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Treatment of Atomic and Molecular Line Blanketing by Opacity Sampling*

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ABSTRACT

An opacity sampling (OS) technique for treating the radiative opacity of large numbers of atomic and molecular lines in cool stellar atmospheres is subjected to several tests. In accord with previous results, we find that the structure of atmospheric models is accurately fixed by the use of 1000 frequency points, and 500 frequency points is often adequate. The effects of atomic and molecular lines are separately studied. A test model computed using the OS method agrees very well with a model having identical atmospheric parameters computed with the giant line (opacity distribution function) method.

I. INTRODUCTION

An opacity sampling (OS) technique appears promising for treating the opacity of large numbers of overlapping molecular and atomic lines in the spectrum of cool stars. In the OS method for model atmospheres, no approximation whatever is made in the calculation of the atomic and molecular opacity at a selected frequency. The resulting flux ($F(\nu, \text{depth})$) consequently contains no errors due to opacity smearing. In a computation of a model atmosphere, then, the only approximation in computing the opacity is in the choice of a particular finite set of frequency points. (The atmosphere would still be subject to such other approximations as plane parallel geometry and LTE, of course.)

The method itself has been derived independently and applied to the treatment of atomic lines in the Sun (Peytremann 1974) and to molecular lines in the atmosphere of a carbon star model (Johnson and Sneden, 1974; Sneden, Johnson, and Krupp, 1975 hereafter referred to as Paper I). These earlier papers have discussed the advantages and disadvantages of the OS method compared to other line blanketing methods.

In the present paper we apply new, stringent tests to the self-consistency of the method and determine the sensitivity of the resulting model atmospheric structure to the number of frequency points used. We then extend the treatment to include the combined effects of atomic and molecular line blanketing. We apply the method to the calculation of model atmospheres for a K giant star and compare our results to those obtained using either straight mean opacities or opacity distribution functions (ODF).

II. TECHNIQUES AND DATA

Since the basic philosophy and a quantitative description of the method of opacity sampling has already been given in the literature (Peytremann 1974; Paper I), we give here only a brief summary of the method. The method itself is the essence of simplicity. At a selected set of frequencies (ν) and optical depths (τ) or mass points (m) one calculates the correct linear or mass absorption coefficient by adding together all the contributions of all the atomic and molecular lines as well as the continuous sources which contribute at that wavelength. The number of such lines may range from a few to a few hundred at each frequency. Such a method obviously requires an enormous data bank, but these are now becoming available. Once one has an accurate value for the absorption coefficient $\kappa(\nu,m)$ one can calculate every monochromatic quantity $Q(\nu,m)$ needed to produce the model atmosphere. Monochromatic fluxes computed by this method should be perfectly accurate, within the usual framework of plane-parallel geometry and LTE. Energy fluxes integrated over the entire spectrum should be exact, the only approximation being in the number of frequency points. Calculations have already indicated that for either atoms or molecules the number of frequency points needed is between 500 and 1000 (Peytremann 1974; Paper I). We investigate this question further in the present paper.

To compute model atmospheres we use a version of the computer code ATLAS5 (Kurucz 1970), which we have modified to include monochromatic molecular and atomic line absorption. The code is based on hydrostatic equilibrium and constancy of total energy flux (radiative plus convective) in a plane-parallel atmosphere. We make the usual assumption that the energy level populations of both atoms and molecules are distributed according to LTE and assume that all lines are formed in pure absorption.

The line data was assembled from several sources. As part of a long term project, we have previously assembled at Indiana University several data tapes containing information on over one million lines of C_2 (Swan, Phillips, and Ballik-Ramsey systems), CN (red and violet systems), CO (infrared), and CH (G-band system). The wavelengths and line strength factors for these lines were obtained from computer programs written by T. D. Fay and based on the formalism of Kovacs (1969), using the best available f-values and constants in the literature. Roger Bell kindly provided us with a data tape containing empirical information on approximately 35,000 atomic lines as well as several thousand lines of MgH, NH, and OH. Finally, in the intervals $\lambda < 3000\text{Å}$ and $\lambda > 6500\text{Å}$ we include Fe I and Fe II lines from a semiempirical data tape provided by Robert Kurucz (1974).

For both the tests of internal consistency and comparisons with other line blanketing methods, only the Doppler core of the line absorption coefficient is considered. The addition of natural and collisional damping to the line blanketing has negligible effect in the models used here. The Ca II H and K lines are not included in these calculations because their great strength would necessitate special treatment, and, for these cool stars, only a small fraction of the energy flux is contained in the spectral interval $\lambda \leq 4000\text{Å}$.

