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AN ANALYSIS OF CH IN THE SOLAR ATMOSPHERE

by

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of the requirements for the degree of
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CHAPTER I

INTRODUCTION

The Solar Photosphere

One of the major problems of solar physics in recent decades has been the search for a physical model of the solar photosphere that would explain satisfactorily the observations of the spectral continuum and the profiles of Fraunhofer lines.

In the lower photosphere the dependence of temperature and pressure on depth is relatively well determined. Most present day studies of this part of the photosphere have the goal of refining the model to take into account various effects such as the influence of the convection zone below the photosphere and the influence of inhomogeneities in temperature as evidenced by the presence of granular contrast on the solar disc.

In the interpretation of the behavior of absorption lines formed in the lower photosphere it has proven useful to assume that the physical conditions in a given small volume element of these layers closely approximate those in a volume element that is in thermal equilibrium. This assumption, that of local thermodynamic equilibrium, implies that a single parameter, the local temperature, determines the relative populations of all continuous and discrete energy levels for the atoms in the volume element. This assumption is probably adequate in the lower photosphere because the internal degrees of freedom of

atoms in this region are strongly coupled to the local radiation field by the high continuous opacity in these layers.

In the upper photosphere the physical conditions become more and more complex as the chromosphere is approached. Thus the derivation of a satisfactory model is more difficult than in the lower photosphere. Since the continuous opacity in the upper photosphere is low, the radiation field and internal atomic degrees of freedom are weakly coupled. Furthermore, as a consequence of the photospheric temperature gradient and the low continuous opacity in the upper photosphere, the radiation field becomes increasingly anisotropic with increasing height. This combination of anisotropic radiation field and poor coupling between the radiation field and internal atomic degrees of freedom implies that the assumption of local thermodynamic equilibrium is possibly not appropriate for the description of conditions in the upper photosphere.

A result of the uncertainty as to the conditions in the upper photosphere is that photospheric temperature-pressure models derived by various techniques often disagree considerably in the upper photosphere. This is illustrated in figure 1-1 where I have plotted as a function of optical depth at $5000 \text{ \AA}$, τ_0 , the temperatures of three different photospheric models.

Purpose of This Investigation

The purpose of this investigation is to use center-limb observations of the profiles and equivalent widths of lines in the $2\Delta-2\pi$ band system of the CH molecule to obtain information about the conditions in the upper photosphere. Molecular lines are especially suitable for such a study because they are formed almost entirely in

the upper photosphere. The CH molecule was chosen for this investigation for two reasons:

1. The CH dissociation energy has been accurately determined in the laboratory.
2. The $\Delta^2-\pi^2$ band system of CH is well developed and falls in a part of the solar spectrum where the blending problems are not too serious.

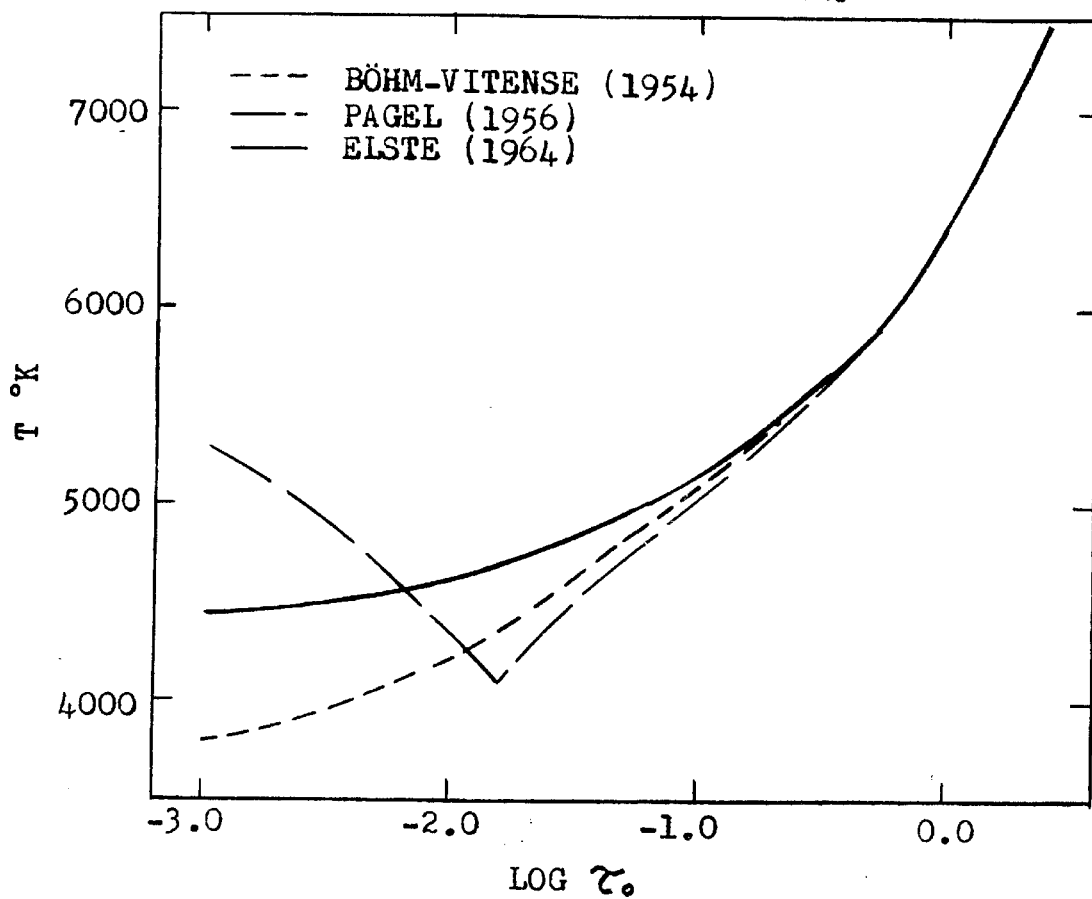


Figure 1-1.--The temperature as a function of $\log \tau_0$ for three photospheric models.

The center-limb behavior of the equivalent widths of the CH lines gives insight into the depth dependence of the number of CH molecules in those atmospheric layers where the lines are formed. This

in turn provides information on the physical conditions in these layers.

The equivalent width of a spectral line depends not only on the number of absorbing particles, but also on the Doppler width which is directly related to the magnitudes of the thermal and microturbulent velocities. Microturbulent velocities are defined as nonthermal motions of groups of atoms in eddies whose scale is small compared to the mean-free-path length of a photon in the line-forming region. Since the thermal velocities are relatively well known throughout the photosphere, the major uncertainty in the value of the Doppler width lies in the magnitude of the microturbulent velocity at the depth of line formation. The equivalent widths of weak and moderately strong lines are affected by variations in the Doppler width in different ways. Therefore, it may be possible to use center-limb observations of the equivalent widths of CH lines of different strengths to study the microturbulence model of the upper photosphere.

Critical data for the study of the physical conditions in the line-forming region may be derived from the profiles of the lines. The shape of a spectral line is very sensitive to the kind of broadening mechanism. It is affected by macroturbulent motions in the photosphere as well as to microturbulent motions. Macroturbulent motions are defined as nonthermal motions of groups of atoms which occur on a scale as large or larger than the region of line formation. It may be possible to use the profiles of CH lines to obtain information about the macroturbulence in the upper photosphere.

Past Studies of Molecular Lines

Since the computed center-limb behavior of the profiles and equivalent widths of CH lines are sensitive to the combined influences of the temperature-pressure model, turbulence model, and the possibility of departures from local thermodynamic equilibrium, it is desirable that we use the results of other investigations to establish a set of preliminary models for the upper photosphere. Of particular interest are previous studies of the upper photosphere based on observations of the center-limb behavior of molecular lines. The investigations of most interest are those of Newkirk (1953, 1957), Pecker (1956), Eugene-Praderie (1960), La Borde (1961), and Cowley (1963).

Newkirk (1953, 1957) studied the center-limb variation of the equivalent widths of the infrared CO lines. In his analysis of the observations Newkirk used temperature-pressure models by Aller and Pierce (1952), Minnaert (1953), and de Jager (1952). The Aller-Pierce model is an empirical model based on limb darkening observations of the continuum. The Minnaert model is a composite model based primarily on limb darkening observations and is very similar to the Aller-Pierce model. The de Jager model was derived from the center-limb behavior of hydrogen line profiles using the Holtzmark theory of line broadening. Since this theory does not account properly for the effect of fast moving electrons on the profiles, the de Jager model is probably inaccurate. Newkirk found that he could explain satisfactorily the CO observations by the assumption of local thermodynamic equilibrium, the assumption of line formation by pure absorption, and the Aller-Pierce and Minnaert photospheric models. When he applied the de Jager model to the observations, Newkirk found that deviations from local

thermodynamic equilibrium of the order of 1000°K were needed for $\log \tau < -1.3$.

Pecker (1956) found that it was not possible to explain the center-limb behavior of the CH equivalent widths by the assumption of local thermodynamic equilibrium, the assumption of line formation by pure absorption, and any of the four model atmospheres that he used. His results do indicate that a model similar to that of Minnaert (1953) but with a boundary temperature of about 3750°K might be suitable. However, since Pecker apparently did not take into consideration the effect of line strength on the center-limb behavior of the CH lines, his results are probably not very useful. Pecker suggested in this paper that a more elaborate investigation of the CH lines should be made using high quality observations.

In a later paper Eugene-Praderie and Pecker (1960) applied Pecker's theory of non-local thermodynamic equilibrium (Pecker, 1959) to the central intensities of CH lines observed at the center of the solar disc. They found deviations from local thermodynamic equilibrium of the order of 300°K when the Minnaert-HAO model photosphere (Pecker, 1956) was used. They suggested that the center-limb behavior of the CH equivalent widths can be explained by deviations from local thermodynamic equilibrium. Since the central intensities of computed lines are sensitive to the assumed temperature-pressure and turbulence models, the departures from local thermodynamic equilibrium found by Eugene-Praderie and Pecker may not be significant.

La Borde (1961) used equivalent widths of lines of six different molecules to determine rotational temperatures at the center of the solar disc and in sunspots. In connection with the present

analysis his investigation of the center-limb variation of the equivalent widths of MgH and C_2 lines is of interest. He found that the MgH observations could be explained by the Minnaert-HAO model (Pecker, 1956) under the assumption of local thermodynamic equilibrium and the assumption of line formation by pure absorption. When he applied the same model as well as several other models to the center-limb behavior of the C_2 lines, he could not obtain agreement between theory and the observations. La Borde suggested several possible reasons for this disagreement but could not give a conclusive explanation for the discrepancy.

Cowley (1963) found that, within the limits imposed by the quality of the observations and the uncertainty of the CN dissociation energy, the center-limb behavior of the violet CN lines could be explained by the assumption of local thermodynamic equilibrium, the assumption of line formation by pure absorption, and the Mutschlecner photospheric model (Mutschlecner, 1963). The observed equivalent widths have to be considered with reservation because of the serious blending problems found in the violet region of the solar spectrum. Nevertheless Cowley's work shows that surprisingly good molecular line equivalent widths can be obtained in spite of blends by using a local continuum level in the vicinity of the measured lines.

The past work on solar molecular lines has provided useful information about conditions in the upper photosphere. The observed equivalent widths of CO, CN, and MgH lines are explained by the Minnaert, Mutschlecner, and Minnaert-HAO models respectively. The dependence on optical depth of the temperatures in these three models is very similar in the upper photosphere. This is shown in figure 1-2.

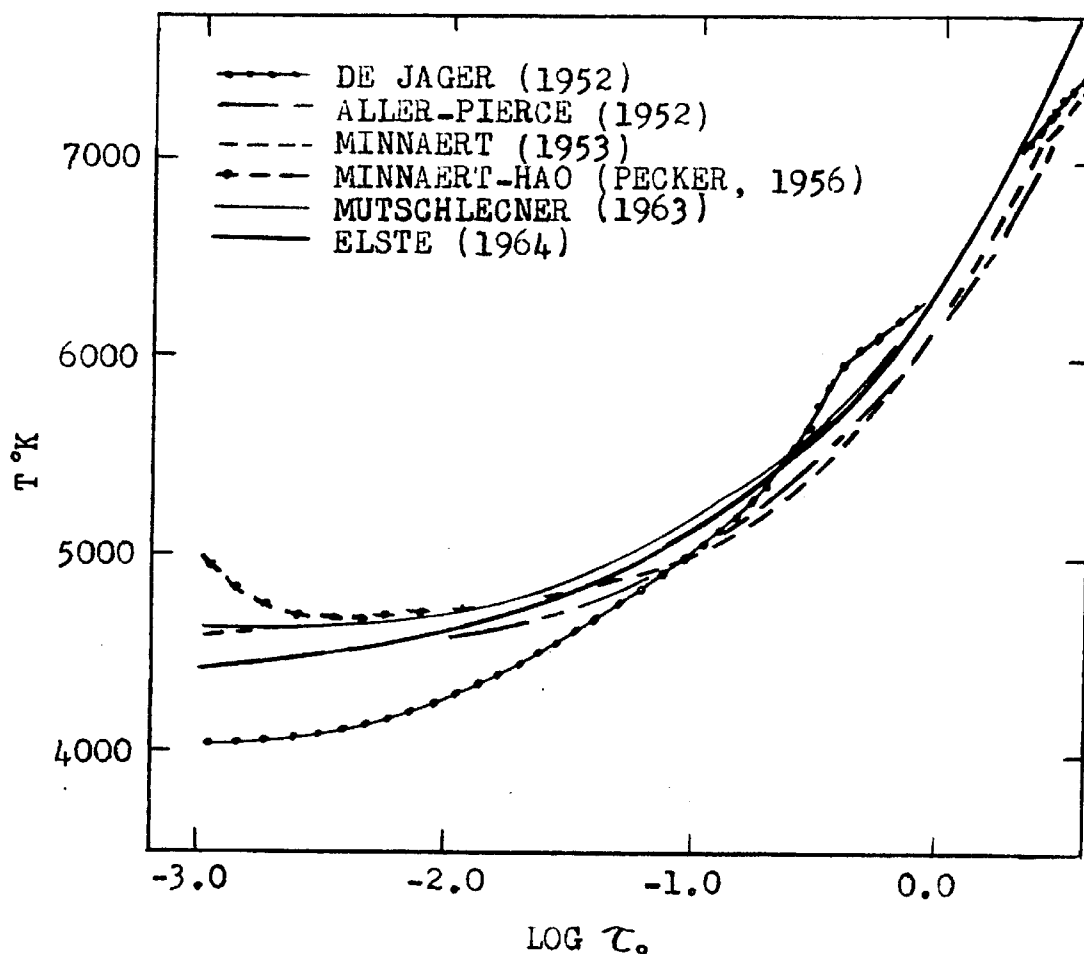


Figure 1-2.--The temperature as a function of $\log \tau_0$ for photospheric models used in studies of molecular lines.

Therefore, we might generalize the results of the investigations of CO, CN, and MgH and conclude that a temperature-pressure model similar to the above models would be a good preliminary model with which to study the CH observations. These studies also indicate that the assumption of local thermodynamic equilibrium and the assumption of line formation by pure absorption may be valid assumptions to apply to the study of molecular lines formed in the upper photosphere.

