THEORETICAL STELLAR ENERGY DISTRIBUTIONS

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SUMMARY. We are working hard to improve model atmospheres because existing models have numerical errors, an unphysical treatment of convection, an inadequate or non-existant treatment of statistical equilibrium, an arbitrarily chosen microturbulent velocity, an arbitrarily chosen helium abundance, and a greatly underestimated line opacity for iron group elements.

In his introduction Roland Buser was sanguine about our ability to determine stellar parameters from theoretical predictions of model atmospheres. Bengt Gustafsson gave an overall review. Here I emphasize the shortcomings in the models so that you will know that much more work remains to be done, and so that you will support efforts to improve the models. I will mention numerical errors and errors in the treatment of convection, non-LTE, microturbulent velocity, abundances, and opacity. The one positive statement I will make is that I now can produce models for A and B stars that reproduce the Balmer, Paschen, and Brackett continua and the Balmer line wings. This implies that even if the physical parameters that characterize the model for a given star are somewhat off, the temperature-pressure structure must be correct in the continuum and line-wing-forming layers. Improved models will have a similar structure but perhaps for a somewhat different effective temperature and gravity.

My published models were produced as long as 15 years ago on computers that are primitive by today's standards. The number of optical depth layers was limited by small memories and slow processors. Now I can compute with many more layers and go to shallower optical depths. This greatly improves the numerical accuracy of the calculated radiation field at wavelengths that have very high or rapidly varying opacity. Fortunately, such wavelengths do not very much affect the structure of a model. There was also a limit to the number of frequencies that I could afford to compute. I am now able to use 1 nm resolution in the ultraviolet for better comparison to satellite observations.

J.-P. Swings (ed.), Highlights of Astronomy, 827–831.

Dave Philip and Don Hayes point out to me at every opportunity that my low gravity models for A stars predict colors that disagree with their observations. This is obviously a non-LTE effect. Computing realistic non-LTE models with all the line opacity is very far beyond the state of the art. Lawrence Anderson at Toledo has made the most progress.

My models for F and G stars are systematically in error and predict color indices that are off by as much as 0.05 mag. I assumed that the error was caused by problems in the mixing length treatment of convection and by the omission of molecular line opacity in the coolest models. Improvements in my treatment of convection, even going so far as having hot and cold streams, have reduced the error somewhat for the hotter convective models, but I am now convinced that most of the error comes from missing line opacity. I hope that Nordlund will be able to produce models with realistic convection cells to take care of the convection physics, so now I am concentrating on the opacity. I will discuss that last.

We do not know much about microturbulent velocity. It has been decreasing as a function of time as the models have improved. In the sun it is depth-dependent varying from about 0.5 to 1.8 km/s. The models assume a constant value. Twenty years ago, I arbitrarily chose 2 km/s as a nice round number. In some stars it can be much larger or may even be 0, so I have experimented with 0, 4, and 10 km/s models. Opacity, radiative acceleration, and model structure vary considerably with the microturbulent velocity. It may turn out that 1 or 1.5 km/s is a good choice for high gravity models. I expect to determine this through spectrum synthesis. I plan to compute grids of models with the microturbulent velocity as a parameter.

The helium abundance is another arbitrary number. I chose 10% by number. Others use a 10% He/H ratio. I am switching to the smaller value because I think it more probable. Small errors in the helium abundance produce errors in the density, electron number, and opacity and consequently produce systematic errors in the derived stellar parameters.

In 1983, working with Lucio Rossi from Frascati and with John Dragon and Rod Whitaker at Los Alamos, I finally completed line lists for all diatomic molecules that produce important opacity in G and K stars. The data are described in a table on the next page. Once the line data were ready, I computed new distribution function opacity tables. The calculations involved 17,000,000 atomic and molecular lines, 3,500,000 wavelength points, 50 temperatures, and 20 pressures, and took a large amount of computer time.

As a test the opacities were used to compute a theoretical solar model, to predict solar fluxes and intensities from empirical models, and (with fudging) to produce improved empirical models that are able to match the Ca II H and K line profiles and both the UV and IR inten-

