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A NEW OPACITY-SAMPLING MODEL ATMOSPHERE PROGRAM FOR ARBITRARY ABUNDANCES

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ABSTRACT I have developed a new version of my model atmosphere program called ATLAS12. It recognizes more than 1000 species, each in up to 10 isotopic forms, including all ions of the elements up through Zn and the first 5 ions of heavier elements up through Es. The elemental abundances are treated as variable with depth. ATLAS12 has 6 input files of line data containing 58,000,000 atomic and molecular lines. For each line the wavelength, identification, lower energy level, gf, radiative, Stark, and van der Waals damping constants are packed into 16 bytes. At each wavelength point in a frequency integration the profiles of all the significant nearby lines are computed and summed. The program and line files will be distributed in the fall of 1992.

There are no significant differences at A0 between an opacity-sampled model computed with ATLAS12 and opacity-distribution-function model computed with ATLAS9. ATLAS12 allows arbitrary abundances but is slower. The new program can be used to produce improved models for Am and Ap stars that include the effects of millions of lines.

LINE LISTS AND OPACITIES

I reported on my line and opacity calculations at a NATO workshop here in Trieste two years ago (Kurucz 1991). The details of my line lists and the opacities can be found in that paper so I will give only a brief outline.

My earlier model calculations used the distribution-function line opacity computed by Kurucz (1979ab) from the line data of Kurucz and Peytremann (1975). We had computed gf values for 1.7 million atomic lines for sequences up through nickel using scaled-Thomas-Fermi-Dirac wavefunctions and eigenvectors determined from least squares Slater parameter fits to the observed energy levels. That line list has provided the basic data and has since been combined with a list of additional lines, corrections, and deletions with the help of Barbara Bell and Terry Varner at the Center for Astrophysics. The line data are being continually, but slowly, improved. We collect all published data on gf values and include them in the line list whenever they appear to be more reliable than the current data. I have also completely recomputed Fe II (Kurucz 1981).

After the Kurucz-Peytremann calculations were published, I started work on line lists for diatomic molecules beginning with H_2, CO (Kurucz 1977), and SiO (Kurucz 1980). Next, Lucio Rossi of the Istituto Astrofisica Spaziale in Frascati, John Dragon of Los Alamos, and I computed line lists for electronic transitions of CH, NH, OH, MgH, SiH, CN, C_2, and TiO. In addition to lines between known levels, these lists include lines whose wavelengths are predicted and are not good enough for detailed spectrum comparisons but are quite adequate for statistical opacities. Work is continuing on other molecules and molecular ions, and on the vibration-rotation spectra.

In 1983 I recomputed the opacities using the additional atomic and molecular data described above which totalled 17,000,000 lines. These opacities were used to produce improved empirical solar models (Avrett, Kurucz, and Loeser 1984), but were found to still not have enough lines. For example, there were several regions between 200 and 350 nm where the predicted solar intensities are several times higher than observed, say, 85% blocking instead of the 95% observed. The integrated flux error of these regions is several per cent of the total. In a flux constant theoretical model this error is balanced by a flux error in the red. The model thus predicts the wrong colors. In detailed ultraviolet spectrum calculations, half the intermediate strength and weak lines are missing. After many experiments, I determined that this discrepancy is caused by missing iron group atomic lines that go to excited configurations that have not been observed in the laboratory. Most laboratory work has been done with emission sources that cannot strongly populate these configurations. Stars, however, show these lines in absorption without difficulty. Including these additional lines produces a dramatic increase in opacity, both in the sun and in hotter stars. A stars have the same lines as the sun but more flux in the ultraviolet to block. In B stars and in O stars there are large effects from third and higher iron group ions. Envelope opacities that are used in interior and pulsation models are also strongly affected.

