Rev. Mexicana Astron. Astrof., **23**, 181-186 (1992)

"FINDING" THE "MISSING" SOLAR ULTRAVIOLET OPACITY

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RESUMEN. Se han calculado nuevas opacidades para modelos de atmósferas y envolventes usando una gran cantidad de tiempo de computación en la Cray del San Diego Supercomputer Center. Las opacidades incluyen 58.000.000 líneas atómicas y de moléculas diatómicas. Se tabulan las funciones de distribución de 12 saltos para 56 temperaturas en el intervalo entre 2000 K y 200000 K, para 21 presiones con logaritmos desde -2 hasta 8, para 1212 intervalos de longitud de onda entre 10 y 10000 nm, para velocidades de microturbulencia de 0, 1, 2, 4 y 8 km/s, y para abundancias solares escaladas de [+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] y [+0.0, sin He] (logaritmo de la abundancia de los elementos más pesados que el helio relativo a la abundancia solar). También se tabulan las opacidades medias de Rosseland para cada caso. Los archivos finales para cada abundancia requieren dos cintas backup de VAX de 6250 bpi cada una. Actualmente se distribuyen copias de estas cintas. Se espera tener copias en CD-ROM en un futuro cercano. Se ha calculado un modelo de atmósfera solar con las nuevas opacidades que se ajusta a la distribución de energía observada.

ABSTRACT. I have computed new opacities for model stellar atmospheres and envelopes using a large grant of Cray computer time at the San Diego Supercomputer Center. The opacities include 58,000,000 atomic and diatomic molecular lines. Twelve-step distribution functions are tabulated for 56 temperatures in the range from 2000 K to 200000 K, for 21 log pressures from -2 to 8, for 1212 wavelength intervals from 10 to 10000 nm, for microturbulent velocities 0, 1, 2, 4, and 8 km/s, for scaled solar abundances [+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] (log abundance of elements heavier than helium relative to solar). Rosseland means are also tabulated for each case. The final files for each abundance require two 6250 bpi VAX backup tapes. I am now distributing tape copies. I hope to have CD-ROMs available in the near future. A solar photospheric model computed with the new opacities matches the observed energy distribution.

Key words: ATOMIC PROCESSES – MOLECULAR PROCESSES – OPACITIES

I. INTRODUCTION

My coworkers and I have developed techniques for statistically including the opacity of millions of lines in model atmosphere calculations (Strom and Kurucz 1966; Kurucz 1970; Kurucz, Peytremann, and Avrett 1975, Kurucz 1979a,b). The opacities have been based upon the atomic line data computed by Kurucz and Peytremann (1975) plus whatever data were available from the literature. The inclusion of line opacity brought about a tremendous improvement in the quality of the models. Systematic errors in the determination of stellar effective temperatures, gravities, and abundances have been greatly reduced, although further improvement is still required. The fluxes computed from these models can be compared directly to stellar observations, or can be convolved with various photometric bandpasses to calibrate the photometric systems in common use (Relyea and Kurucz 1978; Buser and Kurucz 1978). These include solar abundance models for effective temperatures ranging from 5500 K to

50000 K (Kurucz 1979a), and grids for abundances [+1.0], [+0.5], [-0.5], [-1.0], [-1.5], [-2.0], [-2.5], and [-3.0] (log abundance of elements heavier than helium relative to solar).

There are a number of problems with the opacities and consequently with the models. As all these models have been computed with scaled solar abundances and assuming a 2 km/s microturbulent velocity, they can be used only as a first guess for enhanced-or-peculiar-abundance Am and Ap stars, and for stars with no turbulence or with enhanced turbulence. The wavelength intervals, nominally 2.5 nm in the ultraviolet and 5 nm in the visible, are inadequate for comparison to modern observations. There are systematic errors in the cooler models because molecular line opacity has not been included. Figure 1 shows the theoretical model for the solar photosphere that has several per cent error in the flux in the red and, of course, cannot reproduce the molecular features in the ultraviolet. There also have been systematic errors in the models at all effective temperatures caused by missing atomic line opacity which turns out to be quite considerable. This problem has been commonly referred to as the "missing solar ultraviolet opacity".

In the next section I describe my efforts to improve the atomic and molecular line data. Then I briefly describe my method for computing opacity, and finally I describe the results of this work in which I show that the"missing" opacity has been "found".

