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MOLECULAR OPACITY AND STELLAR STRUCTURE

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RESUMEN. Se han construído modelos para estrellas de baja masa de la Secuencia Principal con nuevas opacidades moleculares. Se encuentra que, a pesar de las diferencias entre las nuevas y las viejas opacidades moleculares, los modelos virtualmente no cambian. Estas circunstancias permiten estimar con mayor facilidad la importancia de otros factores físicos en los modelos, tales como la ecuación de estado y la generación de energía.

ABSTRACT. Models of low-mass stars on the Main Sequence have been constructed with the help of new molecular opacities. It is found that, in spite of the differences between the new and old molecular opacities, the models are virtually unchanged. This circumstance permits more easily the assessment of the importance of other aspects of the physics, such as equation of state and energy generation, used in the modelling.

Key words: OPACITIES – STARS: ATMOSPHERES – STARS: LATE-TYPE

1. INTRODUCTION

Stars of masses less than that of the Sun constitute the dwarf end of the stellar population, not just in mass but also in radius and luminosity. With decreasing mass the radius falls off roughly as the mass itself, reaching a radius of 0.1 times the solar radius just below a mass of 0.1 times the solar mass. The luminosity however falls off much more rapidly, reaching 0.1 solar luminosities at about 0.6 solar masses, 0.01 solar luminosities near 0.25 solar masses and 0.001 solar luminosities at 0.1 solar masses. Over the same mass range the central density rises to about $5\text{x}10^2$ g cm^{-3}, the central temperature falls to near $4\text{x}10^6$ K and the photospheric (surface) temperature to almost $3\text{x}10^3$ K. At still lower masses the progression continues past the point where thermonuclear reactions are extinguished. As the luminosity plunges the stellar sequence enters the region of first red, and then brown, and eventually black dwarfs, which are speculated to conceal the unseen and possibly missing mass of the universe. With the decreasing surface temperatures of these stars, the spectra exhibit the increasing dominance of molecular bands, thus testifying to the necessity of including molecular physics, for example, in the equation of state and radiative energy transfer, in the modelling procedures. Other aspects of stellar physics—namely the non-ideal effects in the equation of state, the electron screening of nuclear reactions and the contribution of heat conduction to the opacity—may also have to be considered.

The extreme physical conditions in the low-mass stars, as well as their evolutionary status and possible cosmological significance has attracted the recent attention of many workers. All the usual aspects of stellar physics—equation of state, energy generation and energy transport—have been examined. Among the most recent theoretical investigations are those of VandenBerg *et al.* (1983), Neece (1984), Rappaport and Joss (1984), D'Antona and Mazzitelli (1985), Lunine *et al.* (1986), Dorman *et al.* (1989), Stringfellow (1991) and Luo (1991). A review of theoretical and observational work has been given by Liebert and Probst (1987). In the present paper we give a preliminary report on the use of the very recent molecular opacity results of Carson and Sharp (1991) in the construction of models for low-mass stars. A more detailed account will be given elsewhere.

2. MOLECULAR OPACITY

Molecular band absorption features begin to appear in the spectra of solar-type stars, and become more and more dominant towards later spectral type. For Main Sequence stars, the relationship between photospheric temperature and mass, as outlined above, necessitates the use of Rosseland mean opacities, including molecular absorption, for the modelling of low-mass stars. Among the earliest attempts to compute molecular opacities is the work of Tsuji (1971), who used an Elsasser band model to represent the spectra of 7 molecules including TiO and H_2O. The work of Alexander (1975) extended the study to 17 molecules using straight means and band averages for the absorption coefficient. Later, Alexander *et al.* (1983) adopted a sampling method at 1010 frequencies to treat the band absorption of 7 abundant molecules (except for H_2O for which straight means were used). The 1975 opacities were orders of magnitude greater than earlier estimates, probably due to the inclusion of more sources of absorption. However, the 1983 opacities were smaller by a factor of 10 at 2000 K, probably as the result of replacing straight means by sampling of the absorption coefficient. These 1975 and 1983 opacities have been used extensively in the modelling of cool stars, although Dorman *et al.* (1989) have made use of privately communicated 1986 Alexander opacities.

Very recently, Carson and Sharp (1991) have made new calculations of molecular opacities, including many more molecules and with a greatly increased resolution of the monochromatic absorption coefficient. The dissociation equilibrium, including 40 diatomic molecules (neutral and ionized) and 12 triatomic molecules, is calculated using the empirical spectroscopic constants for the evaluation of partition functions and equilibrium constants (see Carson, 1991). The Rosseland mean opacity is evaluated on a grid of over half a million frequencies, whereon each line of a band is individually profiled. For abundances similar to those used by Alexander, the opacity is considerably reduced at the lowest temperatures. The same techniques applied to zero-metal compositions also give results in good agreement with those of Lenzuni *et al.* (1991).