I was granted a large amount of computer time at the San Diego Supercomputer Center by NSF to carry out new calculations. To compute the iron group line lists I determined eigenvectors by combining least squares fits for levels that have been observed with computed Hartree-Fock integrals (scaled) for higher configurations including as many configurations as I can fit into a Cray. All configuration interactions are included. My computer programs have evolved from Cowan's (1968) programs. Transition integrals are computed with scaled-Thomas-Fermi-Dirac wavefunctions and the whole transition array is produced for each ion. The forbidden transitions can be computed as well. Radiative, Stark, and van der Waals damping constants and Lande g values are automatically produced for each line. The first nine ions of Ca through Ni produced 42,000,000 lines. I will recompute the energy levels and line lists as new analyses become available, and I will compute the heavier and lighter elements. I will make the predictions available to laboratory spectroscopists.

In late 1988 I used the line data described above to compute new solar abundance opacity tables for use in my modelling. The calculations involved 58,000,000 lines, 3,500,000 wavelength points, 56 temperatures from 2000K to 200000K, 21 log pressures from -2 to +8, and 5 microturbulent velocities 0, 1, 2, 4, 8 km/s, and took a large amount of computer time. The opacity is tabulated as 12-step distribution functions for intervals on the order of 1 to 10 nm. There are actually two sets of distribution functions, a higher resolution version with

1212 "little" intervals, and a lower resolution version with 328 "big" intervals. The "little" wavelength intervals are nominally 1 nm in the ultraviolet and 2 nm in the visible. The opacities were tested by computing a solar model as described below.

Since the beginning of 1990 I have been able to take tremendous advantage of the new Cray YMP at the San Diego Supercomputer Center. In a few months I finished more than I had expected to do in two years. I computed opacities ranging from 0.00001 solar to 10 times solar, enough to compute model atmospheres ranging from the oldest Population II stars to high abundance Am and Ap stars. The exact abundances are [+1.0], [+0.5], [+0.3], [+0.2], [+0.1], [+0.0], [-0.1], [-0.2], [-0.3], [-0.5], [-1.0], [-1.5], [-2.0], [-2.5], [-3.0], [-3.5], [-4.0], [-4.5], [-5.0], and [+0.0, no He]. The final files for each abundance require two 6250 bpi VAX backup tapes. I distribute copies of the tapes on request. I hope to produce CD-ROMs of these opacities that can be read on any workstation with a CD reader.

I have just completed Population II opacities with +0.4 enhanced α-process elements (O, Ne, Mg, Si, S, Ar, Ca, Ti) for abundances [+0.5], [+0.0], [-0.5], [-1.0], [-1.5], [-2.0], [-2.5], [-3.0], [-3.5], [-4.0], [-4.5], and [-5.0]. They will soon be ready for distribution.

NEW GRIDS OF MODELS

I rewrote my model atmosphere program to use the new line opacities, additional continuous opacities, and an approximate treatment of convective overshooting. The revised version is called ATLAS9. The opacity calculation was checked by computing a small grid of solar models with various microturbulent velocities and mixing-length-to-scale-height ratios. I adopted a solar model that matches the observed irradiance (Neckel and Labs 1984; Labs et al. 1987) with v_{turb} = 1.5 km/s and l/H = 1.25. I am confident that I have solved the missing opacity problem. See Kurucz 1992 for details and figures.

Thus far I have computed a grid of more than 7000 models for [+1.0], [+0.5], [+0.3], [+0.2], [+0.1], [+0.0], [-0.1], [-0.2], [-0.3], [-0.5], [-1.0], [-1.5], [-2.0], [-2.5], [-3.0], [-3.5], [-4.0], [-4.5], and [-5.0] for 2 km/s microturbulent velocity. The effective temperature range is 3500K to 50000K, from K stars to O stars. Note that since triatomic molecules are not included in the opacity, the models cannot be used for M stars. Gravities range from log g = 5 down to 0 or the radiation pressure limit in steps of 0.5. Models cooler than 9000K are convective with l/H = 1.25. For each model the flux was computed at 1221 wavelengths in the range .01 to 160 μm, enough to treat ionization in H II regions and to calibrate the infrared. The temperature range of this grid should allow photometric calibrations consistent for both cool and hot stars.