In apparent disagreement with the results of the investigations of CO, CN, and MgH are the results of the investigation of C₂ by

La Borde and the investigation of CH by Pecker and Eugene-Praderie. The latter analyses indicate that the Minnaert-HAO model, which combines the photospheric model of Minnaert (1953) with the chromospheric model of Athay, Menzel, Pecker, and Thomas (1955), may be inaccurate in the upper photosphere or that C_2 and CH may be affected by other effects such as departures from local thermodynamic equilibrium. However, since the observations of the lines of these five molecules are of relatively poor quality except for Newkirk's observations of the CO lines, we might expect that some of the differences in the results of the two groups of molecules may be attributed to observational error. One of the goals of this investigation was to obtain observational material which would permit a more thorough analysis of the CH molecule than was possible in the past.

Past Studies of Photospheric Turbulence

The past studies of photospheric turbulence can be grouped into three general categories based on techniques.

Curve of Growth Studies

This technique of studying photospheric turbulence is based upon the effect that turbulent motions have on the equivalent widths of lines of different strengths. The turbulent velocities that come out of such studies are microturbulent velocities. The results of several curve-of-growth studies (Wright, 1944; Huang, Su-Shu, 1950; Claas, 1951) indicate that the magnitude of the radial component of the microturbulence has a velocity of about 1.2 km/sec (most probable speed assuming a Gaussian distribution of speeds). Furthermore, an early center-limb study by ten Bruggencate and Houtgast (1940) indicates that

to a first approximation the photospheric microturbulence is isotropic and independent of depth.

Local Doppler Shift Studies

These studies of photospheric turbulence are based on observations of local Doppler shifts in spectral lines made under conditions of excellent seeing. These line shifts are probably caused by line-of-sight motions of cellular regions extended in depth over at least several hundred kilometers. Therefore, the velocities resulting from such studies are macroturbulent velocities. In general these studies indicate that the magnitude of the radial and tangential macroturbulent components in the upper photosphere is about 0.5 km/sec (most probable speed assuming a Gaussian distribution of speeds). Although the center-limb behavior of the local Doppler shifts is difficult to study because of geometrical foreshortening near the limb, there are indications that the photospheric macroturbulence is anisotropic. This is illustrated in figure 1-3.

Line Profile Studies

Since the profile of a spectral line is influenced by both microturbulent and macroturbulent motions in the line-forming region, the studies based on observations of line profiles give a measure of the total turbulence in the solar photosphere. Several investigations based on observations made at the center of the solar disc (Suemoto, 1957; Unno, 1959; Schmalberger, 1963) indicate that the total turbulence decreases with increasing height in the photosphere. Center-limb investigations (Allen, 1949; Voigt, 1956, 1959; Waddell, 1958; Schmalberger, 1963; de Jager and Neven, 1964) indicate that the total

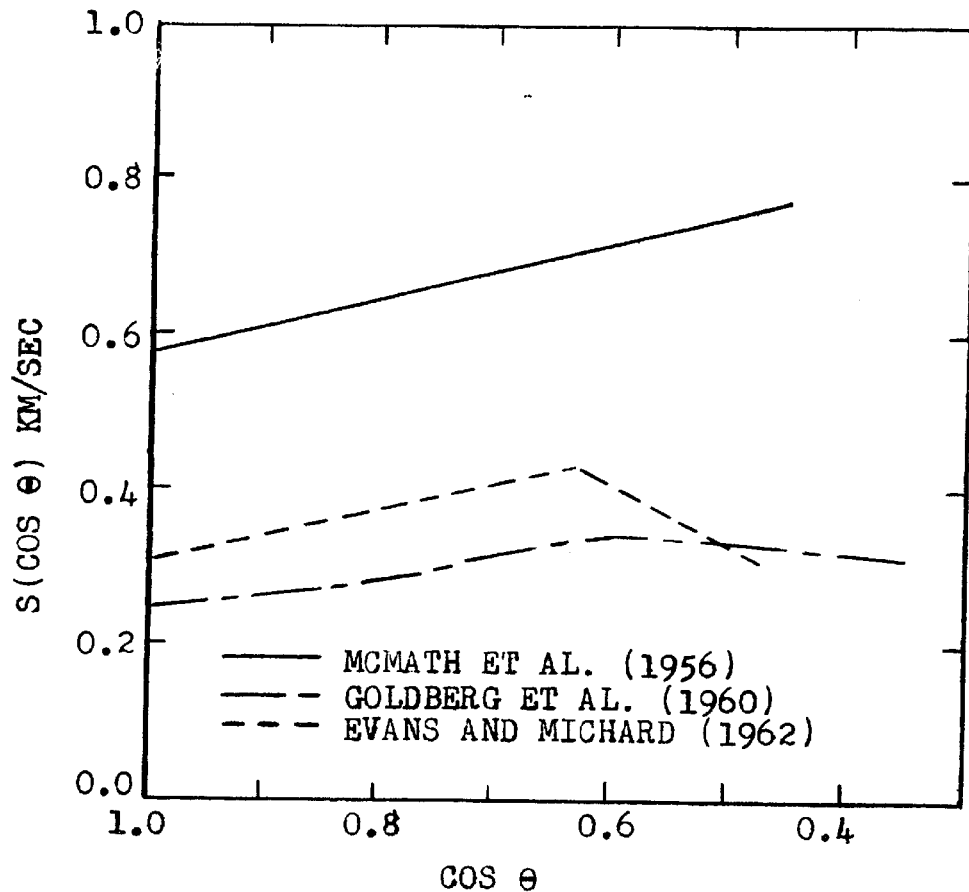


Figure 1-3.--Macro-turbulent velocities determined from the analysis of local Doppler shifts in moderately strong atomic lines. Velocities are random turbulent velocities ($\sqrt{2}$ -root-mean-square velocity).

turbulence increases with increasing distance from the center of the solar disc. This behavior has been interpreted as either an isotropic turbulence that increases with height or an anisotropic turbulence that has a tangential component which is larger than the radial component. Waddell (1958) gives several arguments why the anisotropic model is probably the correct explanation. A later center-limb investigation by Waddell (1960) indicates that the tangential turbulence decreases with height in such a way that the total turbulence is almost isotropic in the upper photosphere. This result is incorporated in the turbulence model of Schmalberger (1963). The latter turbulence model summarizes

fairly well the results of many of the above investigations. However, Schmalberger, like most of the investigators mentioned above, treated the total turbulence as pure microturbulence even though there is strong evidence for macroturbulence in the photosphere. Therefore, his results may not be too accurate. Schmalberger's model is given in figure 1-4.

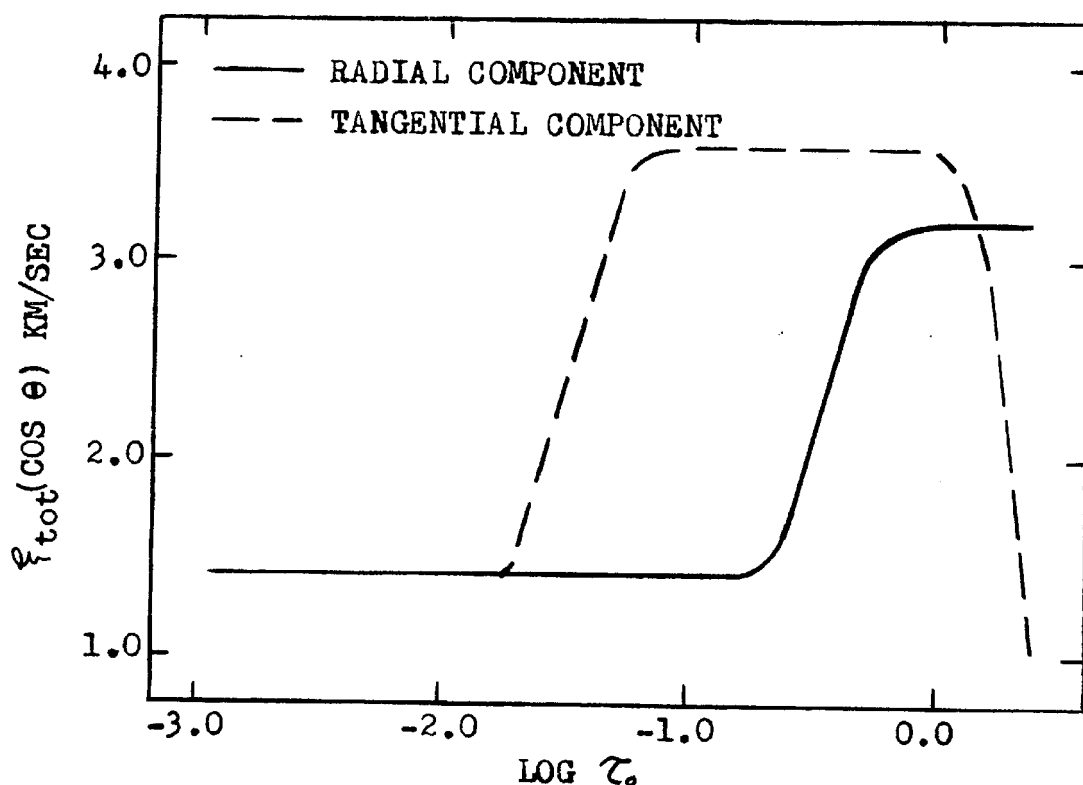


Figure 1-4.--Schmalberger's turbulence model.

The Photospheric Microturbulence

If we compare the results of the three different methods of investigating photospheric turbulence, we note that there are essentially two types of microturbulence models that we can use in analysing the behavior of the CH lines. The simplest model is based on the curve-of-growth results, namely, a microturbulence that is isotropic and independ-

ent of depth, and which has a velocity of about 1.2 km/sec. The other microturbulence model is based on the combined results of studies of line profiles and studies of local Doppler shifts. As a first approximation we may assume (Huang, Su-Shu, 1950) that

$$\xi_{\text{tot}}^2 = \xi^2 + s^2$$

where ξ_{tot} is the total turbulent velocity, ξ is the microturbulent velocity, and s is the macroturbulent velocity. If we accept the small macroturbulent velocities determined from measurements of local Doppler shifts as correct, then the turbulent velocities determined from observations of line profiles are due almost entirely to microturbulence. Therefore, the microturbulence in the lower and intermediate layers of the photosphere may have a large tangential component (see figure 1-4). As we shall see subsequently in Chapter IV, the CH observations tend to rule out such a severely anisotropic microturbulence model and support an isotropic model similar to the one suggested by the curve-of-growth results.

CHAPTER II

THE OBSERVATIONS

The Apparatus

Most of the observations used in this investigation were made by the author with the vacuum spectrograph of the McMath-Hulbert Observatory and with the McMath Solar telescope of the Kitt Peak National Observatory. Since the equipment of both observatories has been described elsewhere (McMath, 1956; Pierce, 1964), we will not discuss it further here. The spectrograph of the McMath-Hulbert Observatory was used in the 6th order in the single pass mode and the spectrograph of the Kitt Peak National Observatory was used in the 6th order in the double pass mode. All of the observations were made photoelectrically. The great majority of these were obtained at Kitt Peak.

Since we wished to study the center-limb behavior of profiles of CH lines, it was necessary to obtain an instrumental profile for the solar spectrograph at Kitt Peak. This was determined by tracing photoelectrically the line of Hg^{198} at $4358 \text{ \AA}$ using the same widths for the entrance and exit slits as were used in the CH observing program. The resulting instrumental profile was almost perfectly symmetrical and had a half-width of $0.0157 \text{ \AA}$ as compared with the width of the exit slit which corresponds to $0.123 \text{ \AA}$.

We also measured the intensity of the scattered light in this spectrograph. This was done by moving the exit slit of the spectrograph

in the direction of the dispersion until it was beyond the cutoff of the intermediate slit. With the exit slit in this position the photometer could receive only light beside the direct beam which is a measure of the spectrographic scattered light. In the 6th order at $4300 \text{ \AA}$ the intensity of the scattered light was about 3 per cent of the intensity of the continuum.

The Observed Lines

In this investigation we shall study lines in the $^2\Delta - ^2\Pi$ band system of the CH molecule. The lines in this system fall between $4130 \text{ \AA}$ and $4470 \text{ \AA}$. Out of the 284 available lines we selected 28 lines belonging to three vibration bands. The criteria for line selection were that they be listed as being unblended in Moore's list of CH lines present in the solar spectrum (Moore, 1959) and that they also appear unblended in the highly resolving McMath-Hulbert Atlas of the Solar Spectrum (unpublished). For the weakest lines we had to relax our criteria somewhat and include several lines which are on the wings of stronger atomic lines.

Observing Procedure (Kitt Peak)

Observations were made each clear morning as soon as the seeing became adequate. The best seeing usually occurred about one hour after sunrise. The periods of excellent seeing lasted about twenty to sixty minutes and were characterized by high contrast in the solar image and a very steady limb. During these periods the irregular shapes of the granules stood out clearly and excursions of the limb amounted to about one second of arc. Deteriorating seeing was characterized by the simultaneous increase in the magnitude of the limb excursions and

the loss of contrast in the image. As soon as the seeing started to deteriorate, it became impossible to observe at $\cos \theta = 0.1$. Shortly later it generally became difficult to observe closer to the limb than about $\cos \theta = 0.3$. The procedure followed was to observe at the extreme limb during periods of excellent seeing and to move closer to the center of the disc as the seeing became worse. Except for observations made at the center of the disc, most of the photoelectric tracings were obtained during periods of good to excellent seeing.

The widths of the entrance and exit slits of the spectrograph were set at 100 microns for all of the observations. Positioning of the solar image on the entrance slit was aided by a cardboard cutout upon which there were inscribed circles of the same radius as the solar image and which corresponded to various desired image positions. These were selected along the solar equator toward the east limb. Anywhere from 3 to 10 tracings were obtained for each line for each limb position. All lines were traced in both directions.

Reduction of the Observations

The equivalent widths of the observed CH lines were measured with a planimeter with each line being circled 10 or more times to reduce scale reading errors. In all cases we used a local continuum defined by the highest level of the continuum in the vicinity of the measured lines. A local continuum can be used for molecular lines because these lines are formed high in the solar photosphere above the layers where most of the continuum and wings of atomic lines are formed. Hence molecules absorb energy from a "continuum" made up of the true continuum minus the energy absorbed by wings of atomic lines. The

intensity of the local continuum was measured with respect to the intensity of the spectrographic scattered light. The measured values of the equivalent widths are given in table 1.