To prepare the line data for use in the model atmosphere program we first select a set of frequencies at which the radiation field is to be calculated. For each of these frequencies, we abstract from the atomic and molecular tapes all those lines which fall within a given interval around the selected frequency. We commonly use the interval $\Delta\nu = \pm 1\text{cm}^{-1}$ for molecular lines and twice that value for atomic lines. All lines are then sorted by wavenumber and stored on a tape ready for use in the model atmosphere program.

The various test models were normally converged until a relative flux constancy to within 0.0005 was achieved; at this point the indicated temperature corrections were usually smaller than 2°K. For a model started from an ordinary guess, approximately 20 iterations were required to restore flux constancy, requiring 1 hour on a CDC 6600 if 1000 frequency points were used. Faster convergence can be achieved by occasional "hand" smoothing of the intermediate model atmospheres, as well as by choosing a better "guess" as to the final model.

III. RESULTS AND DISCUSSION

A. Internal Consistency

For the same set of physical conditions we compute models with differing numbers of frequency points and spacings in order to determine the number of frequencies are required to compute accurate model atmospheres self-consistent in such a way that: 1) a further increase in the number of frequencies does not appreciably change the resulting atmospheric structure, and 2) for that critical number of frequencies, the atmospheric structure is relatively insensitive to the specific frequency points chosen.

Our standard model has the following characteristi T_{eff} = 4000 K; surface gravity = 100 cm/sec^2; v(microturbulence) = 1 km/sec (used only in the line absorption coefficient, not the pressure); solar abundances (Lambert 1968); continuous opacity sources as in ATLAS 5; and line opacities treated by the OS method. This model will be referred to as (4000/2.0/S/HOP,OS).

For purposes of illustration a standard model atmosphere using 1010 frequency points has been adopted (which we, for our convenience, will always call a 1000-frequency set). This number is suggested by previous studies in which 500-1000 frequencies (Paper I) or 600 (Peytremann, 1974) frequencies were found

adequate to specify accurately the structure of a model atmosphere. The 1000 frequency set is equally spaced by 25cm^{-1} from 500 to 25,000 cm^{-1} (20$_\mu$ to 4,000Å); an equal spacing of 250 cm^{-1} is used in the ultraviolet down to a wavelength of 2700Å. A coarser grid of points is employed in the region $2700 < \lambda \leq 4{,}000$Å because this portion of the spectrum transmits only a small portion of the total flux in our models, and the flux shortward of 2700Å is totally negligible for photospheric models at these low temperatures.

To test the effects of the frequency set on the model atmosphere, the following grid of standard models has been calculated: three models with different sets of 100 frequencies, three models with different sets of 500 frequencies, two models with different sets of 1000 frequencies, and one model with a set of 2000 frequencies.

The three 100-frequency sets (R101A, F101B, R101C) are semi-random in their spacing, obtained from a 1000 point set similar to the one described above. That is, one point in every ten is chosen from the larger set with the help of a random number table. This procedure guarantees an appropriate dispersion of points across the entire spectrum, yet each frequency set so generated is completely independent of the others.

Two of the 500-frequency sets (500A, 500B) are spaced equally by 50cm^{-1} below 25,000 cm^{-1}, and above by 500 cm^{-1}. The two sets are shifted with respect to each other by 25cm^{-1}. The third (R500) is made up of random frequencies; to insure coverage of the entire spectrum, however, one point is randomly selected from each interval of 100cm^{-1} for wavenumbers below 25,000cm^{-1} (4,000A) and in each interval of 1000 cm^{-1} for wavenumbers above 25,000 cm^{-1}. All three sets are equally unbiased with respect to the positions of observed spectral lines.

One of the 1000 frequency sets is the standard set described above: the second has a frequencies randomly selected within 50cm^{-1} bins (500cm^{-1} bins for wavenumbers above 25,000 cm^{-1}) across the spectrum.