I have computed preliminary UBV and uvby colors and bolometric corrections following Buser and Kurucz (1978) and Relyea and Kurucz (1978) including the typographic correction from Lester et al (1986). The colors were normalized by finding the model in the grid that best interpolates the spectrophotometry of Vega (Hayes and Latham 1975; Tug, White, and Lockwood 1977), and that best matches the Balmer line profiles (Peterson 1969) and then by forcing the computed colors for that model to match the observed colors. Also considering that Vega has abundances lower than solar (Adelman and Gulliver

1990), that model has T_{eff} = 9400K, log g = 3.90, [-0.5], and v_{turb} = 2 km/s. I have also computed RIJKL, 13-color, and Cousins RI, and will do other systems.

For each model in the grid I have computed the fluxes, photometry in several systems, Balmer line profiles, and limb-darkening. At the present time I can supply a 6250 bpi VAX backup tape with the whole grid computed thus far including fluxes, colors, and Balmer line profiles. I am currently sending out the fourth version of this tape. Earlier versions have a few bad models which have been replaced, and there was an error in the fluxes and colors for the [+1.0] models. The limb-darkening requires a separate tape for each abundance. I will also publish the data on CD-ROMs. Most users will be able to find what they need by simple interpolation.

In the future, for any model, I expect to be able to compute a complete, full-resolution spectrum that can be compared to high resolution observations, or degraded to low resolution, say, 0.1 nm.

The microturbulent velocity is an important parameter that must be considered. Opacity and model structure vary with v_{turb}. If there is diffusion, v_{turb} must be small. In giants it can be large. In pulsating stars, such as Cepheids and RR Lyraes, it varies with phase. I am presently extending the grid calculations to other microturbulent velocities.

I am also computing grids of models using the new α-enhanced opacities, working inward both from the high abundance bulge stars and from the extremely low abundance halo stars.

ATLAS12

In Am and Ap stars, or, perhaps, in all A stars, the atmospheric abundances are not scaled-solar. Scaled-solar grids can produce only an approximate representation of the atmosphere. The cost of computing opacities is so high that it is not practical to pretabulate opacities for individual stars, although it might be possible for subclasses. The alternative is to use opacity sampling to compute individual models for each star. This is not a new idea. Muthsam (1979) computed opacity-sampled models for Ap stars. I have not used it up to now because it is too slow for computing large grids of models.

I have developed a new version of my model atmosphere program, called ATLAS12, that opacity samples from my whole line list. It essentially combines my spectrum synthesis program SYNTHE (Kurucz and Avrett 1981) with my model atmosphere program ATLAS (Kurucz 1970). It recognizes more than 1000 species, each in up to 10 isotopic forms, including all ions of the elements up through Zn and the first 5 ions of heavier elements up through Es. The elemental abundances are treated as variables with depth. It can treat any number of depths.

At present ATLAS12 has 6 input files containing 58,000,000 lines:

NLTELINES: H, He, C, Mg, Al, Si, Ca, etc., the file used by SYNTHE, species that can be treated in non-LTE by Avrett;
LOWIONS: first 5 stages of ionization of all elements;
HIGHIONS: ion stages 6 and higher of elements up through Zn;
DIATOMICS: H, C, N, O, Mg, Si, etc combinations;
TIO: TiO now, VO, ZrO, etc, in the future;
TRIATOMICS: empty now, H_2O, etc., in the future.

For each line the wavelength, identification, lower energy level, gf value, and the radiative, Stark, and van der Waals damping constants are packed into 16 bytes. At each wavelength point in a frequency integration the Voigt profiles of all the significant nearby lines are computed and summed. The lines in file NLTELINES can be treated with more complicated profile functions. The program and line files will be distributed in the fall of 1992.