3. MODELS OF LOW-MASS STARS

Main Sequence models of stars with masses $0.10 \leq M/M_\odot \leq 1.00$ have been constructed (Luo, 1991) with a variety of input physics, including the molecular opacities of Alexander *et al.* (1983) and those of Carson and Sharp (1991). The equation of state and atomic (or high temperature) opacities, to which the molecular opacities were spliced for continuity, were derived from a code based on an average atom treatment of electron occupation using a grand canonical ensemble method for all the elements other than H and He, for which conventional ionization equilibrium was used. Radiative absorption data for H and He were also used, while those for the heavier elements were calculated from hydrogenic formulae (Carson, 1988a,b) using screening constants and effective nuclear charges. After this work had been completed the new opacities of Iglesias and Rogers (1991) appeared and comparisons showed remarkable agreement between both the opacities and the stellar models constructed with them. The electron screening of nuclear reactions, after the work of Ichimuru *et al.* (1984), and conductive opacities of Hubbard and Lampe (1969) were also employed. Other factors which influence stellar modelling are the composition of the stellar material, the convective mixing length/pressure scale height ratio and the photospheric boundary condition. The stellar structure/evolution code by one of us (TRC) is an implementation of the algorithm of Kippenhahn, Weigert and Hofmeister (1967) with facilities permitting the exercise of a choice of several alternatives.

Table 1 and Table 2 give the properties of the zero-age Main Sequence models for Population I ($X = 0.700, Y = 0.280, Z = 0.020$) and Population II ($X = 0.710, Y = 0.289, Z = 0.001$) respectively, using the Carson and Sharp molecular opacities. All quantities are in c.g.s units unless otherwise indicated. Apart from the change of composition from Population I to Population II, the input physics, including the mixing length parameter $\alpha = 1.5$, is kept constant for all the models. It will be observed that, for the same mass, the Population II model is consistently more luminous and of higher effective temperature than the Population I model, with convergence towards lower mass, but that the radius is virtually the same in the two cases. However, on the theoretical Hertzsprung-Russell diagram the Population I models define a sequence which is parallel but *above* and to the *right* of the Population II sequence. All the models have extensive envelope convection zones, and indeed are convective throughout for $M/M_\odot \leq 0.3$. Comparison with the empirical data of Popper (1980) the Population I sequence gives a good overall fit. In view of the rather large uncertainties in the empirical masses, the

Table 1: Zero-age Main Sequence Models for Population I Composition (Carson and Sharp Molecular Opacities)

$M/M_\odot$	$\log(L/L_\odot)$	$\log(R/R_\odot)$	$\log(T_e)$	$\log(T_c)$	$\log(\rho_c)$	$\log(P_c)$
1.00	-0.143	-0.032	3.743	7.121	1.920	17.173
0.80	-0.629	-0.131	3.672	7.041	1.888	17.064
0.60	-1.227	-0.234	3.574	6.949	1.852	16.937
0.50	-1.501	-0.329	3.553	6.909	1.838	16.885
0.40	-1.728	-0.421	3.542	6.880	1.833	16.853
0.30	-1.942	-0.511	3.533	6.846	1.942	16.932
0.25	-2.077	-0.568	3.528	6.818	2.036	17.006
0.20	-2.249	-0.641	3.521	6.781	2.156	17.105
0.15	-2.495	-0.744	3.511	6.727	2.338	17.262
0.12	-2.721	-0.830	3.498	6.676	2.507	17.417
0.10	-3.022	-0.910	3.462	6.611	2.656	17.572

Table 2: Zero-age Main Sequence Models for Population II Composition (Carson and Sharp Molecular Opacities)

$M/M_\odot$	$\log(L/L_\odot)$	$\log(R/R_\odot)$	$\log(T_e)$	$\log(T_c)$	$\log(\rho_c)$	$\log(P_c)$
1.00	0.203	-0.051	3.840	7.176	2.009	17.324
0.80	-0.252	-0.138	3.769	7.099	1.986	17.226
0.60	-0.850	-0.270	3.686	7.004	1.956	17.102
0.50	-1.223	-0.333	3.624	6.946	1.938	17.030
0.40	-1.565	-0.434	3.589	6.896	1.924	16.968
0.30	-1.810	-0.530	3.575	6.857	2.000	17.010
0.20	-2.141	-0.658	3.555	6.786	2.208	17.175
0.15	-2.401	-0.761	3.542	6.729	2.393	17.334
0.10	-3.000	-0.950	3.489	6.592	2.776	17.735

most critical confrontation of theory and observation is via the theoretical Hertzsprung-Russell diagram. There remains however a systematic trend in that at a given mass the models for $\alpha = 1.5$ are cooler for $M/M_\odot > 0.5$ and hotter for $M/M_\odot < 0.5$ compared with observations. The latter conclusion is fortified when comparison is made with the empirical data of Liebert and Probst (1987) which, ignoring those data which do not lie on a well-defined sequence, is better represented by models for $\alpha = 0.5$ or even smaller. It should be noted however that, for a given mass, changes of α change the temperature and radius of the model while leaving the luminosity unchanged. Thus our models suggest that the mixing length parameter α is not constant but a function of mass, with smaller mass favouring a smaller value of α. It is quite feasible that a physical argument can be found for such a variation of α which is not otherwise determined by the mixing-length theory of convection.