II. ATOMIC AND MOLECULAR DATA

My atomic and molecular line data are discussed in my first paper in this volume. My early 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. I also have data for terrestrial atmospheric molecules.

In 1983 I recomputed the opacities using the additional atomic and molecular data described above. These new 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, as shown in Figure 2, 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 Cray computer time at the San Diego Supercomputer Center by SF to compute the iron group line lists. I now have data for 42 million lines for Ca I–IX to Ni I–IX.

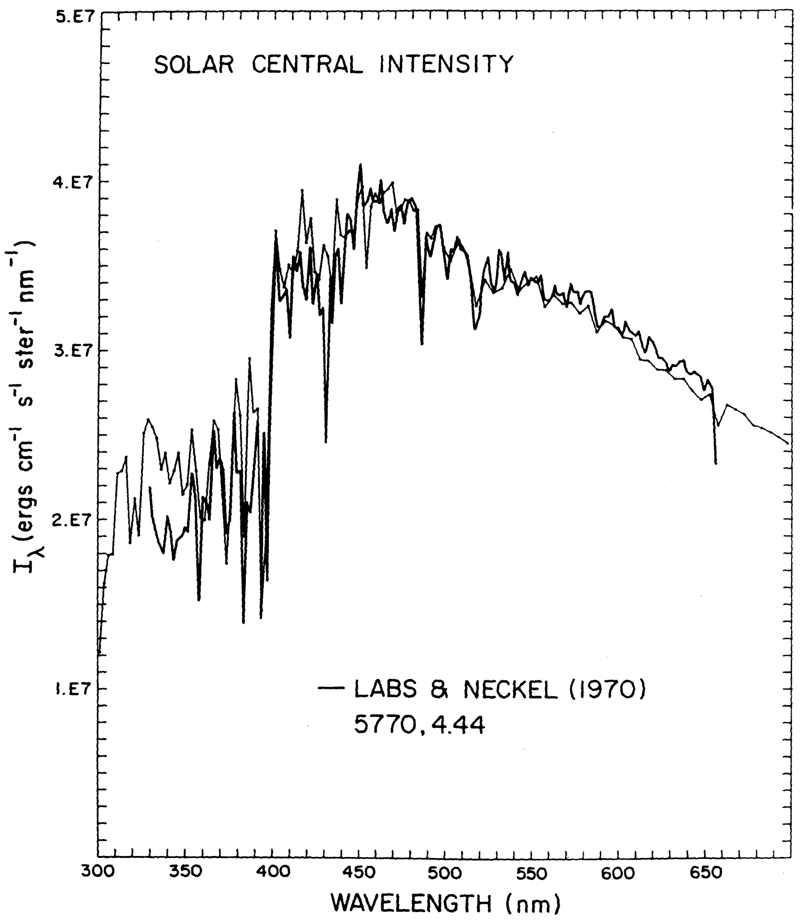

Figure 1 — Predicted central intensity for a solar model compared to observations.

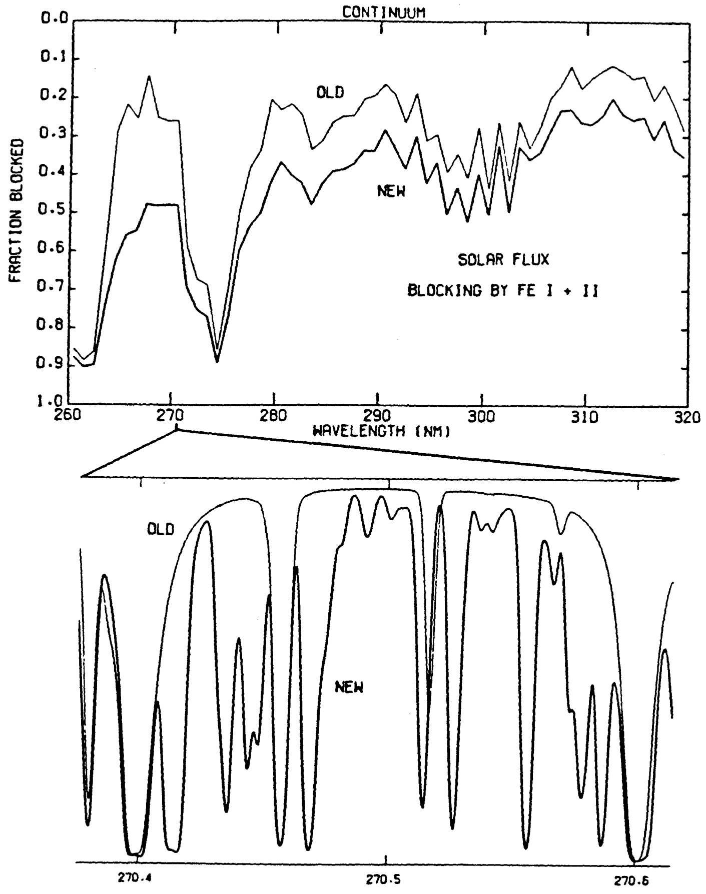

Figure 2 — Comparison between the ultraviolet solar flux computed with my old line data for Fe I and II and with my new line data.