SAMPLE MODELS

I have computed two sample A star models. The models have flux errors less than 0.1%. Each took a day to compute on a VAX 4000. I am aiming for a execution time of overnight or less on a workstation.

The first model is a $T_{\rm eff}$ = 9500K, log g = 4, $v_{\rm turb}$ = 2 km/s , solar abundance model that can be checked against the same model in the grid computed with distribution functions. Figure 1 shows the ATLAS12 and the ATLAS9 temperature distributions. The opacity-sampled model has a lower surface temperature because it has a higher dynamic range in the opacity. The distribution function approach using 12 steps averages the opacity in each step. The maximum opacity that it reproduces is lower than the true maximum. Opacity sampling can be closer to the true maximum, if there are enough sample points. In reality, the surface is not treated physically in either model. Both assume LTE. A non-LTE calculation may not have a temperature drop at the surface. Deeper in, the models are the same. Figure 2 shows the flux computed at 25000 logarithmically-spaced frequencies by ATLAS12. Figure 3 shows the same flux averaged in 21 point blocks to reduce sampling noise compared with the flux computed by ATLAS9. One significant difference is in the wings of $H\gamma$ and $H\delta$. The sampled spectrum is higher and I think will agree better with observations. There must be averaging over the distribution function bandpasses that makes the Balmer line wings appear too strong in the ATLAS9 model. In the Balmer continuum the detailed features do not reproduce well although overall I would say that they match. There are sampling errors in the ATLAS12 spectrum and there are bandpass averaging errors in ATLAS9. I do not know which one is more correctly computed. Both of them suffer from the same errors in the line data, so neither one should match observations exactly.

Next I computed a Vega model with non-scaled solar abundances using the parameters and abundances found by Castelli and Kurucz (1992) and the low helium abundance found by Gulliver et al. (1991): $T_{\rm eff}$ = 9500K, log g = 3.95, $v_{\rm turb}$ = 2 km/s, [-0.5] except with individual abundances He 0.0634, C [-0.35], O [-0.6], Si [-0.6], S [-1.0], Ti [-0.6], Fe [-0.7], Co [-1.0], Ni [-1.0], Zn [-1.0]. Figure 4 compares the opacity-sampled temperature distribution with the scaled-solar Castelli and Kurucz (1992) model and Figure 5 compares the fluxes. The opacity-sampled model is cooler at the surface, hotter at log τ = -3, and cooler between -2 and -1. These differences will affect line profiles and line depths. The fluxes are similar in the infrared and Paschen continuum, but the sampled model is 2% lower at the head of the Balmer continuum and 10% higher at 2×10^{15} Hz (= 150 nm). The Balmer line profiles are not measurably different except at the center of $H\alpha$. It will be necessary to compute a small grid and to iterate to refine the parameters and to match the observational data. The abundances and microturbulent velocity may change as the model changes.