TABLE 1

EQUIVALENT WIDTHS OF THE CH LINES (mÅ)

λ $\cos \theta$	0,0 Band					
	1.0	0.6	0.5	0.3	0.2	0.1
4192.572	69.27	--	76.54	73.46	69.99	--
4210.967 _B	103.80*	106.75*	--	108.75*	100.90*	--
4217.240	99.84	105.13	106.56	103.29	100.38	78.94
4218.725	80.35	85.52	84.94	85.16	80.47	67.98
4248.944	62.98	67.47	68.66	68.96	--	57.21
4255.251	61.33	--	68.22	66.59	64.26	--
4267.389 _B	64.51	--	79.00	78.88	64.34	--
4281.972 _B	87.65*	89.25*	--	--	90.55*	--
4288.736	87.01	--	90.43	92.74	85.18	68.77
4348.338	46.20*	58.35*	--	63.90*	62.00*	--
4387.063	57.18	--	65.70	64.07	59.01	--
4388.870	51.78	--	57.29	55.99	56.51	--
λ $\cos \theta$	1,1 Band					
	1.0	0.6	0.5	0.3	0.2	0.1
4207.408 _B	62.73	--	66.24	69.93	65.18	--
4213.874	55.01	--	66.11	66.92	63.14	--
4216.599	51.78	57.11	59.73	60.03	60.73	45.77
4247.726	40.86	--	49.54	50.76	46.56	--
4253.004	35.96	--	42.26	42.98	41.92	36.04
4253.210	36.17	--	42.21	42.75	42.77	36.04

TABLE 1 continued

		1,1 Band continued					
$\cos \theta$ λ		1.0	0.6	0.5	0.3	0.2	0.1
4263.980		37.18 ⁺	--	47.52 ⁺	48.46 ⁺	--	--
4296.217		41.80 ⁺	--	57.16 ⁺	56.09 ⁺	--	--
4332.169		6.48	--	9.25	9.81	11.60	--
4378.913		49.00 ⁺	--	53.00 ⁺	54.20 ⁺	--	--
		2,2 Band					
4240.199		19.93	--	24.25	25.42	23.58	--
4248.055		27.41	--	34.54	34.72	33.71	--
4328.610		31.90	--	40.19	41.72	39.67	30.21
4329.340 _B		54.75	--	68.79	72.02	73.20	53.20
4335.274 _B		35.10	--	47.17	49.12	48.80	--
4348.636		4.72*	5.95*	6.30*	7.70*	8.08*	6.97

* McMath-Hulbert, by author
⁺ McMath-Hulbert Atlas of the Solar Spectrum, unpublished
 Kitt Peak, by author
 B Probably blended

The profiles of several lines were measured on a two dimensional measuring engine. The level of the spectrographic scattered light was the zero point for all measurements. The observed profiles were corrected for instrumental broadening by Bracewell's technique (Bracewell, 1955). As an example profiles of $\lambda 4248.944$ are shown for several limb positions in figure 4-11, page 57.

Error Analysis

Equivalent Widths

The observed equivalent width of a CH line can be represented by the formula

$$W = (A-B) \cdot d / I_c + S \quad 2-1$$

where A is the measured area of the line, B is a correction for blending by neighboring spectral lines, d is the dispersion of the photoelectric tracing, I_c is the intensity of the local continuum, and S is a systematic correction. If we assume as a first approximation that the parameters in equation 2-1 are independent, then we can define the error in the measured equivalent widths to be

$$\Delta W = \sqrt{\left[\frac{dW}{dA}\right]^2 (\Delta A)^2 + \left[\frac{dW}{dB}\right]^2 (\Delta B)^2 + \left[\frac{dW}{dd}\right]^2 (\Delta d)^2 + \left[\frac{dW}{dI_c}\right]^2 (\Delta I_c)^2 + \left[\frac{dW}{dS}\right]^2 (\Delta S)^2} \quad 2-2$$

From equations 2-1 and 2-2 we obtain

$$\frac{\Delta W}{W} = \sqrt{\left[\frac{\Delta A}{A-B}\right]^2 + \left[\frac{\Delta B}{A-B}\right]^2 + \left[\frac{\Delta d}{d}\right]^2 + \left[\frac{\Delta I_c}{I_c}\right]^2 + \left[\frac{dW}{dS}\right]^2 \left[\frac{\Delta S}{W}\right]^2} \quad 2-3$$

If we wish to use equation 2-3 to compute probable errors for the observed equivalent widths, it is necessary to know the magnitudes of the uncertainties in A, B, etc. Since the CH lines are situated in a rather crowded region of the solar spectrum, it is difficult to estimate accurately the uncertainty in the blending correction, ΔB , and in the intensity of the local continuum, ΔI_c . For the majority of the lines $\Delta B/(A-B)$ is probably of the order of 5 per cent and $\Delta I_c/I_c$ is of the order of 3 per cent. The quantity $\Delta A/(A-B)$, which determines how accurately the lines were planimeted, is about 2 per cent. The dispersion d is accurate to 1 per cent.

The remaining unknown in equation 2-3 is the quantity $(\delta W / \delta S) \cdot (\Delta S / W)$. The major systematic error in W is that caused by the uncertainty in the limb position of observations made near the edge of the solar disc. The limb position of a given observation is uncertain for three reasons: the effect of the finite length of the slit, seeing problems, and guiding errors. Problems of seeing and guiding introduce an uncertainty in the position of the slit of about 1 mm compared to an image diameter of about 800 mm (Kitt Peak). The finite length of the slit (14 mm at Kitt Peak) causes the center of the slit to be 0.62 mm closer to the center of the image than either end. These uncertainties mean that

$$0.183 \leq \cos \theta \leq 0.215 \text{ for } \cos \theta = 0.2$$

and

$$0.059 \leq \cos \theta \leq 0.128 \text{ for } \cos \theta = 0.1.$$

We can account for the effect on W of this uncertainty in limb position, if we define

$$\frac{\delta W}{\delta S} \Delta S = \frac{\delta W}{\delta \mu} \Delta \mu$$

where $\mu = \cos \theta$. The quantity $\delta W / \delta \mu$ can be estimated from the observations. The resulting values for $(\delta W / \delta S) \cdot (S / W)$ are 2 per cent at $\cos \theta = 0.2$ and 10 per cent at $\cos \theta = 0.1$.

If we substitute the above estimates into equation 2-3, we find that

$$\frac{\Delta W}{W} = 6.3 \text{ per cent for } \cos \theta = 0.3,$$

$$\frac{\Delta W}{W} = 6.6 \text{ per cent for } \cos \theta = 0.2,$$

and

$$\frac{\Delta W}{W} = 11.8 \text{ per cent for } \cos \theta = 0.1.$$

These errors do not apply to lines with equivalent widths less than about 20 mÅ. For such weak lines the measured area of the line is very sensitive to the placement of the local continuum. If we take this into consideration, the resulting error in the weak lines is about 20 to 30 per cent.

How accurate are the above error estimates? One way of testing this is to compare them with the random scatter,

$$0.6745 \cdot \sqrt{\frac{1}{N} \sum_{i=1}^N (W_i - \bar{W})^2},$$

in the measured equivalent widths. The quantity W_i is an individual measurement and $\bar{W}$ is the mean equivalent width determined from N tracings of the line. For observations obtained at Kitt Peak the magnitude of the random scatter averaged over all of the lines is

0.62 mÅ at $\cos \theta = 1.0$,

0.61 mÅ at $\cos \theta = 0.5$,

0.73 mÅ at $\cos \theta = 0.3$,

1.10 mÅ at $\cos \theta = 0.2$,

and

2.02 mÅ at $\cos \theta = 0.1$.

This means that for the average line, $W \approx 50$ mÅ, the random scatter in the observations is about one-third to one-fourth of the error predicted by equation 2-3. This suggests that the errors estimated by equation 2-3 may be too conservative. However, since the random error does not take into consideration systematic errors, it is not a true probable error. It is primarily a measure of the consistency of the measuring technique and provides a lower limit to the true error.

Another way of checking the accuracy of the measurements is

to compare them with those made by other investigators using different observations and measuring techniques. We have compared the equivalent widths of table 1 for the center of the solar disc with corresponding values given in the Utrecht catalog (Utrecht, 1960). This comparison is plotted in figure 2-1.

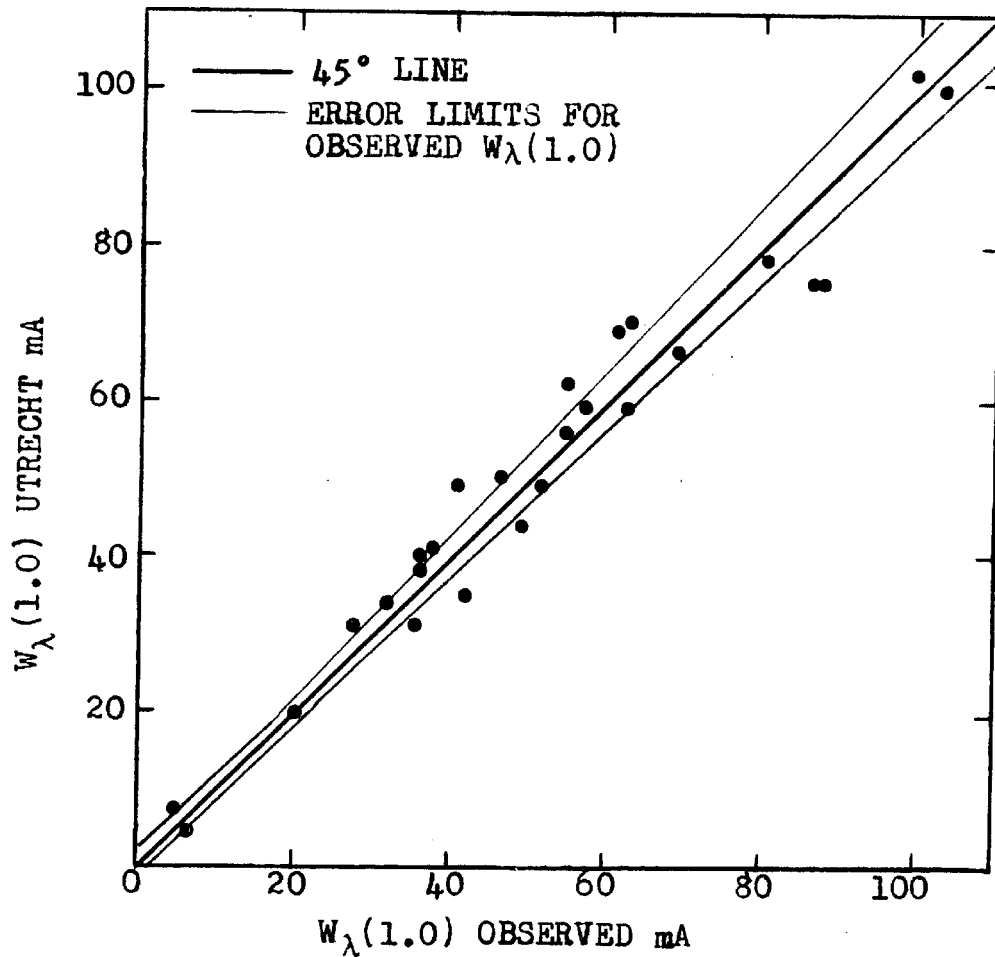


Figure 2-1.--A comparison between Utrecht equivalent widths and those in table 1.

A least squares analysis leads to the relation

$$W_{obs}(mA) = (-1.3 \pm 1.7) + (1.03 \pm 0.03) \cdot W_U(mA)$$

where W_{obs} and W_U are equivalent widths from table 1 and the Utrecht catalog respectively. This result indicates that there are apparently

no significant systematic errors in the equivalent widths used in this analysis.

The Profiles

The profiles of the CH lines are affected by several sources of error besides those mentioned above. For the observations obtained at Kitt Peak the recordings were made with too low linear dispersion on the paper, so that the profiles were slightly too narrow to be measured with high accuracy. A more serious problem was the poor mechanical condition of the entrance and exit slits of the spectrograph. The micrometers of both slits were calibrated at the beginning of the observing program. Unfortunately after most of the observations had been made, we found that the width of the entrance slit was varying from its set position by as much as 50 per cent. The width of the exit slit also varied, but only by about 20 per cent. This uncertainty in the widths of the spectrographic slits consequently reflects itself in the instrumental profile and leads to an inaccurate correction for instrumental broadening. Therefore we can expect errors of the order of a few percent in the central intensities of the observed profiles. The edges of the slit jaws of the spectrograph at Kitt Peak were also imperfect. However, this apparently did not affect the observations very much, since the profiles of $\lambda 4210.967$ obtained at the Kitt Peak and McMath-Hulbert Observatories were almost identical.

Since the effects of all of the above sources of error can be estimated only approximately, it is difficult to assign an accurate probable error to each point on the observed profiles. In Chapter IV we will discuss the profile of $\lambda 4248.944$. The random scatter in the

observations for this line is 1 per cent for $\cos\theta > 0.1$ and 2 per cent for $\cos\theta = 0.1$. There is, however, a possibility that the profiles are affected by systematic errors. The level of the local continuum may be uncertain by as much as 3 per cent. Furthermore, in the extreme wings neighboring spectral lines appear to introduce an uncertainty of about 3 to 5 per cent. These systematic errors are important because the observed profiles will be compared to theoretical profiles computed neglecting the influence of neighboring spectral lines. If we take all of the different sources of error into consideration, the net probable error in the profiles of $\lambda 4248.944$ is about ± 4 per cent.

CHAPTER III

THEORETICAL CONSIDERATIONS

The Theory of Absorption Lines

If we wish to use observations of molecule lines to study the physical conditions in the upper photosphere, we must first develop formulae for computing profiles and equivalent widths of spectral lines.

The flow of radiation in a stellar atmosphere can be described by the equation of transfer. For a plane parallel atmosphere, the equation of transfer

$$\mu \frac{dI_\lambda}{d\tau_\lambda} = I_\lambda(\mu, \tau_\lambda) - S_\lambda(\mu, \tau_\lambda) \quad 3-1$$

has the formal solution

$$I_\lambda(\mu, 0) = \int_0^\infty S_\lambda(\mu, t) e^{-t/\mu} dt/\mu \quad 3-2$$

where, following the usual notation,

I_λ = the monochromatic specific intensity of radiation per unit wavelength at wavelength λ ;

$\mu = \cos \theta$;

θ = the angle of radiation flow measured from the outward normal to the atmospheric surface ;

S_λ = the ratio of the emission and absorption coefficients at wavelength λ ;

and

τ_λ = the optical depth at wavelength λ .

The optical depth τ_λ is defined by

$$\tau_\lambda = \int_0^{t'} \kappa_\lambda \cdot \rho \cdot dt', \quad 3-3$$

where

κ_λ = the absorption coefficient at wavelength λ , per gram of stellar material,

ρ = the density of stellar material in gm/cm^3 ,

and

t' = the geometrical distance from a "surface" level of the sun measured inward normal to the surface.

The proper parameter for describing the behavior of absorption lines is the line depth r :

$$r(\Delta\lambda, \mu) = \frac{I_\lambda(\mu) - I_\lambda(\Delta\lambda, \mu)}{I_\lambda(\mu)}, \quad 3-4$$

where $I_\lambda(\mu)$ is the emergent intensity in the continuum and $I_\lambda(\Delta\lambda, \mu)$ is the emergent intensity in the line at a distance $\Delta\lambda$ from the line center. Before inserting the formal solution of the transfer equation into equation 3-4 we will apply the assumption of local thermodynamic equilibrium to the entire photosphere. This assumption implies that a single temperature completely determines all emission and absorption processes in a given volume element. Under this assumption

$$S_\lambda(\mu, \tau_\lambda) = B_\lambda(\tau_\lambda), \quad 3-5$$

where

$$B_\lambda(\tau_\lambda) = \frac{2hc^2}{\lambda^5} \cdot \left\{ \exp \left[hc/\lambda kT(\tau_\lambda) \right] - 1 \right\}^{-1} \quad 3-6$$

$T(\tau_\lambda)$ = the temperature at optical depth τ_λ in degrees Kelvin,

h = Planck's constant,

c = the speed of light,

and

k = Boltzmann's constant.