In Table 3 we give, in the same format as earlier, the properties of the Population I models, for the same physics input as before but using the Alexander *et al.* molecular opacities instead of those of Carson and Sharp. Perhaps unexpectedly the two Population I sequences are found to be almost identical, with properties varying only in the third-decimal place of the logarithm. The explanation is probably to be found in the fact that in the upper part of the mass range the molecular opacities are not making a significant contribution to the stellar model structure, while in the cooler lower part of the mass range the models are either largely or completely convective. It should however be noted that greater difficulty was encountered in obtaining converged models at the lowest masses when the larger Alexander *et al.* molecular opacities were used.

Table 3: Zero-age Main Sequence Models for Population I Composition (Alexander *et al.* Molecular Opacities)

$M/M_\odot$	$\log(L/L_\odot)$	$\log(R/R_\odot)$	$\log(T_e)$	$\log(T_c)$	$\log(\rho_c)$	$\log(P_c)$
1.00	-0.143	-0.032	3.743	7.121	1.920	17.173
0.80	-0.629	-0.131	3.672	7.041	1.888	17.064
0.60	-1.228	-0.233	3.573	6.949	1.851	16.937
0.50	-1.504	-0.328	3.551	6.908	1.837	16.884
0.40	-1.731	-0.420	3.541	6.880	1.833	16.852
0.30	-1.945	-0.509	3.530	6.845	1.938	16.928
0.20	-2.251	-0.641	3.521	6.781	2.156	17.104
0.15	-2.495	-0.743	3.511	6.727	2.338	17.262

The above results would indicate that the models of low-mass stars are not very sensitive to the particular molecular opacities employed, at least for the range of masses explored here, and might suggest that other factors may be more important in any further attempts to fine-tune models to the observational data. Thus, secure in the expectation that the opacities are not *per se* introducing unknown variations, as a result of variations in composition, or in the absorption data used, or in the methods of computation of the opacities, we turn to examine briefly other aspects of the input physics. We have used two different forms of the outer photospheric boundary condition without any appreciable change in the properties of the models. The use of an alternative composition to the Population I and Population II compositions detailed above induces changes in the models, but mainly for $M/M_\odot > 0.5$. It is therefore conceivable that an intermediate composition coupled with a lower value of α would have the combined effect of improving the global fit of the models to all the empirical data. We have also repeated all the Population I models for $\alpha = 1.5$ and using Carson and Sharp molecular opacities, excluding in turn the electron screening of nuclear reactions and the conductive opacity contribution. This exercise showed that the inclusion of electron screening of nuclear reactions increases the luminosity by less than 1% for $M/M_\odot = 1.0$ increasing to less than 10% for $M/M_\odot = 0.1$, with an attendant increase in the effective temperature everywhere less than 0.5%. On the other hand the inclusion of conductive opacity increased the luminosity by from 0.2% to 3.0% over the same mass range, while the change of effective temperature was everywhere less than 0.2%. None of these effects however makes any appreciable difference to the Main Sequence in the Hertzsprung-Russell diagram, or to the curves representing the mass–luminosity and mass–effective-temperature relations. There remains for investigation the equation of state as an aspect of the physics entering the construction of stellar models. Here our indications are that the treatment of the equation of state, particularly the handling of non-ideal effects such as pressure ionization, has more important consequences for stellar models than the other aspects of the physics. To see this it is sufficient to point to the variations between the results of earlier workers, whose models have been founded upon different equations of state rather than other aspects of physics. For example, the several main sequences collated by Dorman *et al.* (1989) differ markedly from one another and from the empirical main sequence.

4. DISCUSSION

Our primary objective has been the testing of the new Carson and Sharp molecular opacities in modelling low mass stars in the range $0.1 \leq M/M_\odot \leq 1.0$. It was found that the results are not appreciably different from those obtained using the molecular opacities of Alexander *et al.* However it would be premature to conclude the irrelevance of the method of calculation or accuracy of molecular opacities on the basis of grey radiative transfer under conditions of local thermodynamic equilibrium. Nevertheless the insensitivity of the models to the molecular opacities used helps to, at least temporarily, remove from consideration one aspect of the input physics in order to assess better the role played by uncertainties in other areas of physics. It is expected that the equation of state is still the source of considerable uncertainty. This together with the electron screening of nuclear reactions seem to be important factors in the modelling of the low-mass stars. Both these factors can only become more significant as we enter the regime of masses where $M/M_{\odot} < 0.1$ which we do not discuss here. It should also be borne in mind that evolutionary effects must also enter into the interpretation of observational data and its confrontation with the predictions of theoretical models.

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