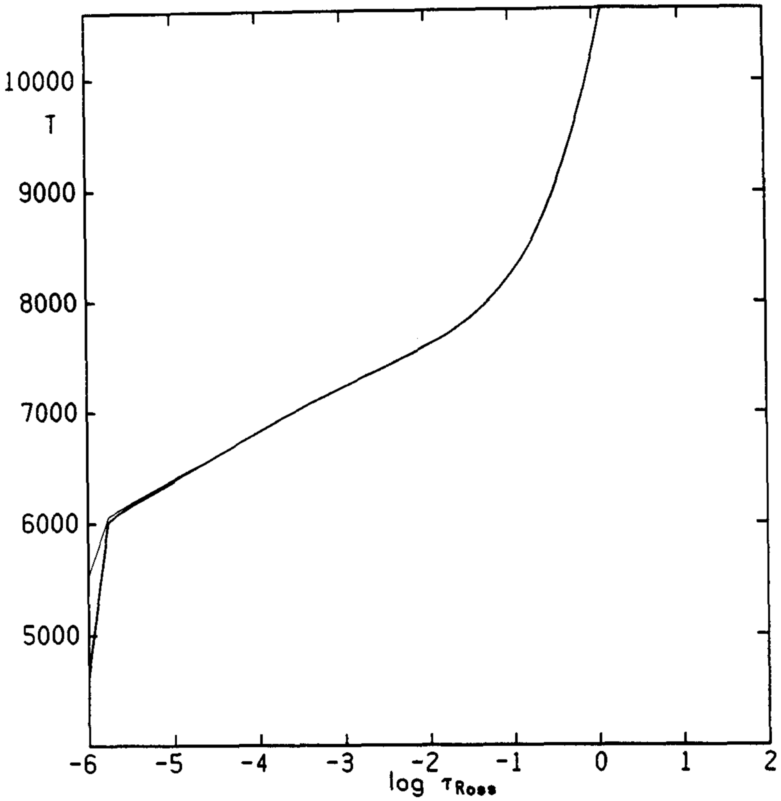

Fig.1. Comparison between ATLAS12 opacity-sampled temperature structure (thick line) and ATLAS9 distribution-function temperature structure (thin line) for T_{eff} = 9500K, log g = 4, [0.0], v_{turb} = 2 km/s.

FUTURE WORK AND PROGRAM DISTRIBUTION

ATLAS12 is still under development. At present it runs slowly and is being added to and modified every day. Now I am concentrating on speeding up the continuous opacity routines. In October 1992, I expect to distribute the line data and a version of ATLAS12 that works for A stars. If I am lucky, I will also have finished the new molecular equation of state, and it will also work for G and K stars. I will produce a Rosseland opacity version that can generate envelope opacities for arbitrary abundances. Obviously, the program can be modified to treat diffusion problems. I will eventually produce a non-LTE version.

I will make specialized versions of ATLAS12 or of SYNTHE with reduced line lists for computing β indices, or other indices, from previously computed models. It should be easy for the user to do this for a favorite index.

As the line data are still in need of much improvement, I will concentrate on computing the heavier and lighter elements, and the diatomics.