III. THE OPACITY PROGRAM

The opacities are calculated with a version of my spectrum synthesis computer program that has been under development since 1965 and has been described by Kurucz and Furenlid (1981) and by Kurucz and Avrett (1981). The algorithms for computing the total line opacity are extremely fast because maximum use is made of temperature and wavelength factorization and pretabulation. On a Cray computer a 500,000 point spectrum can be computed in one run. The same programs run on a VAX, only much more slowly. There is no limit to the number of spectrum lines that can be treated.

The spectrum calculations require a pre-existing model atmosphere. For computing opacities it is just a table of temperatures and pressures. Quantities that need be computed only once for the model atmosphere are pretabulated, i.e, number densities, partition functions, doppler widths. The equation of state and continuum opacities are computed with a version of the model atmosphere program ATLAS (Kurucz 1970). Solar abundances are taken from Anders and Grevesse (1989). Photoionization continua are put in at their exact positions, each with its own cross-section and with the series of lines that merge into each continuum included so that there are no discontinuities in the spectrum.

Hydrogen line profiles are computed using a routine from Peterson (1979) that approximates the Vidal, Cooper, and Smith (1973) profiles, works to high n, and includes Doppler broadening, resonance broadening, van der Waals broadening, and fine-structure splitting. Autoionization lines have Shore-parameter Fano profiles. Other lines have Voigt profiles that are computed accurately for any value of the damping parameter a which includes radiative, Stark, and van der Waals broadening. For small parameter a, table lookup is used for speed. Line wings are truncated when they are weaker than 0.001 times the continuum. Lines weaker than 0.001 times the continuum are not considered.

The opacity spectrum is computed only for zero microturbulent velocity. Other velocities are obtained by convolution. The spectral resolution is 500000, high enough to reproduce the line profiles. The spectrum is computed at 3,500,000 points uniformly spaced in $\Delta\lambda/\lambda$ (velocity) from 8.97666 nm to 10000 nm. The distribution function for a wavelength interval is determined by statistically analyzing the total line opacity spectrum in that interval. In practice the spectrum is divided into 36 subintervals because of file size limitations. The input line files must be be subdivided, and the output opacity files must be combined to produce the final opacities.

IV. SOLAR OPACITIES AND A NEW SOLAR MODEL

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 2000 K to 200000 K, 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 both as 12-step distribution functions for intervals on the order of 1 to 10 nm, and as opacity sampling where, simply, every hundredth wavelength point in the calculation was saved. 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.

I have rewritten my model atmosphere program to use the new line opacities, additional continuous opacities, and an approximate treatment of convective overshooting. The opacity calculation was checked by computing a new solar model that matches the observed irradiance (Neckel and Labs 1984; Labs et al. 1987) as shown in Figure 3. The model has $T_{\rm eff} = 5777$ K, $\log g = 4.4377$, $V_{\rm turb} = 1.5$ km/s, and convective mixing-length-to-scale-height ratio 1.25. I am confident that I have solved the "missing opacity" problem.