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FILE	NUMBER LINES	WAVELENGTH RANGE (NM)		COMMENT
KP	265587	5.2682	9997.2746	Kurucz-Peytremann atomic
PREDKP	696704	6.6681	9995.4359	Predicted KP
GFFILE	28420	2.4898	65101.684	Additions to KP
NLTELINE	53594	22.7838	9999.3740	Can be treated NLTE
FE2	431933	51.2159	9988.4949	Fe II
H2	28486	84.4941	184.4573	Lyman and Werner
HYDRIDES	331268	203.6264	3245.1715	CH,NH,OH,MgH,SiH all iso
CNAX12	484709	292.5406	99912.800	12C14N Red
CNAX13	503631	295.1871	99924.784	13C14N Red
CNAX15	289887	341.5994	99776.188	12C15N Red
CNBX	323818	201.9947	715.7552	CN Violet all isotopes
C2AX	406236	271.8071	9999.6289	C2 Phillips all isotopes
C2BA12	462803	389.6061	99957.754	12C12C Ballik-Ramsay
C2BA13	387809	511.6587	99980.746	12C13C Ballik-Ramsay
C2BA33	313319	527.1495	80319.395	13C13C Ballik-Ramsay
C2DA12	329771	344.9621	2541.6874	12C12C Swan
C2DA13	253014	374.0201	991.5625	12C13C Swan
C2DA33	217545	376.2757	959.4157	13C13C Swan
C2EA12	487232	176.0052	862.4585	12C12C Fox-Herzberg
C2EA13	332214	177.3769	560.9010	12C13C Fox-Herzberg
C2EA33	260883	178.6938	543.2282	13C13C Fox-Herzberg
COAX	396004	111.3365	460.6524	CO 4th Pos all isotopes
COIR	118920	963.5078	9998.8853	CO vib-rot all isotopes
SIOAX	760378	177.3128	546.2833	SiO A-X all isotopes
SIOEX	947015	143.0468	462.4214	SiO E-X all isotopes
TIOAX6	325116	528.5640	1875.4212	46Ti16O gamma
TIOAX7	327496	528.7059	1771.6149	47Ti16O gamma
TIOAX8	647203	490.4263	2146.0045	48Ti16O gamma
TIOAX9	332113	528.9757	1864.4024	49Ti16O gamma
TIOAX0	334222	529.1046	1860.9887	50Ti16O gamma
TIOBX6	343598	246.6118	1232.9218	46Ti16O gamma'
TIOBX7	345990	246.3570	1209.4093	47Ti16O gamma'
TIOBX8	861488	235.9828	1362.8784	48Ti16O gamma'
TIOBX9	350530	246.7795	1187.2650	49Ti16O gamma'
TIOBX0	352802	247.3491	1186.9649	50Ti16O gamma'
TIOCX6	232718	350.0947	1562.0368	46Ti16O alpha
TIOCX7	234318	350.0471	1554.5985	47Ti16O alpha
TIOCX8	503950	257.0800	1316.1735	48Ti16O alpha
TIOCX9	237430	350.0113	1540.7715	49Ti16O alpha
TIOCX0	238827	349.9744	1534.3348	50Ti16O alpha
TIOEX6	241398	630.6768	2002.6215	46Ti16O epsilon
TIOEX7	242954	631.0335	1997.7022	47Ti16O epsilon
TIOEX8	510074	549.4411	2273.1493	48Ti16O epsilon
TIOEX9	245978	631.7067	1988.4477	49Ti16O epsilon
TIOEX0	247466	632.0252	1984.0965	50Ti16O epsilon
TIOBA	310376	541.4458	2250.2486	TiO delta all isotopes
TIOCA	223850	446.7588	1669.0456	TiO beta all isotopes
TIOFA	153496	432.0083	816.6252	TiO f-a all isotopes
TIOBD	158000	593.4372	2662.9648	TiO phi all isotopes
TIOED	102107	332.9690	562.5112	TiO e-d all isotopes

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sities formed near the temperature minimum. The work on empirical models is in collaboration with Avrett and Loeser.

There are 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 model this error is balanced by a flux error in the red. The model predicts the wrong colors. After many experiments with convection and opacities, and after synthesizing the spectrum in detail, I have 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 lines in absorption without difficulty.

I have used Bob Cowan's Hartree-Fock programs at Los Alamos to compute Slater single- and configuration interaction integrals for the lowest 50 configurations of the first 10 stages of ionization for elements up through Zn and for the first 5 for heavier elements. These calculations allow me to determine eigenvectors by combining least squares fits for levels that have been observed with computed integrals (scaled) for higher configurations. Each least squares iteration takes a significant amount of time on a Cray and many iterations are required. Thus far I have completed new line lists only for Fe I and II, but they produce the strongest effect on the spectrum. Radiative, Stark, and van der Waals damping constants and Lande g values are automatically produced for each line. The complexity of these calculations is illustrated by this table,

	Fe I		Fe II	
	even	odd	even	odd
number of configurations	26	20	22	16
number of levels	5401	5464	5723	5198
largest Hamiltonian matrix	1069	1094	1102	1049
number of least squares parameters (many fixed at scaled HF)	963	746	729	541
total number of lines saved	583,814		1,112,322	

The figure on the next page shows the blocking in the solar ultraviolet spectrum produced by Fe lines. The calculation was done once with the old line data mentioned above and again with the newly calculated data. The increase in opacity is dramatic. I expect there to be similar effects in hotter stars. I am currently trying to get computer time from the NSF to complete the calculations for the iron group elements including higher stages of ionization. Once the line data are complete, I will recompute the opacity tables for a range of abundances, then compute new grids of models, and finally predict the colors for every photometric system.