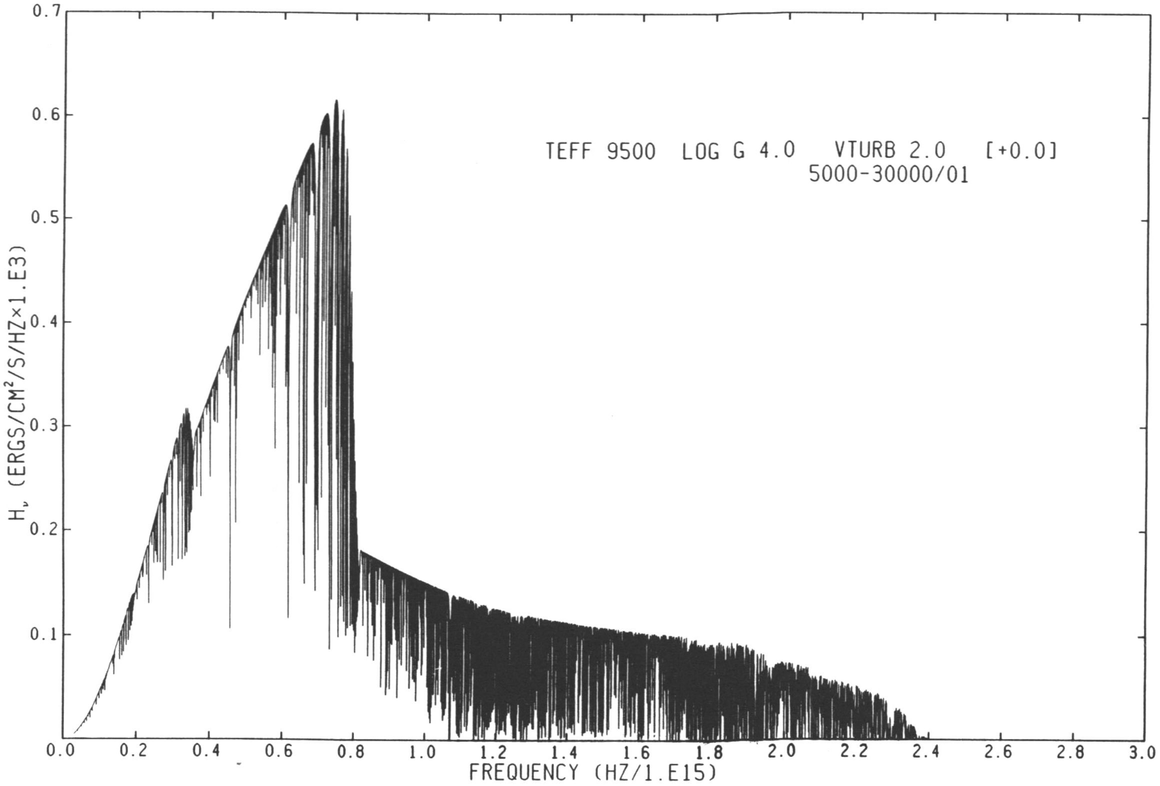

Fig.2. Opacity-sampled flux predicted by ATLAS12 at 25000 logarithmically-spaced frequencies for $T_{\rm eff} =$ 9500K, $\log g = 4$, [0.0], $v_{\rm turb} = 2$ km/s.