The results of these model atmosphere calculations are shown in Figures 1 and 2, in which are plotted the temperature versus the mass parameter RHOX = $\int \rho dx$, which represents the mass in a unit column (g cm^{-2}) above that point. Since total pressure = surface gravity x RHOX, these graphs are T-P relations at the same time. Figure 1 shows the three 100-frequency point models plotted together with the 1000-point standard model, represented by a solid line. Vertical bars indicate a few selected values of log τ_R (where $\tau_R \equiv$ Rosseland optical depth). At RHOX = 1 there is a spread of 250°K among the various models, showing that the upper atmosphere is not well represented by a 100-point frequency set. The spread is even greater at smaller values of RHOX, with a maximum deviation of about 350°K. However, the photospheric temperature-pressure structure (in the region $0.01 \leq \tau_R \leq 5$, where the continuum is formed) is matched quite well.

Figure 2 is a similar diagram involving the three 500 frequency point models. At RHOX = 1 there is a spread of approximately 100°K among the various models, a value substantially smaller than in the previous case. A temperature difference of this order would be marginally detectable by observations. Once again, the photospheric structure is matched quite well.

The thermal structures of the two 1000-frequency models are generally identical to within a few degrees, with a few differences as large as 30°K. The differences are smaller than the computational and observational noise. The model computed with 2000 frequency points (with equal spacing of 12.5 cm^{-1} below 25000 cm^{-1}, and 125 cm^{-1} above) is nearly identical with the equally-spaced 1000-frequency model. These comparisons are not illustrated since the models are indistinguishable if drawn on the same scale as Figure 1 and 2.

Figures 1 and 2 and the results of the previous paragraph strongly suggest the self-consistency of the OS treatment. Imagine the envelope of all models computed with different sets of N frequencies. As the number of frequency points N is increased, the resulting envelope of model atmospheres narrows nicely, until (near N = 1000 points) it defines a unique model structure. In addition, the envelopes determined for successively greater numbers of frequencies fall within those

specified by the coarser grids. Altogether these tests provide persuasive evidence of the convergence of the OS method in both of the ways outlined at the beginning of this section.

It appears that 1000 frequencies are sufficient to fix the structure of a model atmosphere within 30°K. This uncertainty is very acceptable, even for fine analysis abundance determinations or synthetic spectra. In fact, the 500-frequency models are sufficiently precise for most purposes. This conclusion on the critical number of frequency points agrees well with that of Peytremann (1974). The only important consideration in the selection of the frequency points is that they be distributed over the entire spectrum.

B. Comparison of Atomic and Molecular Line Blanketing

The separate influence of atomic and molecular lines on atmospheric structure is illustrated in Figure 2, which compares standard atmospheres (4000/2.0/S/HOP,OS) computed with different amounts of blanketing. The curves correspond to: (1) continuum opacity only, (2) continuum plus atomic line opacity, or (3) continuum plus atomic line plus molecular line opacity. The effect of the atomic lines is as expected: the surface layers are cooled (to 2400°K) in the blanketed model compared to the unblanketed model (which has 3250°K), and the deepest layers are warmed slightly. The additional blanketing of the molecular lines further cools the outer layers (to 2040°K and raises the temperature of the deepest layers slightly more. For the standard model, most of the effect from the molecules is due to CO. The strong surface cooling effect and slight backwarming for CO has already been demonstrated through the use of straight mean opacities (Johnson 1973), and is confirmed in a more precise way here.

C. OS and Straight Mean Opacities

Figure 3 also shows a curve for an atmosphere computed with straight mean opacities taken over intervals of 100 cm^{-1}. Straight mean opacities, which are simply the average of the opacity across a chosen spectral interval, have the great advantage of simplicity and have been used by a number of investigators (for references, see Paper I). The particular model shown in Figure 3 includes a fraction of the MK atomic line blanketing (Mutschlecner and Keller 1972) and straight mean opacities of H_2O, CO, and CN. While some of the differences between the straight mean and the OS models may be due to slightly different atomic and molecular data, most of the differences must be due to the more accurate treatment of the line opacities in the OS models. The principal error in the stright mean opacity arises from the smearing of the opacity and the consequent filling of the opacity windows, through which more flux would otherwise flow. The straight mean therefore tends to overblanket a model, resulting in higher temperatures in the upper atmosphere and perhaps throughout the model (Carbon 1974).

