full line-by-line treatment of water vapor in the computation of model atmospheres and Rosseland mean opacities is of great importance. The spectral region around 1.6 μm is still not very well reproduced by the synthetic spectra; this is probably at least partly caused by the incompleteness of H_2O lines in this regions or by the lack of sufficient data for other important opacity sources. It will be very interesting for the modeling of cool stars and for molecular physics to identify the source of these discrepancies. In future work we will compute and present a larger grid of model atmospheres and synthetic spectra for cool dwarfs and giants computed using the method described here.

We would like to give special thanks to Hugh Jones and John Fernley for first bringing together all the players in this project, and to Robert Kurucz for his valuable comments as referee. We also want to thank E. Baron, J. M. Matthews, and S. Starrfield for stimulating discussions. This work was supported in part by grants to G. Fontaine and F. Wesemael from FCAR (Québec) and G. F. Fahlman and H. B. Richer from NSERC (Canada); as well as a NASA LTSAA grant to Arizona State University and grants from SERC (UK).

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