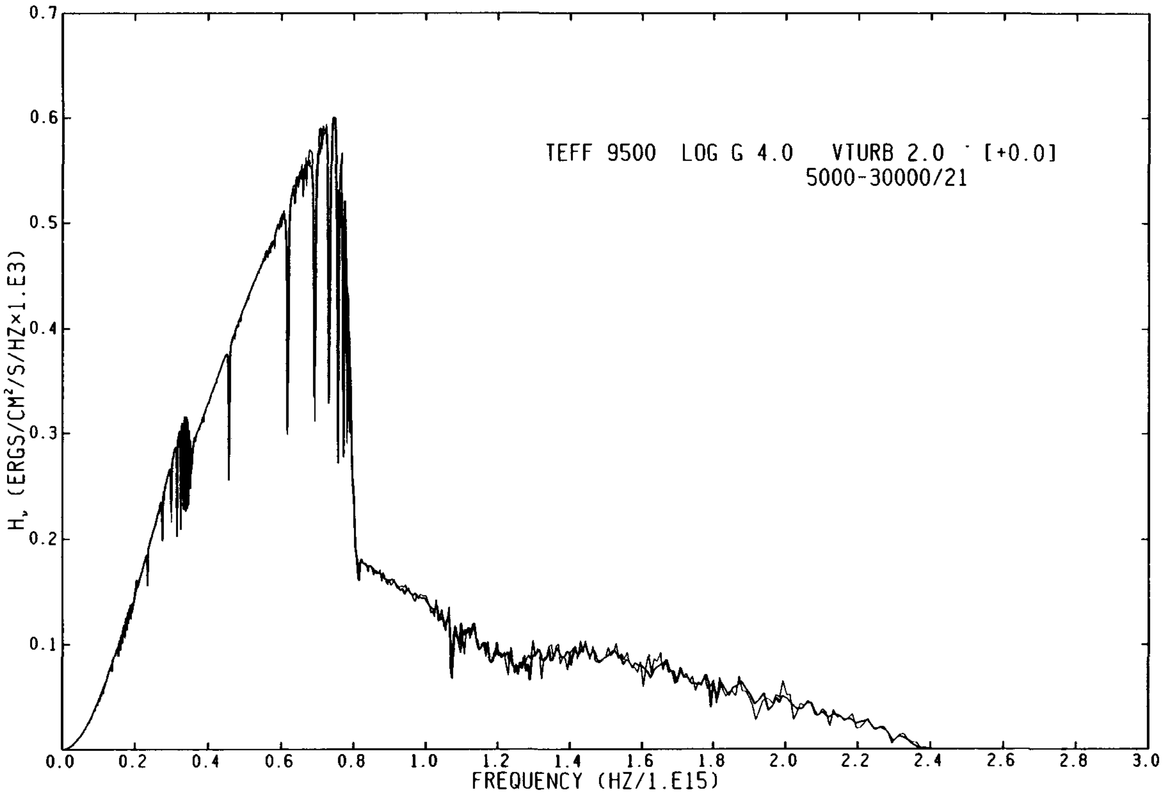

Fig.3. Opacity-sampled flux predicted by ATLAS12 at 25000 logarithmically-spaced frequencies averaged in blocks of 21 for $T_{\mathrm{eff}} = 9500$K, log g = 4, [0.0], $v_{\mathrm{turb}} = 2$ km/s (thin line) compared to ATLAS9 distribution-function flux at 1221 frequencies (thick line).