We caution, however, against uncritical inferences about the straight mean method from this comparison. Like other such comparisons in the literature, we have here compared a stright mean model calculated with only 100 frequency points with an OS model computed with 1000. Clearly, the accuracy of the straight mean must depend on the size of the frequency interval over which the opacities are averaged. To our knowledge, the effect of the interval size on the resultant model has never been carefully investigated, though some appreciation for the effect for the CN red system can be gained from the figures in Johnson, Marenin, and Price (1972). In the limit of an infinitesimally small spectral interval, the straight mean must be exact of course. The crucial question can then be stated as follows: What is the critical size of the spectral interval over which

the straight mean is taken in order that the resultant model approach the "correct" model within an arbitrary accuracy? This would appear to be an interesting area for further investigation. The question has recently been touched upon by Van Paradijs and Vardya (1975), who claim that even the opacity distribution function is a certain kind of straight mean. Perhaps it is more meaningful to think of the straight mean opacity as a one-picket ODF. A closer examination of the relationship betwen the straight mean, the ODF, and the OS method would appear fruitful.

D. Comparison of the OS and ODF Model

A crucial test of the ODS method would be the comparison of a model using the OS with one computed using the accurate opacity distribution function (ODF). This has not generally been possible in the past because different investigators have used different sets of lines, differing dissociation energies, oscillator strengths, and compositions; however, close agreement between the two methods has been achieved in a particular solar model (Peytremann 1974). Now Bell, et. al. (1975) have computed models using their giant line method of line blanketing which is an ODF method described in detail by Gustafsson, et. al. (1975). Using the precise data employed by these authors in computing their ODF models, we make such a comparison for a model (Bell 1974) with the parameters (4000/2.25/S). The results of this test are shown in Figure 4. As is apparent, the models produced by the two methods are in excellent agreement. This accord is heartening on all counts since it verifies the validity both of the opacity sampling method and the giant line method. The slight differences which arise in the very outer layers of the atmosphere are not to be regarded as serious. In the outermost atmospheric layers, the giant line method fails because the strongest lines are artificially truncated by the highest picket in the ODF, and the temperature plateau reached is slightly too hot.

The OS method on the other hand, fails in the very outer layers because the energy balance there is controlled by a very few strong lines and the statistics connected with these very few lines are poor. This is of no importance, however, because other more serious neglects (departures from LTE and radiative equilibrium) would likely make the results there inapplicable to real stars anyway. The excellent agreement of both methods throughout the remainder of the stars provides substantial evidence that we have found the "correct" model.

E. Effect of Line Wings on Models

The above tests were performed with the assumption of the Doppler absorption profile only for both atomic and molecular lines. When wings are added to the atomic lines as described by the usual Voigt function, the atmosphere is very slightly warmed in the outer layers from $\leq 10°K$ for $\tau(R) \geq 10^{-4}$ to as much as 100°K at $\tau(\text{Rosseland}) = 10^{-6}$ (where the atmosphere is very uncertain, however). Deep backwarming is negligible. In these calculations the total damping constant $\Gamma = \Gamma(\text{radiation}) + \Gamma(\text{Van der Waals})$. For simplicity we assume Γ (radiation)$= 3\gamma$ (classical), although the models are rather insensitive to the precise value used. With $\Gamma(\text{radiation}) = 1.5\ \gamma$ (classical) the thermal structure is changed by less than 2°K anywhere.

IV. CONCLUSIONS

We have subjected an opacity sampling (OS) technique for calculating the opacities of large numbers of atomic and molecular lines to a number of tests, with very promising results for the method. Our conclusions follow.

(1) For a giant star of solar composition and effective temperature of 4000°K, we find that 1000 frequency points, spaced either randomly or uniformly, produce atmospheric models which are identical within 30°K at the worst point in the atmosphere. Changing the location of the frequency points or adding

additional frequency points beyond this critical number produces no further changes in the atmosphere. In that sense it is "converged". A set of 500 frequency points, picked randomly or equally spaced, produces an atmosphere which agrees with the above standard atmosphere within 30°K except in the extreme outer atmosphere, where the agreement is within 100°K at the worst point. Atmospheric models computed with as few as 100 frequency points spread randomly across the entire spectrum agrees quite well (within 50°K) with the standard model throughout most of the photosphere but are rather badly in error in the outer layers where the τ(Rosseland) is less than 0.001.

(2) For a particular model with the parameters (4000/2.0/S) we find that the addition of atomic lines in the OS technique cools the boundary temperature from about 3250°K to 2400°K and warms the deeper layers of the photosphere slightly. The addition of molecular lines of CO, CN, CH, and C_2 (of which CO is the only significant absorber for this model) cools the boundary to a temperature of 2040°K and warms the deep photosphere even more.