V. ADDITIONAL OPACITIES

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

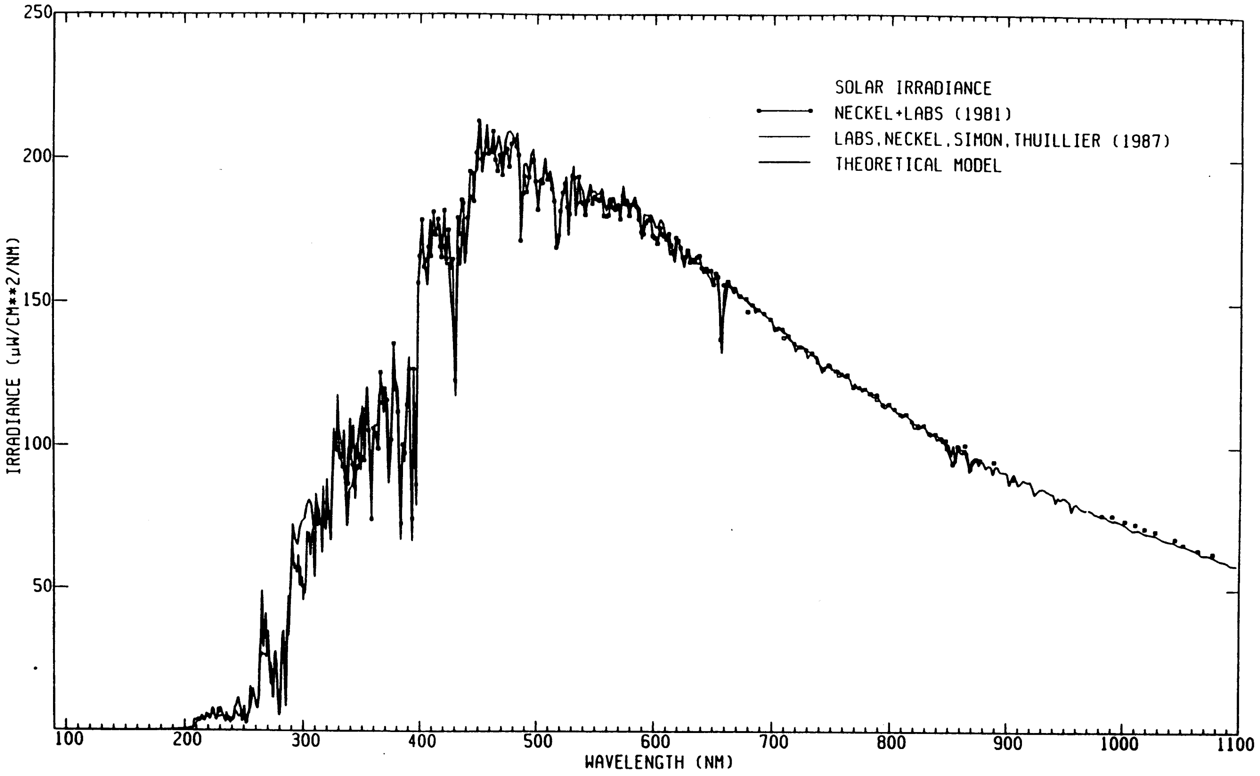

Figure 3 — Predicted solar irradiance compared to observed.

oldest Population II stars to high abundance Am (metallic line) and Ap (peculiar) stars. The hardest part was transmitting the results (200 tapes) back to Cambridge over Internet, but even that usually worked quite well. 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 three 6250 bpi VAX backup tapes. I have begun to distribute copies of the tapes. I plan to produce 600 megabyte CD-ROMs of these opacities that can be read on any workstation with a CD reader.

Rosseland mean opacities have been computed for each abundance for temperatures up to 200000 K for use in interiors and envelope calculations. The mass density and electron number were also saved to allow changing variables. These Rosseland opacities should be much better than the Los Alamos opacities in the same temperature region because they treat all the lines explicitly and with detailed profiles, and because the equation of state and the opacity spectra are computed for the actual composition, not as a post facto mixture. The numerical accuracy of any sort of mean opacity must be more reliable in my calculation.

I am open to suggestions for computing opacities for other abundance mixes. At the present time I am planning to compute C/O variations, Population II opacities with enhanced light even elements, and some Am and Ap mixes.

Currently I am testing a new opacity program that tabulates monochromatic opacity for a limited temperature-pressure range at all 3.5 million wavelength points using 16 bit packed integers, or for the whole temperature-pressure grid in a small wavelength range, say for a Mg index or a β index. I am running the program on all the lines of a single element or ion. Georges Michaud from Montreal is going to use these opacities to compute diffusion of elements up or down in an atmosphere.

My opacity routines will be rewritten in the next year or two to include as many levels as possible and to include new calculations and measurements, especially the Opacity Project data as they become available. I do not expect any major changes in the results at stellar atmospheric temperatures.

ACKNOWLEDGEMENTS

This work is supported in part by NASA grants NSG-7054, NAG5-824, and NAGW-1486, and has been supported in part by NSF grant AST85-18900. The most important contribution to this work is a large grant of Cray computer time at the San Diego Supercomputer Center.

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