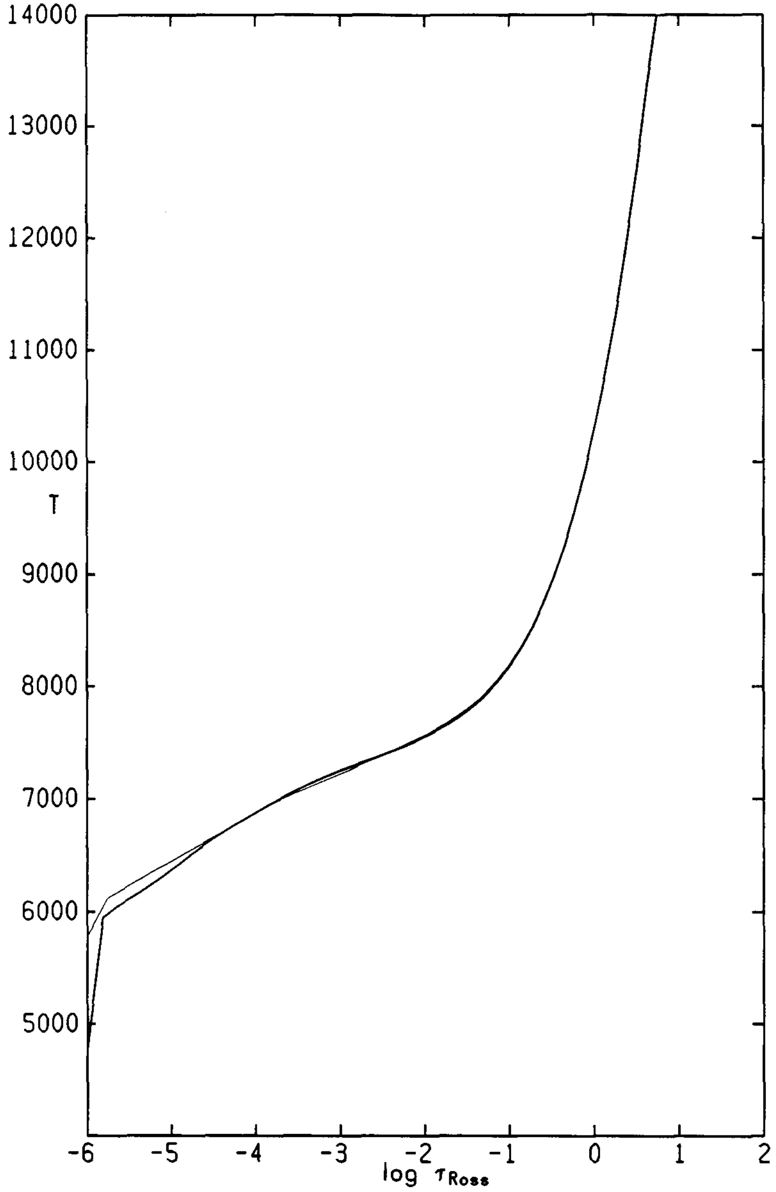

Fig.4. Comparison between the ATLAS12 opacity-sampled temperature structure (thick line) for a Vega model with T_{eff} = 9500K, log g = 3.95, v_{turb} = 2 km/s, with individual abundances and the ATLAS9 distribution-function temperature structure (thin line) with scaled solar abundances.

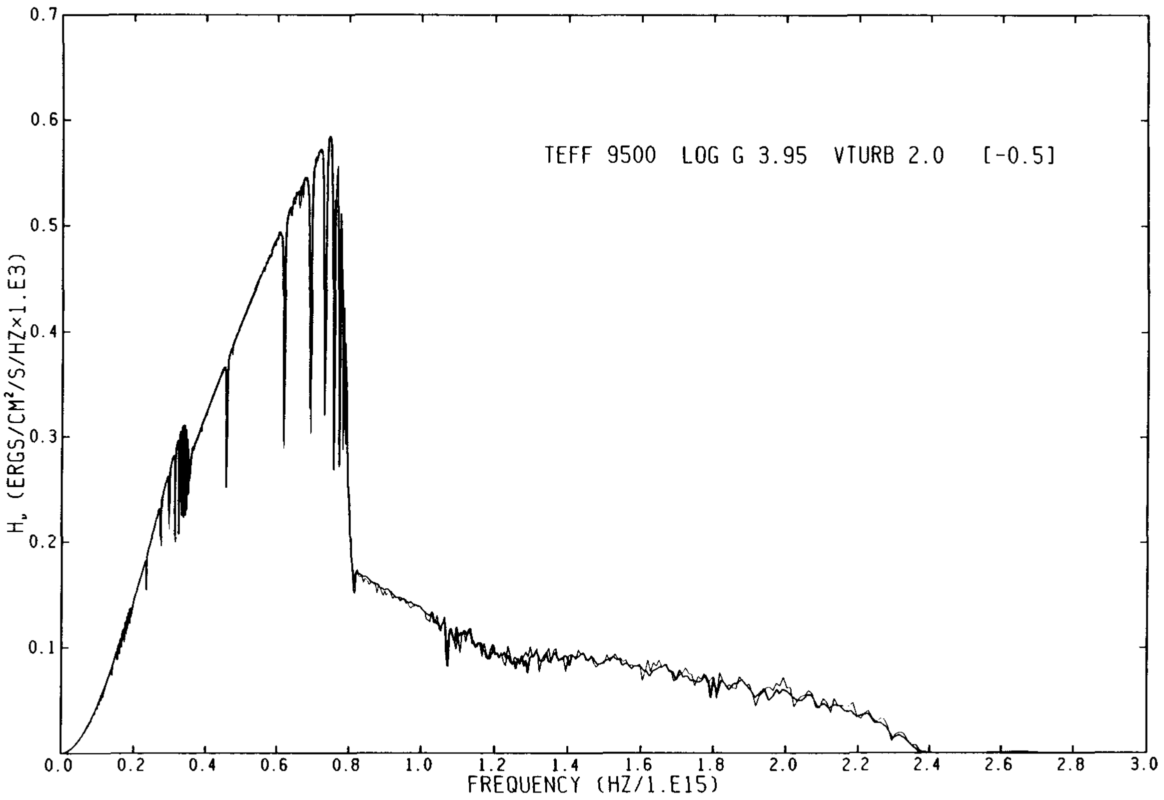

Fig.5. Comparison between fluxes predicted by the ATLAS12 Vega model (thick line) and fluxes predicted by the ATLAS9 Vega model as described in Figure 4.

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