If we define the optical depth at 5000 Å, τ_0 , as the independent variable, it is possible to use equations 3-2, 3-4, and 3-5 to derive a theoretical expression for r (Aller, 1960):

$$r(\Delta\lambda, \mu) = \int_0^{\infty} \frac{\kappa_\ell(\Delta\lambda, \tau_0)}{\kappa_0(\tau_0)} e^{-\tau_\ell(\tau_0)/\mu} g_\lambda^\mu(\tau_0) d\tau_0/\mu, \quad 3-7$$

where

$\kappa_\ell(\Delta\lambda, \tau_0)$ = the line absorption coefficient per hydrogen particle at optical depth τ_0 corresponding to a distance $\Delta\lambda$ from line center,

$\kappa_0(\tau_0)$ = the continuous absorption coefficient per hydrogen particle at optical depth τ_0 ,

$$\tau_\ell(\tau_0) = \int_0^{\tau_0} \frac{\kappa_\ell(\Delta\lambda, \tau_0)}{\kappa_0(\tau_0)} d\tau_0, \quad 3-8$$

and

$$g_\lambda^\mu(\tau_0) = \frac{\int_0^{\infty} B_\lambda(t) e^{-t/\mu} dt/\mu - B_\lambda(\tau_0) e^{-\tau_0/\mu}}{\int_0^{\infty} B(t) e^{-t/\mu} dt/\mu} \quad 3-9$$

The weighting function $g_\lambda^\mu(\tau_0)$ is a function only of $T(\tau_0)$ and the wavelength λ . One advantage of using this function is that for a series of lines in a spectral region 50 to 100 Å wide a single weighting function can be used. This saves a large amount of computing time.

The line depth $r(\Delta\lambda, \mu)$ is an extremely fine tool with which to study conditions in the solar atmosphere. Somewhat more general is

the integral over the line depth, the total absorption or equivalent width $W_\lambda(\mu)$:

$$W_\lambda(\mu) = \int_{-\infty}^{\infty} r(\Delta\lambda, \mu) d(\Delta\lambda). \quad 3-10$$

It expresses the total energy that is subtracted from the continuum by an absorption line. This parameter is useful for rough analyses of stellar atmospheres, since equivalent widths are much easier to measure than are line profiles.

The physical conditions in the photosphere may be represented by a model which gives the electron temperature, electron pressure, coefficient of continuous opacity, and the radial and tangential components of the microturbulence and macroturbulence as a function of optical depth. We would like to express equation 3-7 in terms of these parameters and write it in a form that will permit efficient computing procedures. Furthermore, since it takes considerable time and effort to write a computer program for calculating line profiles and get it working properly, we will develop a procedure that can be used for either atomic or molecular lines. The approach which we shall use is similar to one described in a paper by Aller, Elste, and Jugaku (1957). This method was developed for computation of atomic lines and, as will be shown below, can be easily modified to handle molecular lines.

For atomic lines the line absorption coefficient per absorbing atom is

$$\alpha_o = \frac{\sqrt{\pi} e^2}{mc} f_\lambda \frac{H(\alpha, v)}{\sqrt{\dots}}, \quad 3-11$$

where

e = the electronic charge,

m = the electronic mass,

f = the oscillator strength of the line being computed,

λ = the wavelength of the line,

$$\sqrt{\dots} = \sqrt{\xi^2 + \xi_{th}^2},$$

$$\xi_{th}^2 = \frac{2RT}{\mu_{at}} = \frac{83.83}{\theta \cdot \mu_{at}},$$

ξ_{th} = the thermal velocity of the atom or molecule producing the line,

μ_{at} = the molecular weight of the atom or molecule,

θ = 5040/T,

and

ξ = the microturbulent velocity, which behaves like additional thermal motion, and results from the nonthermal motion of eddies in the photosphere whose sizes are small in comparison with the size of the region of line formation.

The wavelength-dependent part of the line absorption coefficient is given by

$$H(\alpha, v) = \frac{\alpha}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{\alpha^2 + (v - y)^2} dy,$$

3-12

where

$$\alpha = \frac{\Gamma \lambda}{4 \pi \sqrt{\dots}},$$

$$v = \frac{\Delta \lambda + s \cdot \lambda / c}{\Delta \lambda_D} = \frac{\Delta \lambda + s \cdot \lambda / c}{\lambda \sqrt{\dots} / c},$$

s = the macroturbulent velocity, which enters as a Doppler shift of the line, and is the result of motions of the entire line forming region,

and

Γ = the total damping constant.

From equations 3-7 and 3-11 we have:

$$r(\Delta\lambda, \mu) = \int_0^{\infty} \frac{n_{r,s}}{N_H K_0} (f\lambda)_{r,s} \frac{H(\alpha, v) \sqrt{\pi} e^2}{\sqrt{\dots} mc} e^{-\tau_e/\mu} g_{\lambda}^{\mu}(\tau_0) d\tau_0/\mu, \quad 3-13$$

where $n_{r,s}$ is the number of atoms per cm^3 with electrons in the lower level r,s of the transition. If we change the integration variable from τ_0 to $x = \log \tau_0$, we obtain:

$$r(\Delta\lambda, \mu) = \int_{-\infty}^{\infty} \frac{N_{el} 10^x n_{r,s} (gf\lambda)_{r,s} \sqrt{\pi} e^2}{N_H K_0 g_{r,s} \sum n_r \text{Mod} mc} \cdot \frac{H(\alpha, v)}{\sqrt{\dots}} e^{-\tau_e/\mu} g_{\lambda}^{\mu}(x) dx/\mu, \quad 3-14$$

where

$$\tau_e/\mu = \int_{-\infty}^x \frac{N_{el} 10^x n_{r,s} (gf\lambda)_{r,s} \sqrt{\pi} e^2 H(\alpha, v) dx}{N_H K_0 g_{r,s} \sum n_r \text{Mod} mc \sqrt{\dots} \mu}, \quad 3-15$$

N_{el} = the number of atoms per cm^3 for the element "el" summed over all ionization states,

N_H = the number of hydrogen atoms per cm^3 summed over all ionization states,

n_r = the number of atoms per cm^3 of element "el" which are in the r th stage of ionization,

$\text{Mod} = 0.43429448,$

and

$g_{r,s}$ = the statistical weight of the sth excitation level in the rth ionization state.

If we separate out those quantities which are depth-independent from those quantities which depend on depth, we can write the final expression for the line depth

$$r(\Delta\lambda, \mu) = \int_{-\infty}^{\infty} A \cdot Z(x) \frac{H(\alpha, \nu)}{\sqrt{\dots}} \exp \left[- \int_{-\infty}^x A \cdot Z(x) \frac{H(\alpha, \nu)}{\sqrt{\dots} \mu} dx \right] g_{\lambda}^{\mu}(x) \frac{dx}{\mu}, \quad 3-16$$

with

$$A = \frac{N_{el}}{N_H} (gf\lambda)_{r,s} \frac{\sqrt{\pi} e^2}{mc} \frac{1}{\text{Mod}} \quad 3-17$$

and

$$Z(x) = \frac{1}{N \cdot \sum n_r} \frac{n_{r,s}}{g_{r,s}} 10^x \quad 3-18$$

Let us examine the function $Z(x)$ more closely. Under the assumption of local thermodynamic equilibrium the excitation rate is

$$\frac{n_{r,s}}{n_r} = \frac{g_{r,s}}{u_r} 10^{-\theta \chi_{r,s}}, \quad 3-19$$

where u_r is the partition function for the rth ionization state of the element in question and $\chi_{r,s}$ is the excitation potential of the line.

If we define the rth state of ionization as being the most abundant ionization state, we can write

$$\frac{n_{r,s}}{g_{r,s} \sum n_r} = \frac{n_{r,s}}{g_{r,s} n_r \left(\dots + \frac{n_{r-1}}{n_r} + 1 + \frac{n_{r+1}}{n_r} + \dots \right)} \quad 3-20$$

From equations 3-19 and 3-20 we find that

$$\frac{n_{r,s}}{g_{r,s} \sum n_r} = \frac{10^{-\theta \chi_{r,s}}}{u_r \frac{n_{r-1}}{n_r} + u_r + u_r \frac{n_{r+1}}{n_r}} \quad 3-21$$

We also define the quantity U_r ,

$$U_r = u_r \frac{n_{r-1}}{n_r} + u_r + u_r \frac{n_{r+1}}{n_r} \quad 3-22$$

For the number ratio in two successive ionization states under equilibrium conditions the Saha equation gives:

$$\log \frac{n_{r+1}}{n_r} = \log \frac{u_{r+1}}{u_r} - \chi_r \cdot \theta - \frac{5}{2} \log \theta + 9.0801 - \log P_e, \quad 3-23$$

which allows us to write equation 3-22 in the form:

$$\begin{aligned} U_r = & 10^{\log u_{r-1} + \chi_{r-1} \cdot \theta - (9.0801 - 5/2 \log \theta - \log P_e)} \\ & + 10^{\log u_r} \\ & + 10^{\log u_{r+1} - \chi_r \theta + (9.0801 - 5/2 \log \theta - \log P_e)}. \end{aligned} \quad 3-24$$

Using the definition of U_r we can write equation 3-21 as

$$\frac{n_{r,s}}{g_{r,s} \sum n_r} = \frac{10^{-\theta \chi_{r,s}}}{U_r} \quad 3-25$$

Inserting equation 3-25 into equation 3-18 and writing it in logarithmic form gives:

$$\log Z(x) = x - \log N_o - \log U_r - \theta \chi_{r,s} \quad 3-26$$

If we have a temperature-pressure model and a turbulence model, we can use equations 3-9, 3-12, 3-17, 3-24, and 3-26 in 3-16 to compute theoretical profiles of atomic lines. Our next step is to derive a

similar set of expressions for molecular lines and put them in such a form that profiles of both atomic and molecular lines are obtained with equal ease using essentially the same computing procedure.

If we examine equations 3-16, 3-17, and 3-18, we note that the quantity which will be different for atoms and molecules is

$(N_{el} \cdot n_{r,s}) / (N_H g_{r,s} \sum n_r)$. Since we are interested primarily in the CH molecule, we will derive the corresponding expression for this molecule.

A similar derivation can be used for other molecules. In place of the atomic line parameter $n_{r,s}$ we have $n_{v,K,e}$ which is the number of molecules excited to the lower level of the desired transition. The subscripts v and K are the vibrational and rotational quantum numbers of the lower level and the subscript e represents the electronic lower level.

If we assume local thermodynamic equilibrium, we get from the Boltzmann equation the excitation ratio:

$$\frac{n_{v,K,e}}{n_{CH}} = \frac{g_{v,K,e}}{u_{CH}} \cdot e^{- (E_e + E_v + E_r)/kT} \quad 3-27a$$

$$= \frac{g_{v,K,e}}{u_{CH}} \cdot e^{- E_t/kT} , \quad 3-27b$$

where

E_e = the electronic energy above the ground level,

E_v = the vibrational energy of the lower level of the transition
 $= hc \cdot [w_e(v + \frac{1}{2}) - w_e x_e(v + \frac{1}{2})]$

E_r = the rotational energy of the lower level of the transition
 $= hc [B_e - \alpha_e(v + \frac{1}{2})] \cdot K(K+1) - hc [D_e - \beta_e(v + \frac{1}{2})] \cdot K^2(K+1)^2$,

$E_t = E_e + E_v + E_r$,

and $B_e, \alpha_e, w_e, \beta_e, D_e$, and $w_e x_e$ are the appropriate rotational and

vibrational constants (Hertzberg, 1950).

The dissociation of molecules under equilibrium conditions is described by the equation

$$\frac{n_C \cdot n_H}{n_{CH}} = \frac{u_C u_H}{u_{CH}} \left(\frac{2\pi M k T}{h^2} \right)^{3/2} e^{-D/kT}, \quad 3-28$$

where

D = the dissociation energy,

n_C = the number of neutral carbon atoms per cm^3 ,

n_H = the number of neutral hydrogen atoms per cm^3 ,

n_{CH} = the number of CH molecules per cm^3 ,

$$M_{CH} = \frac{M_C \cdot M_H}{M_{CH}}$$

M_i = the mass of atom or molecule i ,

u_C = the partition function of neutral carbon,

u_H = the partition function of neutral hydrogen,

and

u_{CH} = the partition function of the CH molecule.

From equations 3-27, and 3-28 we obtain the following expression for $n_{v,K,e}$:

$$n_{v,K,e} = g_{v,K,e} \frac{n_C}{u_C} \frac{n_H}{u_H} \left(\frac{2\pi M k T}{h^2} \right)^{-3/2} e^{+(D-E_t)/kT} \quad 3-29$$

We now define the quantity A exactly as we did in the atomic case (equation 3-17) with $N_{e1}/N_H = N_C/N_H$, where N_C/N_H is the abundance of carbon. From equations 3-17, 3-18, and 3-29 we find that the quantity $Z(x)$ for CH becomes

$$Z(x) = \frac{10^x}{K_0} \sum \frac{n_C}{n_{r_c} u_C} \frac{n_H}{n_{r_h} u_H} \left(\frac{2\pi M k T}{h^2} \right)^{-3/2} e^{+(D-E_t)/kT} \quad 3-30$$

Furthermore, if we define

$$\log Z(x) = x - \log K_0 + (D' - \chi_t) \cdot \theta - \log U_{CH} , \quad 3-31$$

where

$$D' = 6.24 \cdot 10^{11} \cdot D$$

is the dissociation energy in electron volts and

$$\chi_t = 6.24 \cdot 10^{11} \cdot E_t$$

is the total energy of the lower level of the desired transition in electron volts; then the quantity U_{CH} must be defined as

$$U_{CH} = u_C \sum \frac{n_{r_c}}{n_C} \frac{u_H}{n_H} \left(\frac{2\pi m k T}{h^2} \right)^{3/2} . \quad 3-32$$

If we compare equation 3-32 with equation 3-22 we see that

$$U_{CH} = u_C \frac{u_H}{n_H} \left(\frac{2\pi m k T}{h^2} \right)^{3/2} . \quad 3-33$$

Now we have to express the number of hydrogen atoms per cm^3 , n_H , in terms of the gas pressure P_g and electron pressure P_e . By definition

$$\begin{aligned} P_g &= P_m + P_H + P_e \\ &= P_H (\sum \epsilon_i + 1) + P_e , \end{aligned} \quad 3-34$$

where P_m is the partial pressure of all of the elements except hydrogen, P_H is the partial pressure of hydrogen, and

$$\sum \epsilon_i = \sum N_i / N_H ,$$

N_i / N_H being the abundance of the element i relative to hydrogen. From equation 3-34 we find that

$$P_H = \frac{P_g - P_e}{1 + \sum \epsilon_i} = n_H k T . \quad 3-35$$

Here we have assumed that n_H , the number of hydrogen atoms per cm^3 , equals the total number of hydrogen particles per cm^3 . This is a valid assumption because only a negligible fraction of hydrogen atoms are ionized in the upper layers of the photosphere.