(3) In a precise comparison of atmospheric models produced with the opacity sampling (OS) method and the opacity distribution function (ODF) method for the parameters (4000/2.25/S), we find the temperature-pressure to be identical to within 30°K at the worst point in the atmosphere. This test provides persuasive evidence that both of these methods produce a "correct" atmosphere.

(4) For models of giant stars, the line wings add no significant opacity to the atmosphere, except a slight warming in the outermost atmospheric layers.

(5) The results of this paper strongly support the results of a previous paper (Paper I) regarding the advantages of the OS method.

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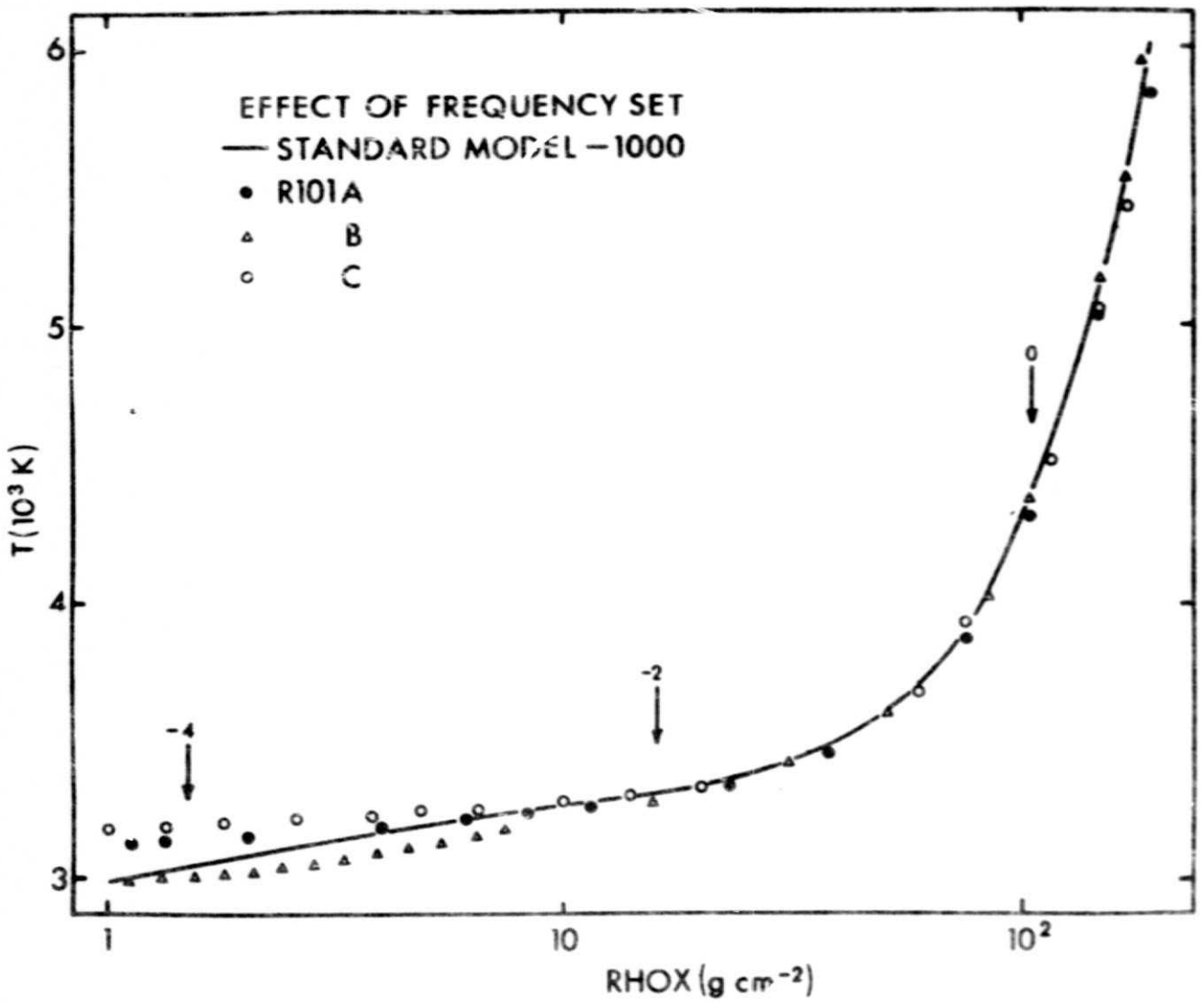
Captions for Figures