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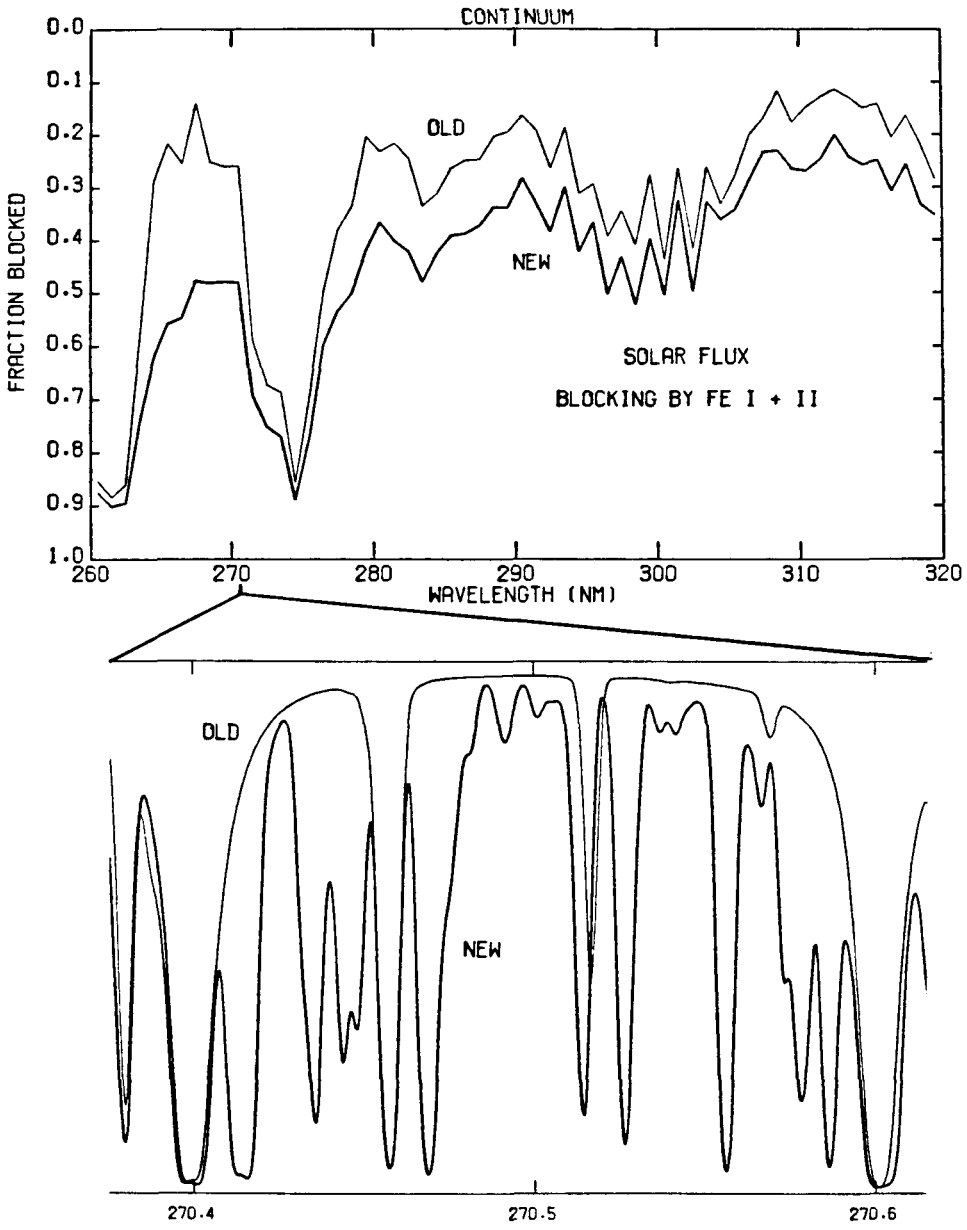

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