If we substitute the expression for n_H given by equation 3-35 into equation 3-33 and assume $P_g \gg P_e$ as is the case throughout the photosphere, the resulting expression for U_{CH} is

$$U_{CH} = U_C \frac{n_H}{P_g} (1 + \sum \epsilon_i) \left(\frac{2\pi M}{h^2} \right)^{3/2} (kT)^{5/2} \quad 3-36$$

$$= U_C \cdot 10^{(13.9786 - 2.5 \log \theta - \log P_g)}.$$

Thus we find that it is possible to develop a procedure which can be used for computing profiles of either atomic or molecular lines. The only major difference between computing profiles of neutral carbon lines and CH lines is in the difference between the quantity U_C for carbon as given by equation 3-24 and the corresponding expression U_{CH} given by equation 3-36. Also instead of $\chi_{r,s}$ the quantity $(D' - \chi_t)$ must be used in the equation for $Z(x)$ (equations 3-26 and 3-31).

Since the computation of profiles by hand would be a time consuming and laborious task, a computer program was written in order that we might take advantage of the available high-speed IBM 7090 computer. This program is described briefly in Appendix I.

The Oscillator Strength of CH

In order to evaluate the quantity A (equation 3-17), which contains all of the depth-independent terms used in computing a line profile, it is necessary to know the f -value of the particular CH line being computed. The f -value of a specific vibration-rotation line in a

given electronic transition is (Hertzberg, 1950)

$$f(\text{line}) = f_{\text{CH}} \cdot \left(\int \psi_{\nu'}^* \cdot \psi_{\nu} \cdot dr \right)^2 \cdot \frac{S_{J''}}{2J'' + 1} \quad 3-37$$

where

f_{CH} is the oscillator strength of the entire $\Delta - \pi$ band system,

$\int \psi_{\nu'}^* \cdot \psi_{\nu} \cdot dr$ is the overlap integral or vibrational factor,

and

$\frac{S_{J''}}{2J'' + 1}$ is the rotational factor.

The overlap integrals used were computed from quantum mechanics by Pillow (1955). The rotational factors were evaluated by using the formulae given by Mulliken (1927).

The Formation of Molecules Other than CH

Implicit in the above derivation is the assumption that molecular formation does not significantly reduce the number of neutral carbon and hydrogen atoms in the solar photosphere. How adequate is this assumption?

In studies of molecular formation in stellar atmospheres the procedure developed by Russell (1934) is often used. We define a fictitious pressure P_A of element A as the pressure that atoms of this element would exert if no molecules containing this element were formed. Then by definition

$$P_A' = P_A + \sum_i P_{AB_i} \quad 3-38$$

where P_A is the partial pressure of the unbound atoms and P_{AB_i} is the

partial pressure of molecule AB_i . We also define the dissociation constant K_{AB} :

$$K_{AB} = \frac{P_A P_B}{P_{AB}}. \quad 3-39$$

If we refer to equation 3-28 we see that

$$K_{AB}(T) = \frac{n_A n_B}{n_{AB}} kT = \frac{u_A u_B}{u_{AB}} \left(\frac{2\pi m_{AB}}{h^2} \right)^{3/2} (kT)^{5/2} e^{-D_{AB}/kT}, \quad 3-40$$

where all of the variables have definitions similar to those in equation 3-28. Tables of $K_{AB}(T)$ have been published by several authors (e.g. Russell, 1934; Pecker and Peuchot, 1956; Stanger, 1964). Once a set of equations of the form 3-38 have been set up, they can be solved simultaneously by an iterative process for the partial pressures of the neutral atoms and molecules.

The most extensive investigation of molecular formation in the solar photosphere is that of de Jager and Neven (1956). They found that the number of neutral carbon and hydrogen atoms in the photosphere is not affected very much by molecular formation. De Jager and Neven based their work on dissociation constants determined by Pecker and Peuchot (1956).

Recent computations by Stanger (1963) indicate that the dissociation constant for CO is a factor of 30 smaller than the value given by Pecker and Peuchot (1956). We have confirmed Stanger's value by using the expression for $K_{CO}(T)$ given by Newkirk (1953). Newkirk's formula, which appears to be correct, is

$$\log K_{CO}(T) = -\frac{5040}{T} D_{CO} + \frac{3}{2} \log T + \log(1 - e^{-3107.17/T}) + 8.022 \quad 3-41$$

where $D_{CO} = 11.1$ electron volts.

If we use values of $K_{CO}(T)$ given by equation 3-41, we find that CO formation does significantly affect the population of neutral carbon atoms in the upper photosphere. Since the partial pressures of CH, CN, C_2 , etc. are much lower than that of CO, we can use equation 3-38 to write:

$$P'_C = P_C (1 + P_O / K_{CO}). \quad 3-42$$

Similarly for oxygen we obtain:

$$P'_O = P_O (1 + P_C / K_{CO}). \quad 3-43$$

We can solve equations 3-42 and 3-43 by an iterative process and find $P_C/P'_C = n_C / (n_C + n_{CO})$, where the quantity n_i is the number of atoms or molecules of type i per cm^3 . Values of the ratio P_C/P'_C computed for Elste's model (see figure 1-1) are plotted as a function of $\log \tau_o$ in figure 3-1.

Since CH and CO molecules are formed in much the same layers of the photosphere, it is possible that CO formation will influence the behavior of CH spectral lines. We can account for this by introducing the factor P_C/P'_C into equation 3-36, so that

$$U_{CH} = U_C \frac{P'_C}{P_C} 10^{(13.9786 - 2.5 \log \theta - \log P_g)} \quad 3-44$$

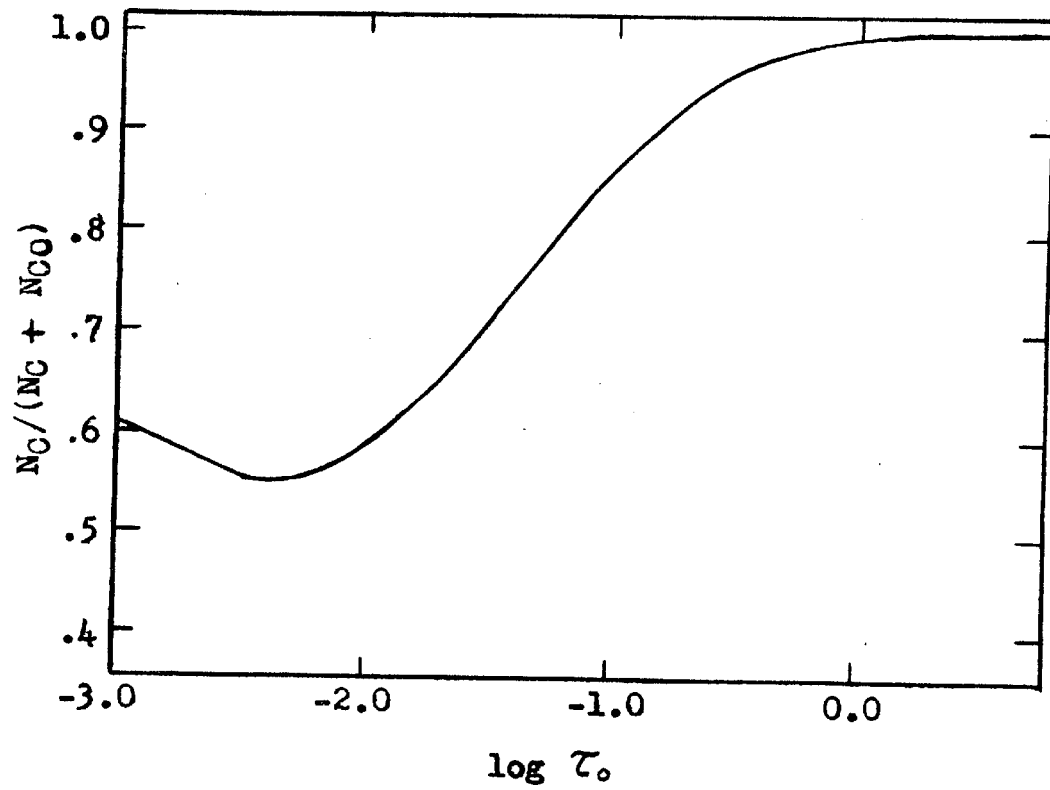


Figure 3-1.--The influence of CO formation on the number of neutral carbon atoms in the photosphere (for Elste's model).

CHAPTER IV

THE ANALYSIS OF THE OBSERVATIONS

At the present time the physical conditions in the solar photosphere can be represented relatively well by a homogeneous model in which the atmospheric parameters are a function of depth only. Nevertheless, the observation of granular contrast on the solar disc is evidence for the existence of inhomogeneities in the photosphere not considered in the above model. For this reason we feel that it will be useful to analyse the CH observations in two ways, first on the basis of a homogeneous model and secondly through an inhomogeneous three stream model.

An Analysis of the CH Observations

Based on a Homogeneous Model

The Adopted Temperature-pressure Model

Typical photospheric temperature-pressure models give the electron temperature and pressure, total gas pressure, and coefficient of continuous opacity as a function of optical depth at $5000 \text{ \AA}$. Methods for computing such models can be found in standard astrophysics texts (e.g. Aller, 1963).

The major problem in deriving a photospheric model is the accurate determination of the electron temperature as a function of depth. The most straight forward way of doing this is through use of

limb darkening observations of the spectral continuum. This method gives the relationship between depth and electron temperature directly. Another way of determining the electron temperature is through use of center-limb observations of spectral lines. The latter method depends upon the assumption of local thermodynamic equilibrium, that is, that the local ionization and excitation temperatures are equal to the local electron temperature. Theoretical arguments indicate that this assumption may not be valid in the upper layers of the photosphere (e.g. Böhm, 1960). Therefore, since observations of the continuum give the depth-dependence of the electron temperature directly, temperature models based on such observations are to be preferred.

In our interpretation of the CH observations we have used a recent photospheric model developed from limb darkening observations. This model, Elste's model 10 (Elste, 1964), takes into account the continuous absorption by heavy elements in the blue and violet spectral regions as well as that by the various hydrogenic sources of opacity. This model is an improved version of Elste's model 9. The latter model was used by David (1961) in a study of hydrogen Balmer lines and by Mattig and Schröter (1961) in an interpretation of observations made at the extreme limb of the wings of the Na D lines and the continuum at 5893 Å. It was also used by Mugglestone (1964) in a study of the wings of the Na D lines. As is apparent in figure 1-2, page 8, the temperature variation in Elste's model 10 is similar to the temperature run in models which have been used to explain CO, CN, and MgH observations. Elste's model 10 is given in table 2.

The Adopted Microturbulence Model

One of the purposes of this investigation is to study the

TABLE 2

ELSTE'S PHOTOSPHERIC TEMPERATURE-PRESSURE MODEL 10

$\log \tau_0$	θ	$\log P_e$	$\log P_g$	$\log \kappa_0/P_e$
-3.00	1.135	-.6679	3.7041	-24.8817
-2.80	1.131	-.5971	3.7825	-24.8919
-2.60	1.125	-.4907	3.9002	-24.9067
-2.40	1.118	-.3846	4.0158	-24.9225
-2.20	1.107	-.2725	4.1300	-24.9443
-2.00	1.093	-.1554	4.2432	-24.9708
-1.80	1.076	-.0329	4.3554	-25.0021
-1.60	1.056	.0955	4.4668	-25.0384
-1.40	1.034	.2288	4.5772	-25.0782
-1.20	1.009	.3707	4.6864	-25.1232
-1.00	.982	.5223	4.7937	-25.1718
-.80	.952	.6917	4.8976	-25.2257
-.60	.918	.8918	4.9951	-25.2867
-.40	.879	1.1385	5.0822	-25.3571
-.20	.834	1.4459	5.1546	-25.4400
.00	.784	1.8086	5.2108	-25.5346
.20	.730	2.2138	5.2521	-25.6382
.40	.675	2.6339	5.2815	-25.7405
.60	.633	2.9601	5.3038	-25.8113
.80	.603	3.1970	5.3240	-25.8542
1.00	.584	3.3517	5.3449	-25.8773
1.20	.572	3.4495	5.3582	-25.8896