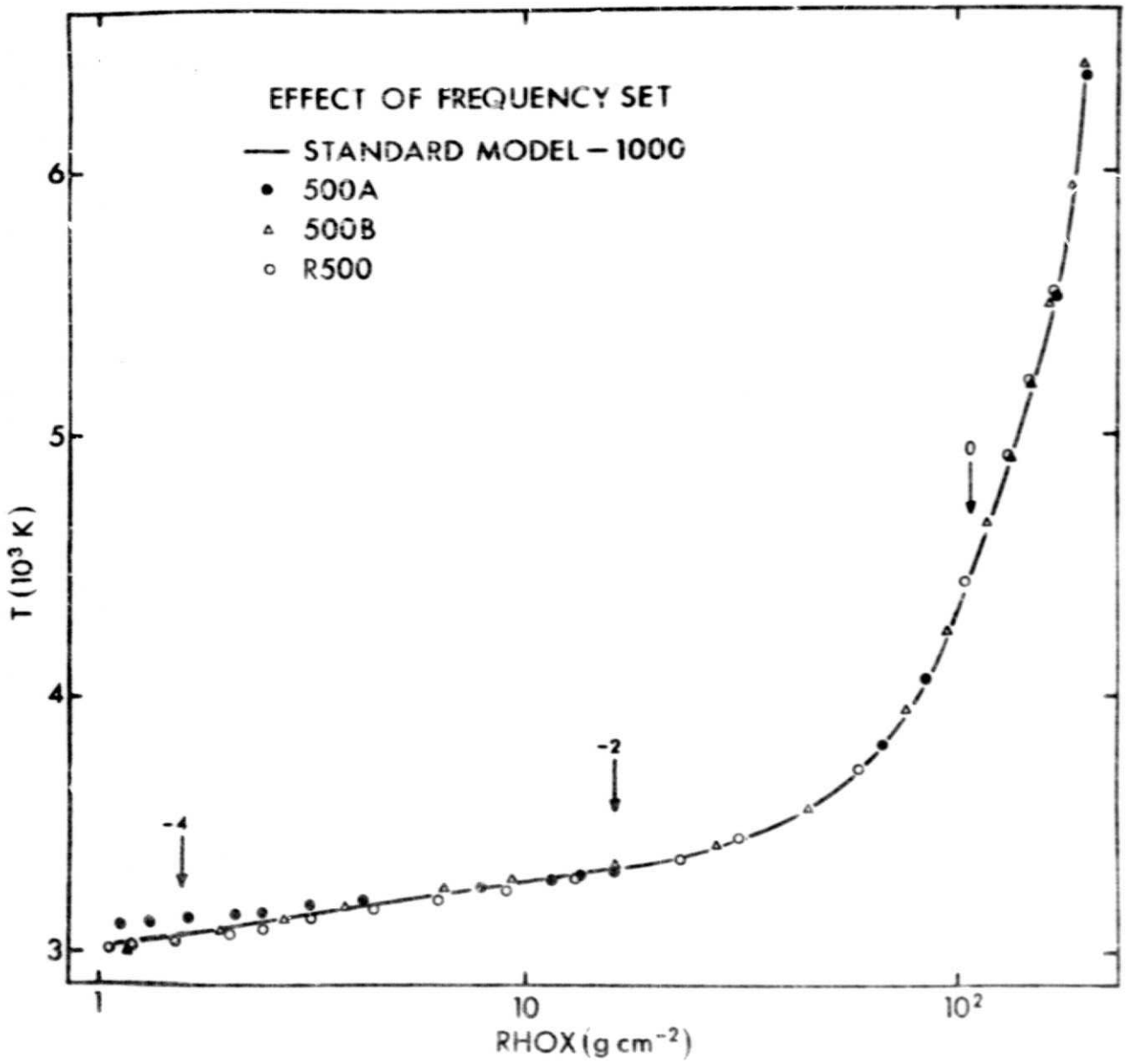
Figure 1: Temperature-pressure structure of a standard atmosphere (as in Fig. 1) converged with different sets of 100 frequencies and one set of 1000 frequencies (solid line).

Figure 2: Temperature - pressure structure of a standard atmosphere (4000/2.0/S) converged with different sets of 500 frequencies and one set of 1000 frequencies (solid line).

Figure 3: Effect of atomic lines and of both atomic and molecular lines compared to continuous opacities alone on the structure of a standard model (as in Fig. 1). A model with straight mean opacities is also given for comparison.