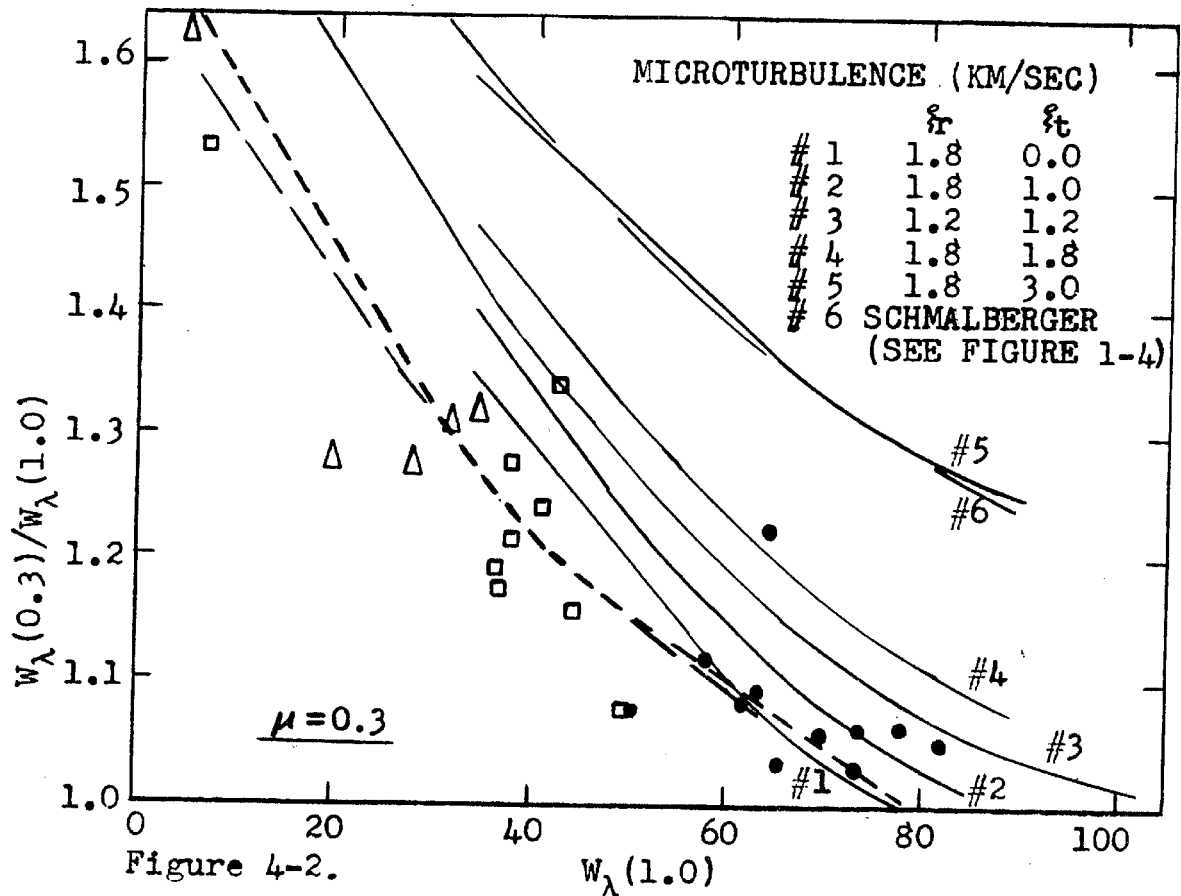
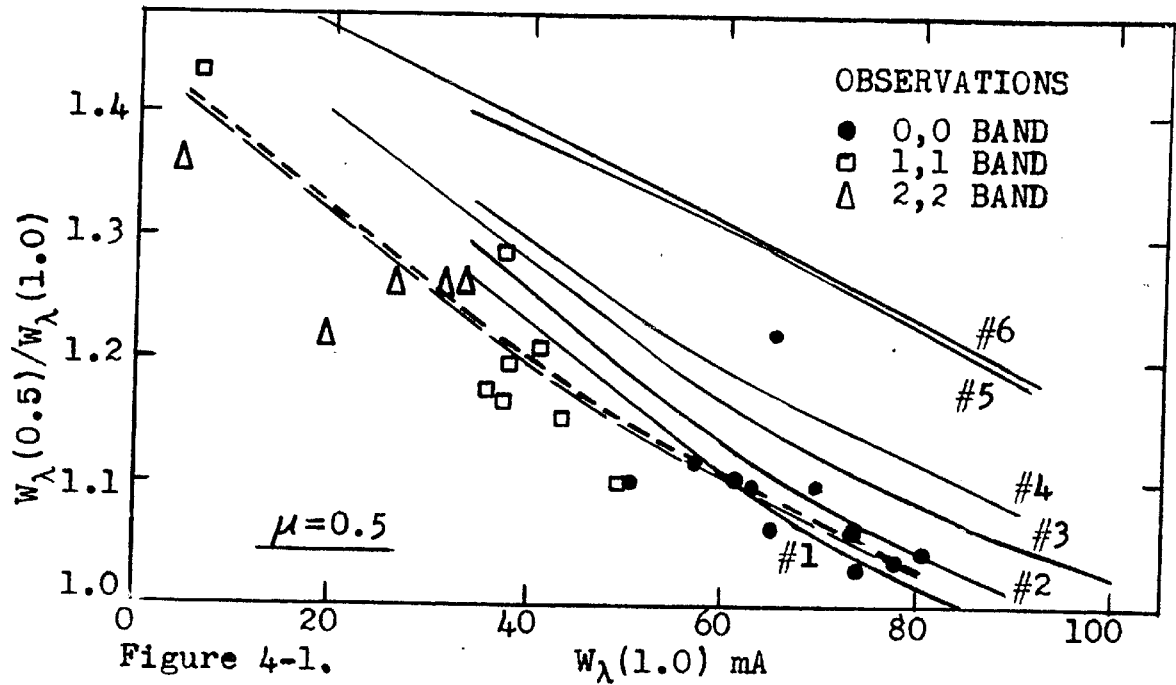
microturbulence in the upper layers of the photosphere. A convenient way of doing this is to compare the computed and observed behavior of $W_\lambda(\mu)/W_\lambda(1.0)$ when this ratio is plotted as a function of $W_\lambda(1.0)$. Such graphs are useful because they display simultaneously the center-limb behavior of a large number of both weak and strong lines. Furthermore, the observed values of $W_\lambda(\mu)/W_\lambda(1.0)$ are relatively insensitive to errors in the choice of the local continuum and in the correction for blending.

The observed values of this ratio are plotted in figures 4-1 and 4-2. Some difficulty was caused by the fact that many of the CH lines are doublets. Since a doublet has a center-limb behavior different from a singlet of the same strength, it was necessary to allow for this effect. The method for doing this is described in Appendix II. We have drawn as lines in figures 4-1 and 4-2 the dependence of $W_\lambda(\mu)/W_\lambda(1.0)$ on $W_\lambda(1.0)$ computed for several microturbulence models using Elste's temperature-pressure model and assuming local thermodynamic equilibrium. In these preliminary computations the effect of CO formation was neglected.

As is apparent in figures 4-1 and 4-2, the computed center-limb behavior of the CH equivalent widths is sensitive to the assumed values of ξ_r and ξ_t in the microturbulence model. The reason for this is that the equivalent widths of absorption lines of moderate strength depend upon the magnitude of the line-of-sight Doppler velocity $\xi(\mu)$. This velocity is given by

$$\xi(\mu) = \sqrt{\xi_t^2 - (\xi_t^2 - \xi_r^2) \cdot \mu^2 + \xi_{th}^2}$$

where ξ_t and ξ_r are the tangential and radial components of the



Figures 4-1 and 4-2.-- The effect of microturbulence on the behavior of $W_{\lambda}(\mu)/W_{\lambda}(1.0)$. (The long and short dashed lines represent the results of the final computations made with and without CO formation respectively.)

microturbulence and ξ_{th} is the thermal velocity of the CH molecules. Since the magnitudes of the thermal and microturbulent velocities are comparable in the solar photosphere, the value of $\xi(\mu)$ depends rather critically on ξ_r and ξ_t . Therefore, the computed value of $w_\lambda(\mu)/w_\lambda(1.0)$ is sensitive to the assumed microturbulence model.

Past investigations of photospheric turbulence (see Chapter I) indicate that the microturbulence model in the upper photosphere lies somewhere between models #3 and #6 in figure 4-2. The simplest of these that comes close to predicting the observed center-limb behavior of the CH equivalent widths is a microturbulence which is isotropic and independent of depth.

Departures from Local Thermodynamic

Equilibrium

Preliminary computations indicated that it would be difficult to explain the center-limb behavior of the CH equivalent widths with the assumption of local thermodynamic equilibrium, Elste's temperature-pressure model, and a microturbulence model that is consistent with other observations. In general the computed values of $w_\lambda(\mu)/w_\lambda(1.0)$ were systematically larger than the observed values. This is shown in figures 4-1 and 4-2 by lines #3 through #6. The effect of formation of CO molecules was neglected in the computation of these lines. Even though CO formation affects the population of neutral carbon atoms considerably for $\log \tau < -1.0$ (see figure 3-1, page 40), there is surprisingly little change in the behavior of the CH equivalent widths if it is included. This is illustrated in figures 4-3 and 4-4 where we have compared the behavior of $w_\lambda(\mu)/w_\lambda(1.0)$ computed with and without CO formation for Elste's temperature-pressure model and a microturbulence

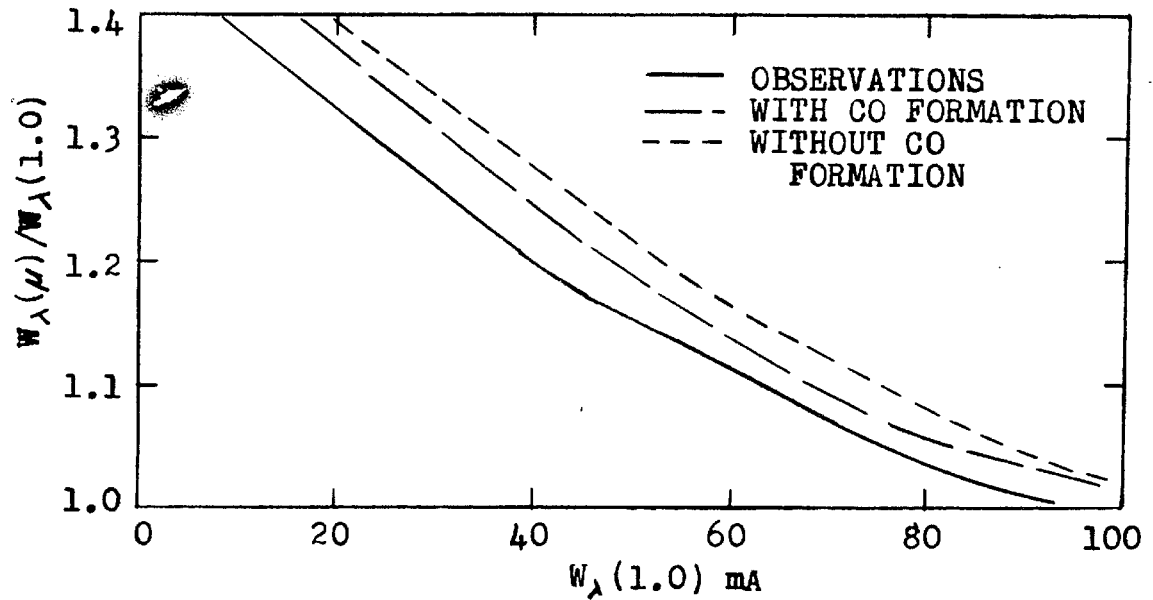


Figure 4-3.--The effect of CO formation on the behavior of $W_{\lambda}(\mu)/W_{\lambda}(1.0)$ for $\mu = 0.5$.

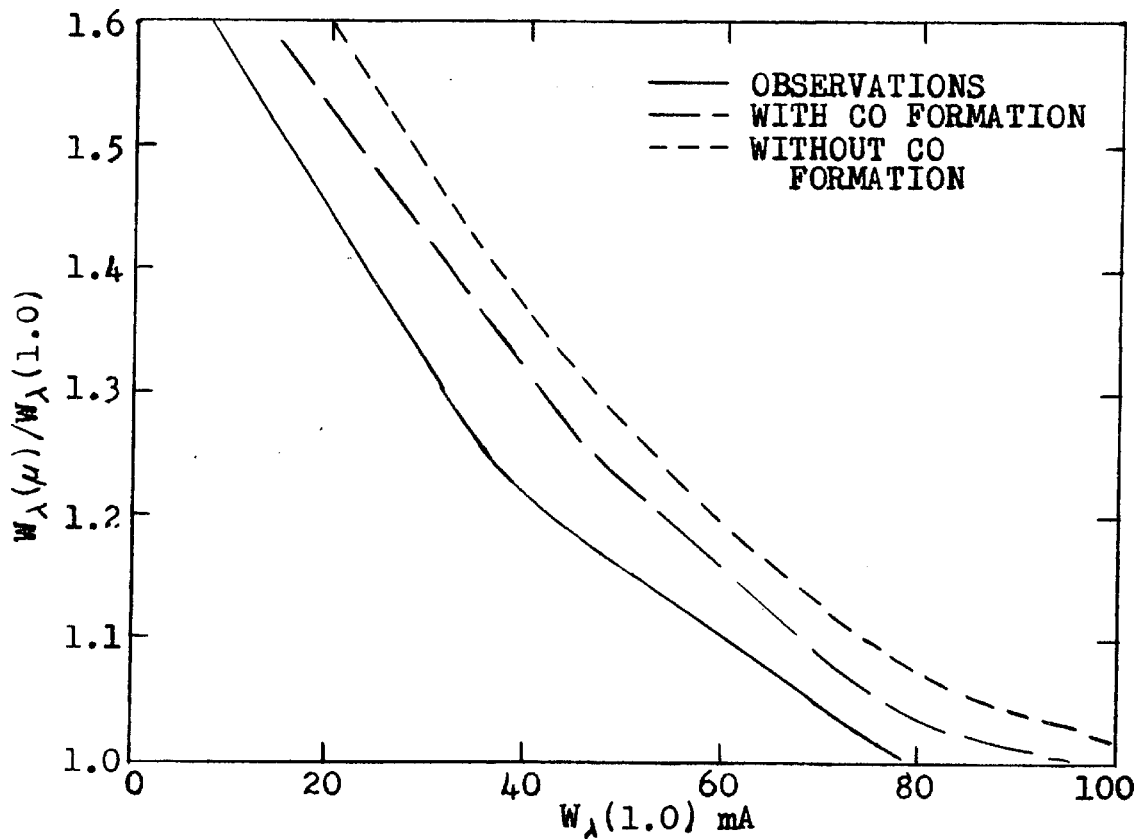


Figure 4-4.-- The effect of CO formation on the behavior of $W_{\lambda}(\mu)/W_{\lambda}(1.0)$ for $\mu = 0.3$.

which is isotropic, independent of depth and has a velocity of 1.2 km/sec. Although the inclusion of CO formation does improve the agreement between the computations and the observations, the computed values of $W_{\lambda}(\mu)/W_{\lambda}(1.0)$ still fall systematically above the observed values. This suggests that the CH lines may be affected by departures from local thermodynamic equilibrium.

A simple way of treating the problem of non-local thermodynamic equilibrium is to assume that formulae such as Planck's law, Boltzmann's equation, etc., are valid in a region with departures from local thermodynamic equilibrium but that the temperatures used in each formula may be different. We may assume that in a stellar atmosphere the velocity distributions of the electrons and atoms are Maxwellian and that the kinetic temperatures of the atoms are equal to the kinetic temperature of the electrons (Böhm, 1960). We may also assume that the source function for the continuum is given by the Planck function using the local electron temperature (Swihart, 1956; Pagel, 1956; Thomas and Athay, 1961).

The next question is whether or not the local ionization, excitation, and dissociation temperatures will be equal to the local electron temperature. These temperatures will be equal if collisional excitation, ionization, and dissociation processes are dominant over the corresponding radiative processes. Böhm (1954, 1960) has studied this problem in some detail for atomic excitation and ionization.

The first problem is the determination of the ratio of the number of collisional excitations per second to the number of radiative excitations per second for rotational and vibrational energy levels in the $^2\Pi$ electronic level. If we apply the appropriate formulae given by Böhm (1954, 1960), we find it probable that the populations of these

levels are determined by collisional processes for conditions similar to those in the upper photosphere. Therefore, we shall assume that the local rotational and vibrational temperatures of the CH molecule are equal to the local electron temperature.

The second problem was the evaluation of the ratio of the number of radiative to collisional dissociations per second. Since the cross sections necessary to compute this ratio are unknown, one cannot say a priori what its value will be. If one assumes as a very crude first approximation that Böhm's formula for ionization (Böhm, 1954, 1960) can be applied to dissociation, then the value of this ratio is about 3 at $\log \tau_0 = -1.0$ and 30 at $\log \tau_0 = -3.0$. These values imply that the dissociation of the CH molecule may be influenced by the anisotropy of the radiation field in the upper photosphere.

In order to investigate this effect in more detail we assumed that the CH molecules are radiatively dissociated and computed dissociation temperatures for Elste's model. The computations are discussed in Appendix III and the resulting temperatures are plotted as a function of $\log \tau_0$ in figure 4-5. These temperatures are higher than the corresponding electron temperatures. Thus it appears that if radiative dissociation is important, the CH molecule will be affected by departures from local thermodynamic equilibrium.

The third problem is whether or not the source function of the CH lines is identical to the source function of the continuum. These functions will be identical if the local excitation temperature governing the relative populations of electrons in the $^2\Delta$ and $^2\Pi$ electronic levels is equal to the local electron temperature. It is difficult to predict if these two temperatures will be equal because the $^2\Delta$ electronic level

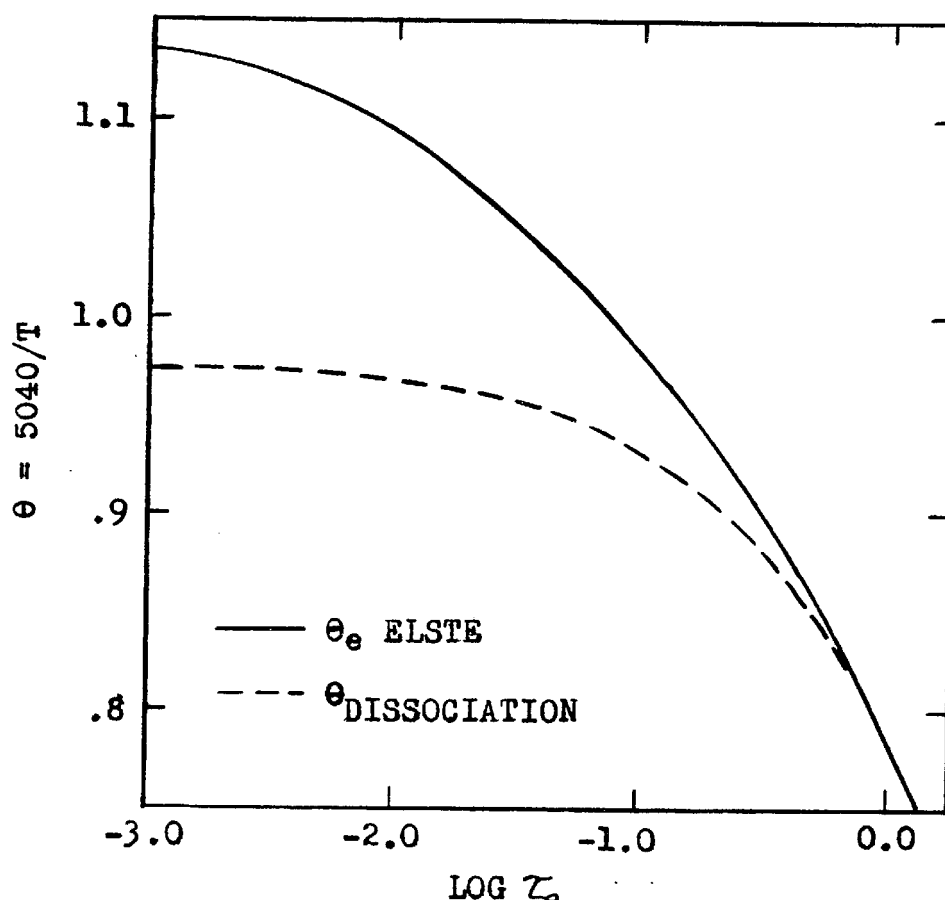


Figure 4-5.--The depth-dependence of the CH dissociation temperature.

is close to the dissociation limit of the CH molecule. Since this problem is not readily tractable, we shall assume for simplicity that the populations of the $^2\Delta$ and $^2\Pi$ levels are determined by the local electron temperature.

The Results of the Computations

The CH equivalent widths--As we have already indicated above, the computed values of $W_\lambda(\mu)/W_\lambda(1.0)$ were systematically larger than the observed values when local thermodynamic equilibrium was assumed. These discrepancies between the computations and observations disappear as soon as we introduce departures from local thermodynamic equilibrium in

accordance with the form predicted by the mechanism of radiative dissociation. Since CO formation turned out to have such a small effect on the behavior of the CH equivalent widths, it can probably be neglected in most of the computations.

When CO formation is neglected, we find that we can obtain excellent agreement between the computed and observed center-limb behavior of the CH equivalent widths with Elste's temperature-pressure model (table 2), the theoretical dissociation temperature model (figure 4-5), and an isotropic microturbulence which is independent of depth and has a velocity of 1.4 km/sec. In order to illustrate the general agreement between the observations and the above computations, we have plotted by short dashed lines in figures 4-1 and 4-2 the behavior of $W_{\lambda}(\mu)/W_{\lambda}(1.0)$ computed for this set of conditions. In figures 4-6 to 4-10 we have compared the computed and observed equivalent widths of lines in three vibration bands for five limb positions.

The only significant change that results when CO formation is included is that the microturbulence becomes slightly anisotropic ($\xi_r = 1.4$ km/sec, $\xi_t = 1.6$ km/sec). The behavior of $W_{\lambda}(\mu)/W_{\lambda}(1.0)$ computed using this microturbulence model and including CO formation is given by long dashed lines in figures 4-1 and 4-2. As is apparent the curves computed with and without CO formation are very similar.

If we examine figures 4-6 to 4-10, we note that the agreement between the computations and observations is satisfactory for lines in the 0,0 and 1,1 vibration bands. The scatter of these points is consistent with the expected accuracy of the observations. The points corresponding to lines in the 2,2 band show a fair amount of scatter. However, since these points fall on both sides of the 45° line, this

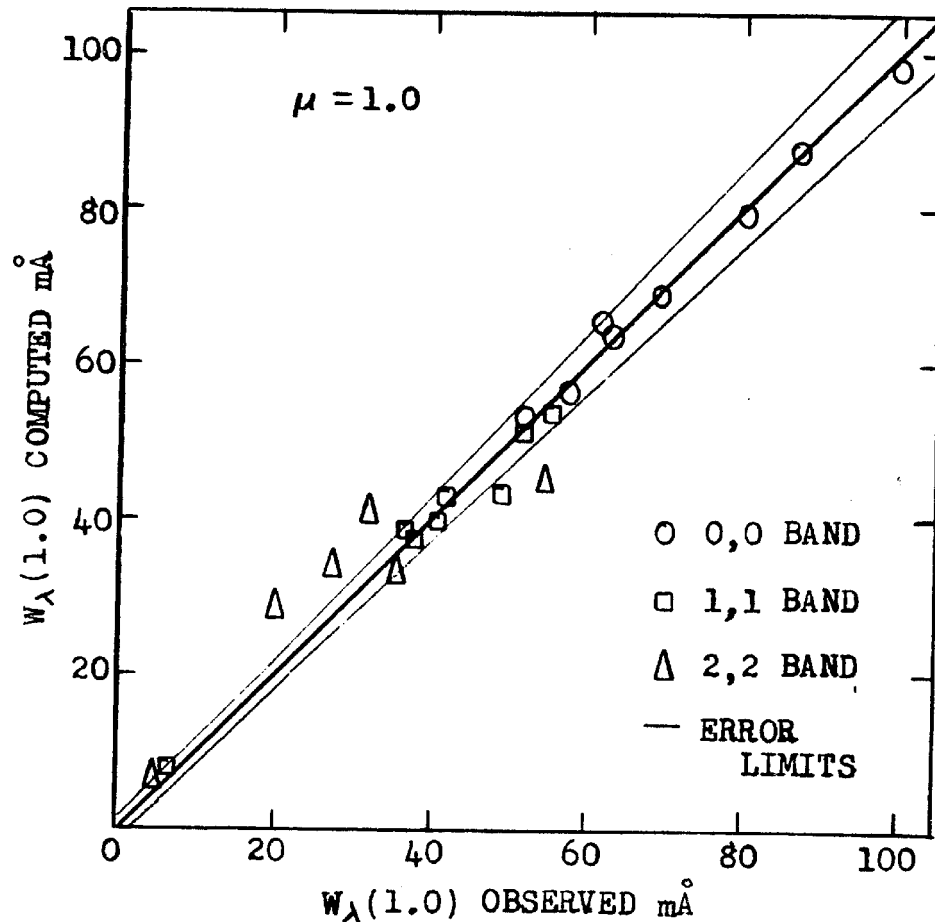


Figure 4-6.--A comparison between the computed and observed equivalent widths for $\mu = 1.0$.

scatter is probably caused by errors in the empirical equivalent widths. Apparently we have underestimated the uncertainties in the observations for these lines.

In the above computations we have allowed for the doublet splitting of the close doublets even though these lines were listed in the literature as having zero separations between the two components forming them. From the observed width and shallowness of these lines at $\mu = 1.0$ the assumption of zero separations seemed untenable.

In order to determine the magnitudes of the separations we did the following. The doublet splitting is a strong function of the rotational

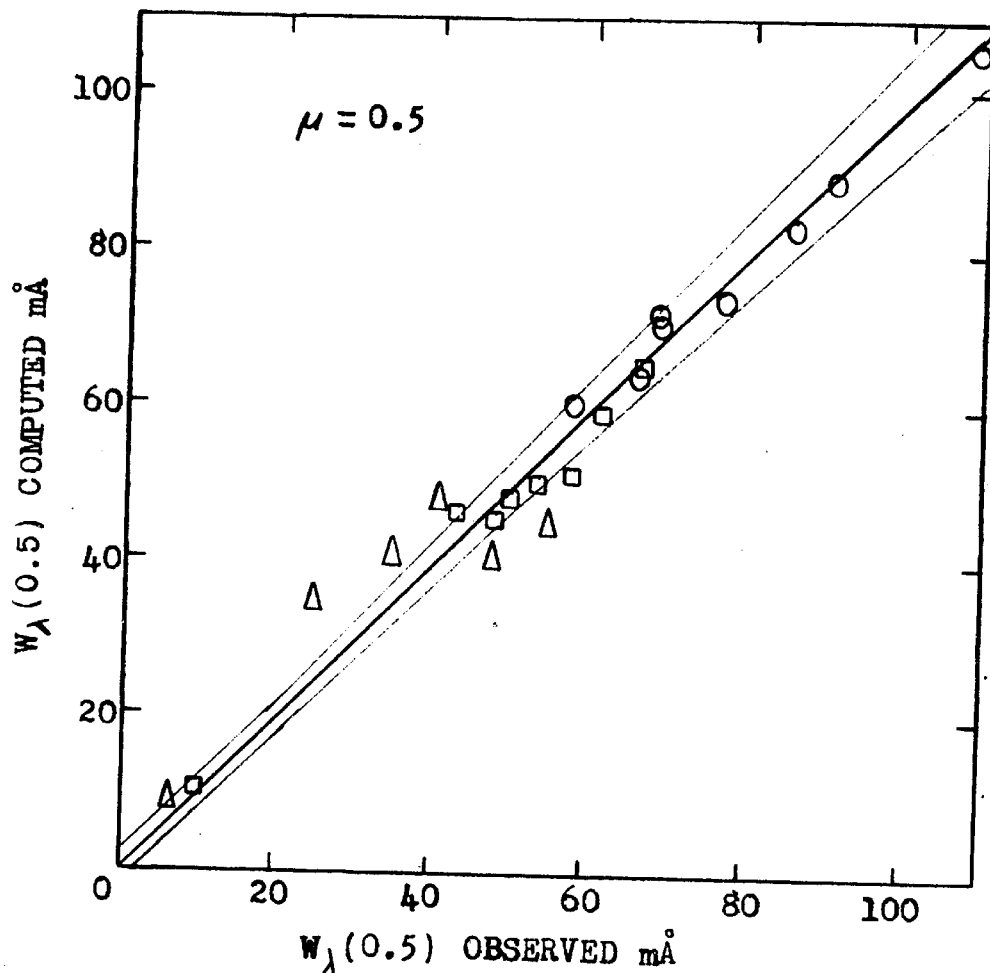


Figure 4-7.--A comparison between the computed and observed equivalent widths for $\mu = 0.5$.

quantum number K . Most of the CH doublets are sufficiently separated for the magnitude of the splitting to be measured in the laboratory (Gero, 1941). By plotting the measured separations as a function of K it was possible to estimate the magnitude of the separations for the close doublets. In some cases, where the observed lines were free from blending, these estimates were improved upon by comparing the observed and computed profiles for the center of the disc. The resulting doublet separations are listed in table 3.

The CH profiles--Detailed computations were made on the center-limb behavior of the profile of $\lambda 4248.944$. This line is the only

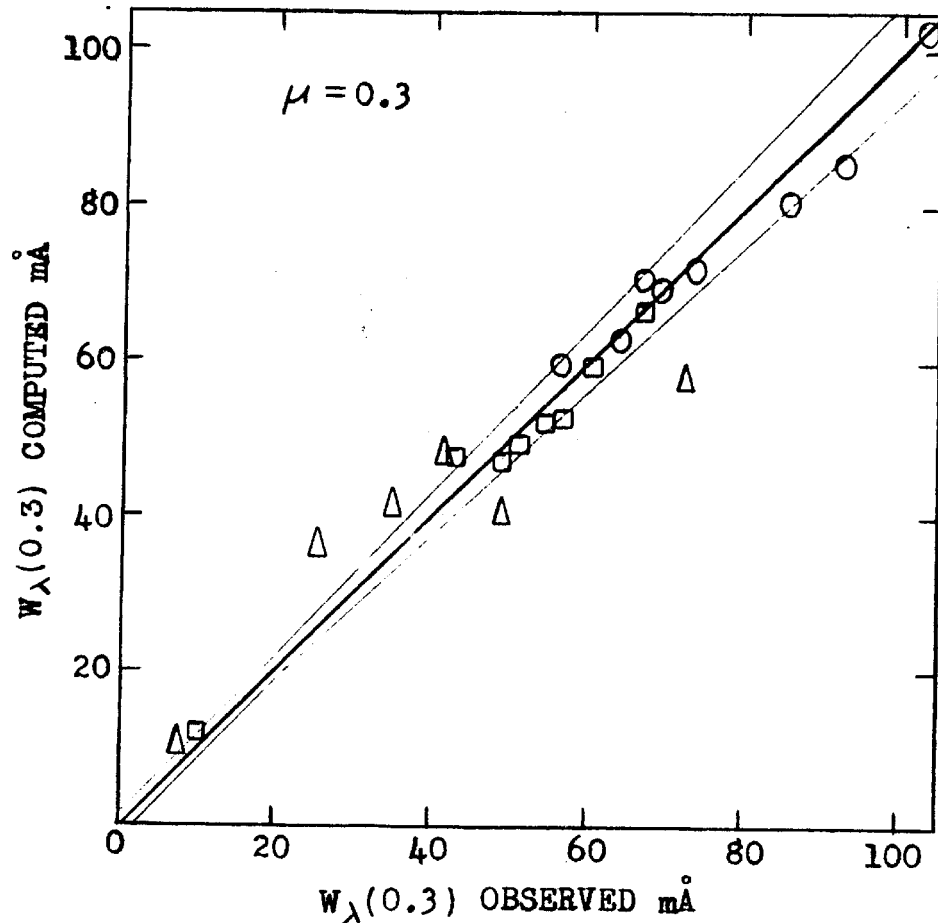


Figure 4-8.--A comparison between the computed and observed equivalent widths for $\mu = 0.3$.

satisfactory CH singlet in the observations. Since the center-limb behavior of the central intensity and half-width of this line is similar to that of other CH lines of comparable strength, it has been assumed that its center-limb behavior is representative in all respects of that of other comparable CH lines.