Figure 4: Comparison of models (4000/2.25/S) computed by the giant line (ODF) method and by the opacity sampling (OS) method for essentially the same set of atomic and molecular parameters.


EFFECT OF FREQUENCY SET
— STANDARD MODEL – 1000
• R101A
△ B
○ C
6
5
4
3
T(10³ K)
-4
-2
0
1
10
10²
RHOX (g cm⁻²)


EFFECT OF FREQUENCY SET
STANDARD MODEL – 1000
500A
500B
R500
T (10^3 K)
RHOX (g cm^{-2})
6
5
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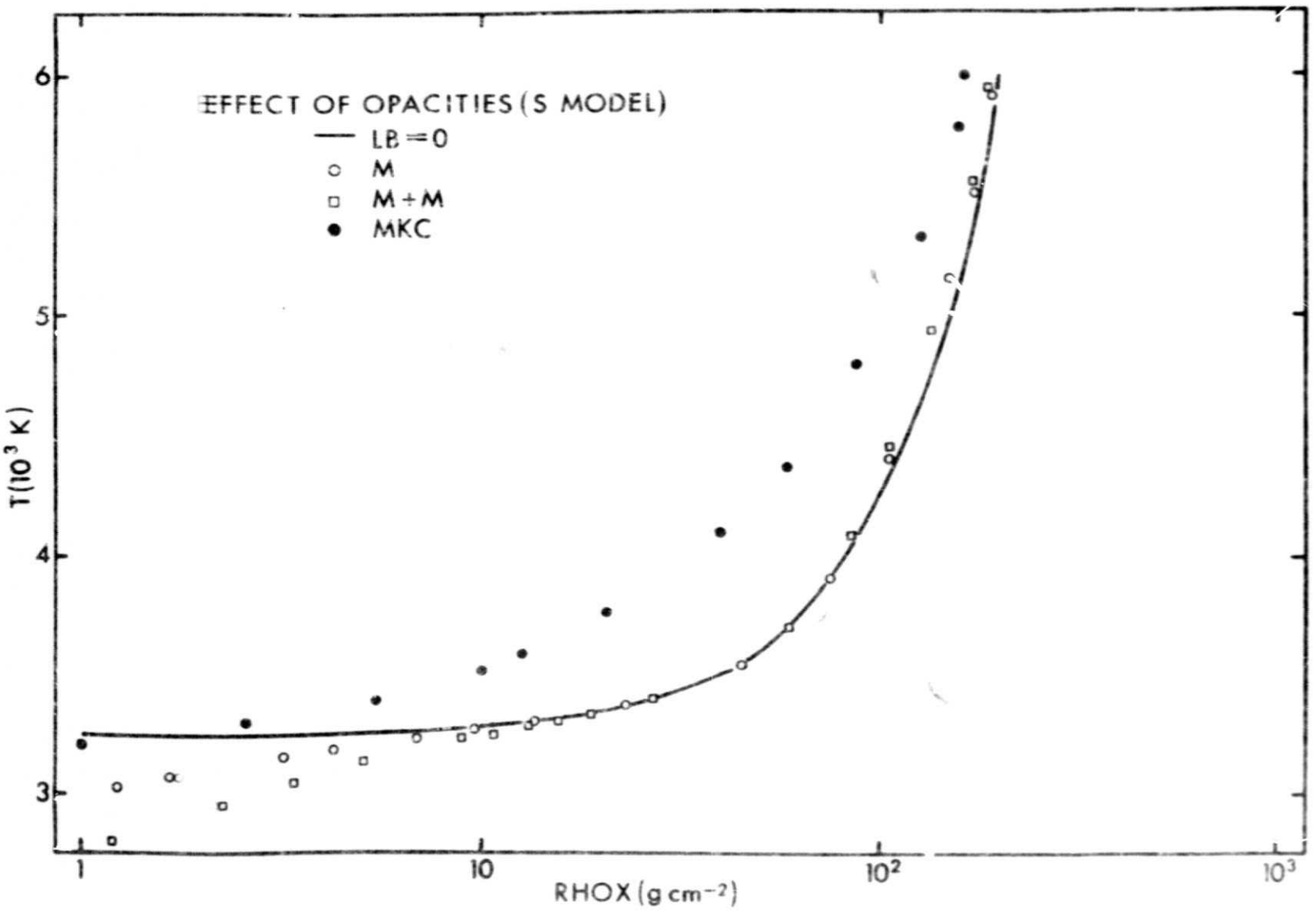
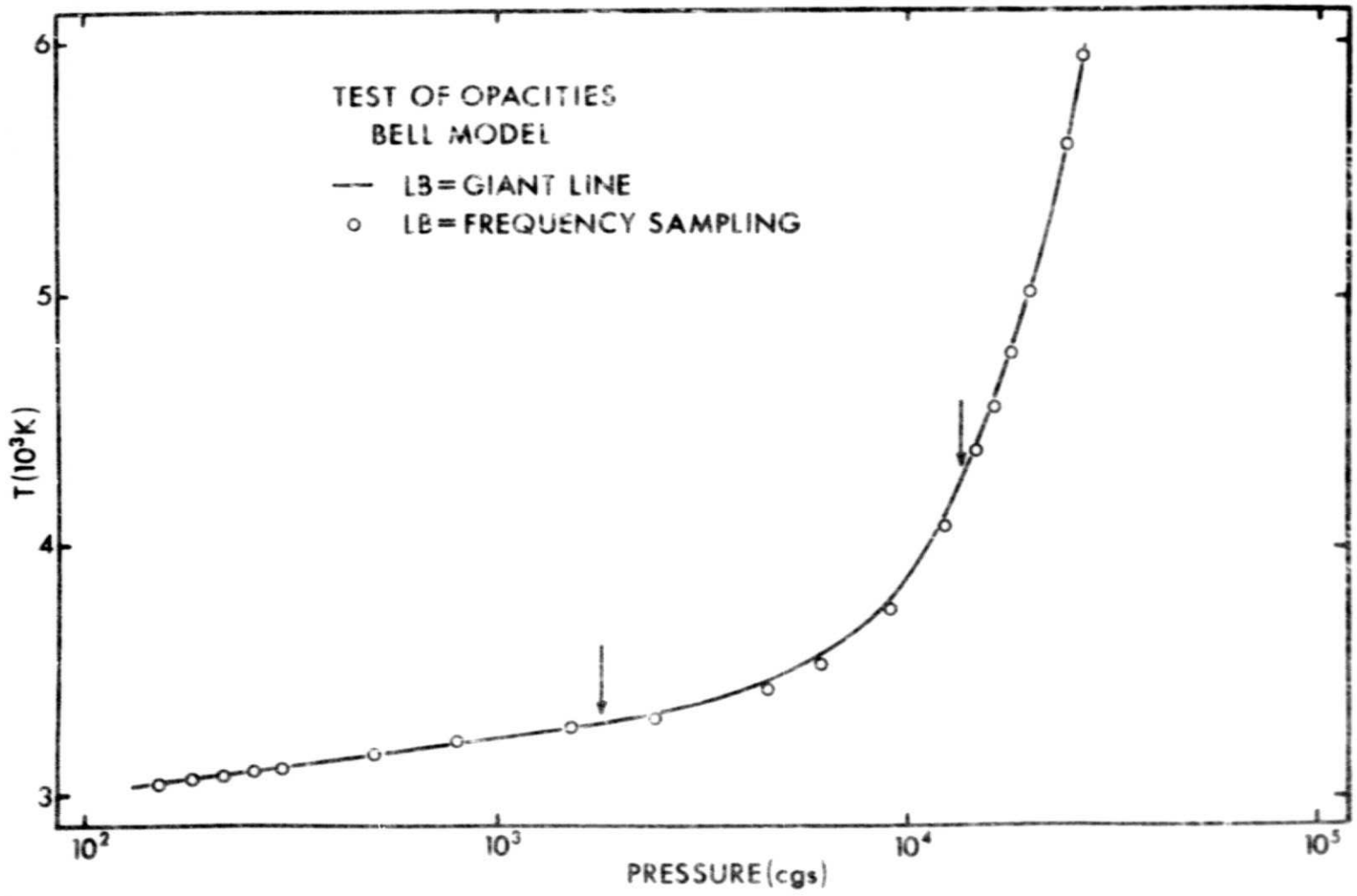
1
10
10^2
-4
-2
0


EFFECT OF OPACITIES (S MODEL)
LB = 0
M
M + M
MKC
T(10³ K)
6
5
4
3
1
10
10²
10³
RHOX (g cm⁻²)


TEST OF OPACITIES
BELL MODEL
— LB = GIANT LINE
o LB = FREQUENCY SAMPLING
T(10³K)
6
5
4
3
10²
10³
10⁴
10⁵
PRESSURE (cgs)