We found that we could explain the center-limb behavior of the CH equivalent widths with either one of two microturbulence models depending upon whether or not we included the effects of CO formation in the computations. In both models the computed profiles of $\lambda 4248.944$ were narrower than the corresponding observed profiles for all limb

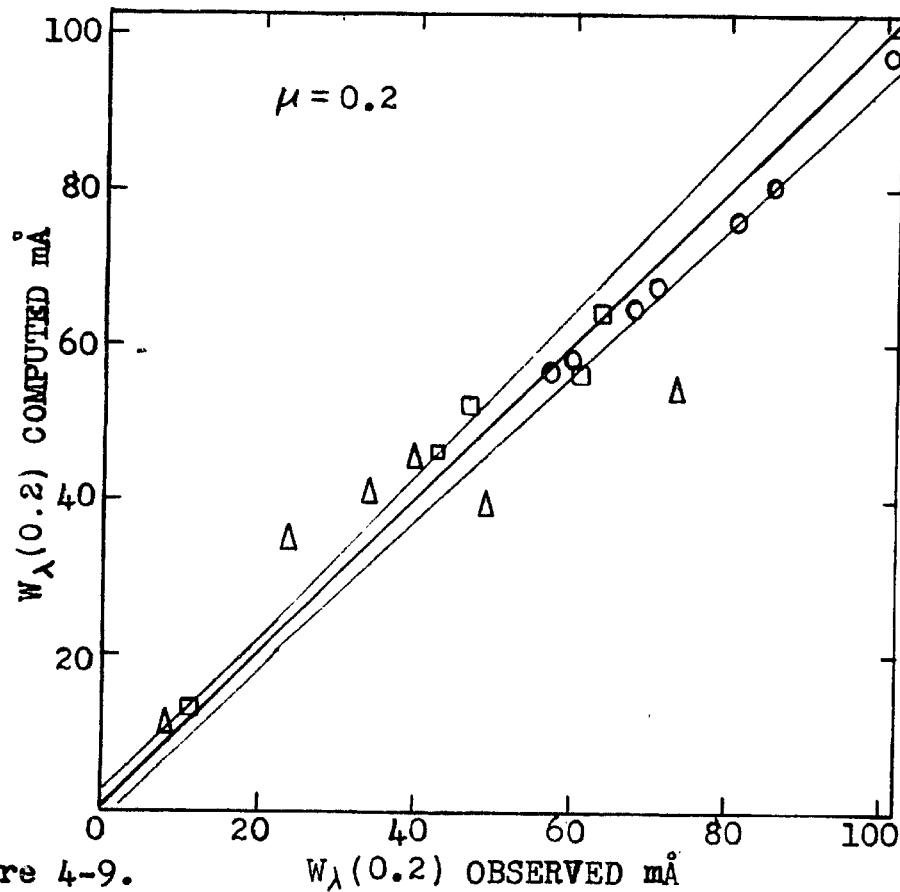


Figure 4-9.

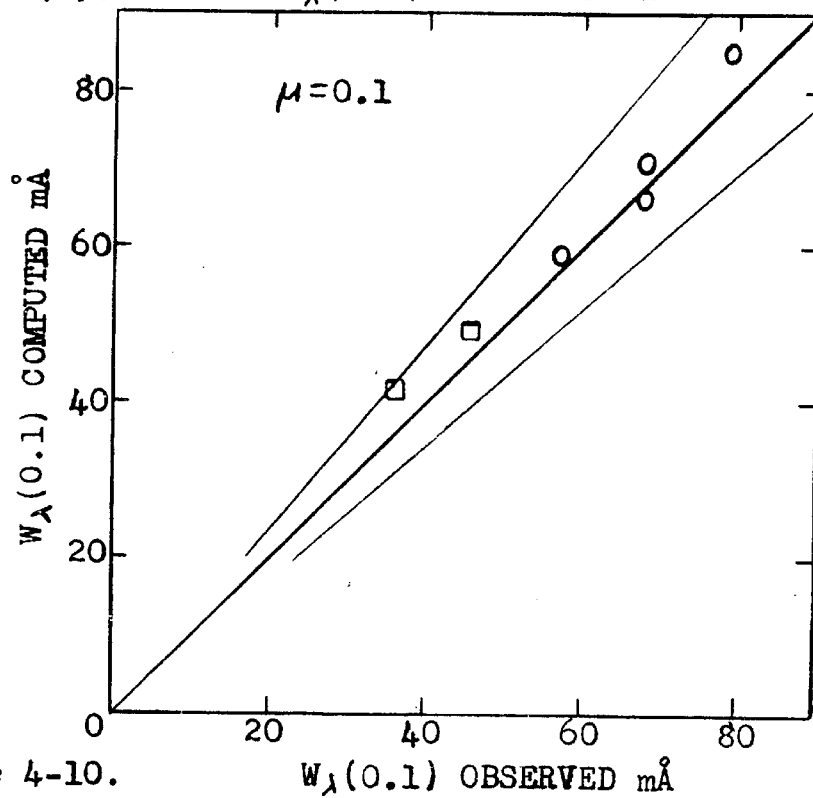


Figure 4-10.

Figures 4-9 and 4-10.--A comparison between the computed and observed equivalent widths for $\mu = 0.2$ and $\mu = 0.1$.

TABLE 3

WAVELENGTH SEPARATIONS BETWEEN COMPONENTS OF CH DOUBLETS			
λ	($\text{\AA}$)	λ	($\text{\AA}$)
4192.572	0.000	4288.736	0.009
4207.408	0.030	4296.217	0.000
4210.067	0.040	4328.610	0.000
4213.874	0.070	4329.340	0.112
4216.599	0.025	4332.169	0.058
4217.240	0.069	4335.274	0.026
4218.725	0.012	4378.917	0.023
4240.199	0.007	4387.063	0.008
4248.055	0.017	4388.870	0.000
4281.972	0.040		

positions. This indicates that we need to introduce another line-broadening agent into the model. The simplest, physically plausible mechanism that we can use to broaden out the profiles without affecting their equivalent widths is macroturbulence. If we assume that the magnitudes of the line-of-sight macroturbulent velocities have a Gaussian distribution, then the required vertical and tangential velocities are 1.0 km/sec and 1.75 km/sec.

In figure 4-11 we have drawn the observed profile of $\lambda 4248.944$ and have plotted points to indicate two types of theoretical profiles. One of these is affected only by microturbulence; and the other by both microturbulence and macroturbulence. The microturbulence model used was the isotropic model with $\xi_r = 1.4$ km/sec. If the slightly anisotropic model had been used ($\xi_r = 1.4$ km/sec, $\xi_t = 1.6$ km/sec), the computed profiles would be almost identical to those illustrated and the required

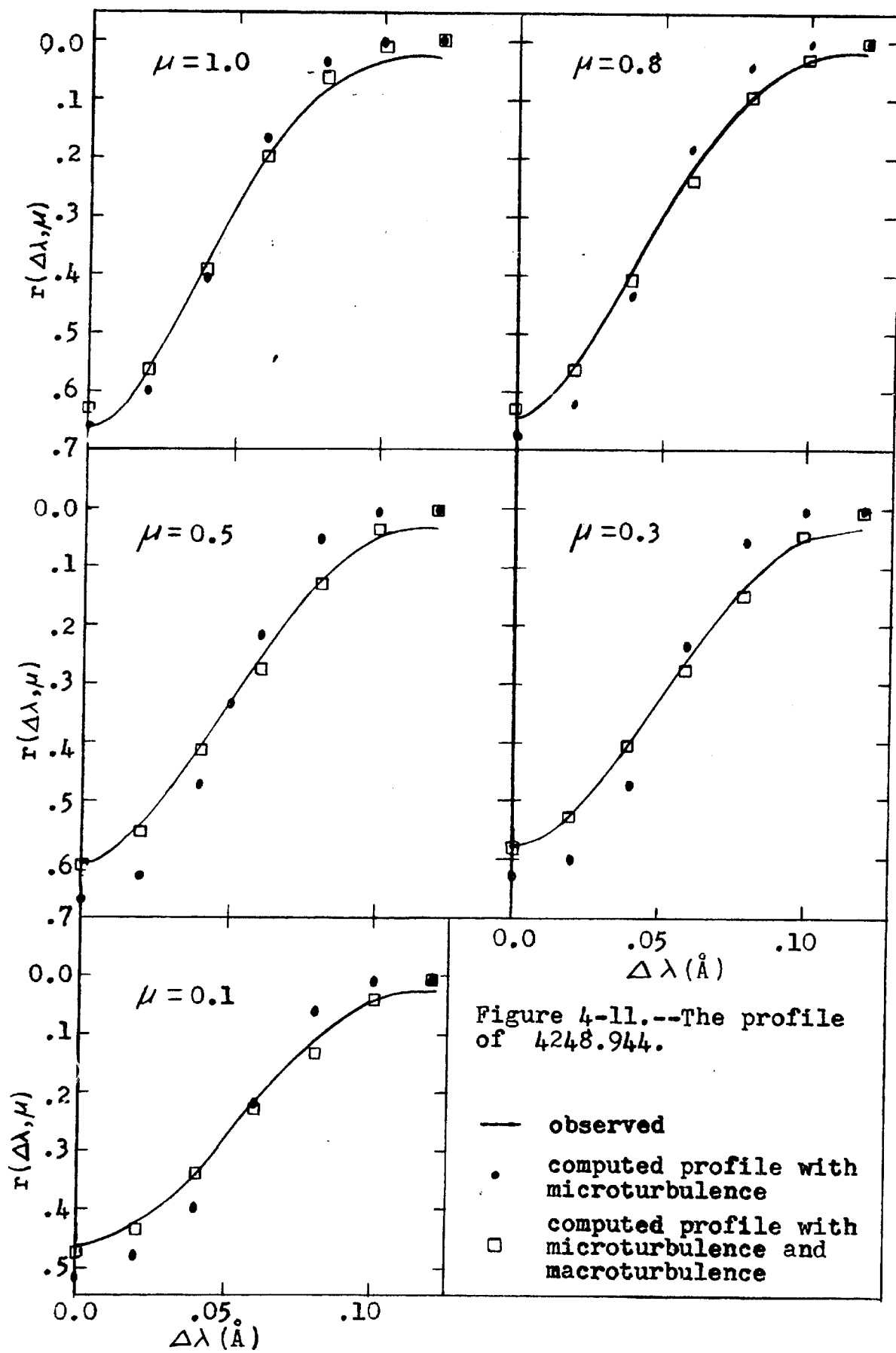


Figure 4-11.--The profile of 4248.944.

tangential macroturbulent velocity would be reduced to about 1.6 km/sec.

A Discussion of the Results

A brief summary of the results of the homogeneous model computations is given in table 4. It is of interest to know what layers of the photosphere these computations refer to and therefore to know where the CH lines are formed. One way of finding this out is to use the information contained in the contribution functions of CH lines. The contribution function $C(\Delta\lambda)$ for a given position $\Delta\lambda$ on a line profile is a plot of the integrand of the equation for $r(\Delta\lambda, \mu)$, equation 3-16, as a function of $\log \tau_0$. Contribution functions for the center of $\lambda 4248.944$ are given for several limb positions in figure 4-12. If one examines the contribution functions for the center and wings of typical CH lines, one finds that the CH lines are formed primarily between $\log \tau_0 = -0.5$ and $\log \tau_0 = -2.5$.

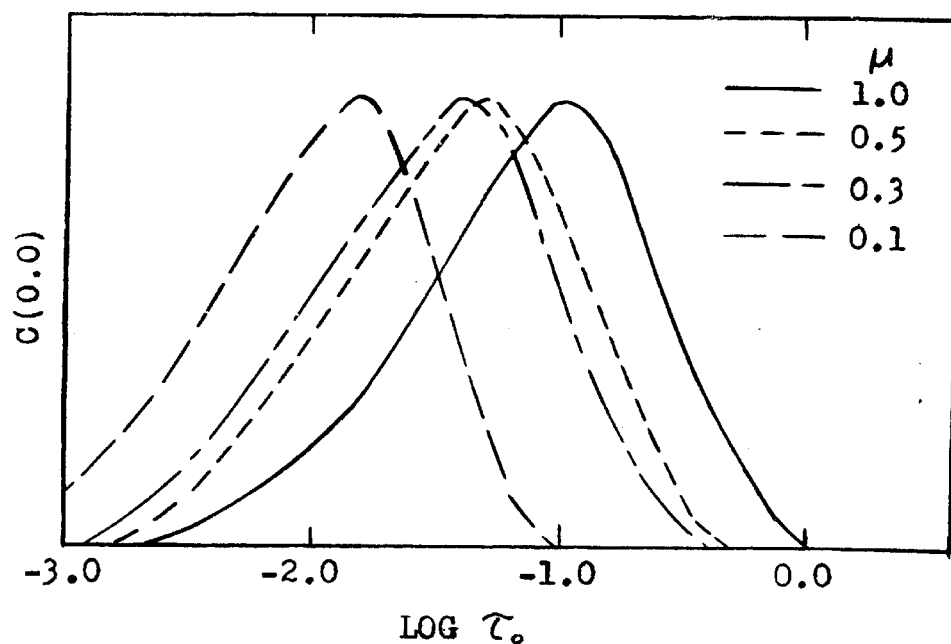


Figure 4-12.--Contribution functions for $r(\Delta\lambda = 0.0, \mu)$ for $\lambda 4248.944$.

TABLE 4.--A SUMMARY OF THE RESULTS OF THE COMPUTATIONS

TABLE 4.--A SUMMARY OF THE RESULTS OF THE COMPUTATIONS										
Model	CO	$\frac{\theta_{CH}}{\theta_e}$	Turbulence (km/sec.)				$W(\mu)_c/W(\mu)_o$		Profiles (comparison with observations)	
			ξ_r	ξ_t	s_r	s_t	0.5	0.3		
Model 10	no	1.00	1.2	1.2	--	--	>1.0	>1.0	--	
	yes									
	no	.92	1.4	1.4	1.0	1.75	1.0	1.0	good	
	yes	.92	1.4	1.6	--	--	1.0	1.0	--	
Three Stream	yes	1.00	1.4	1.4	--	--	<1.0	--	--	
	yes	1.00	1.4	1.7	0.0	0.0	1.0	--	$\mu=1.0$ core too wide	
	yes	1.00	1.0	1.1	1.8	2.5	<1.0	--	$\mu=1.0$ line too wide except in wings, too asymmetric $\mu=0.5$ good	
	yes	1.00	1.0	1.1	1.0	2.5	<1.0	--	$\mu=1.0$ too narrow in wings, slightly too wide core $\mu=0.5$ good	
	yes	1.00	1.0	1.4	1.0-2.0	2.3	1.0	--	$\mu=1.0$ fair, core slightly too wide, slightly too asym. $\mu=0.5$ good	
	yes	.92	1.0	1.5	1.0-2.0	2.2	1.0	--	$\mu=1.0$ same as with $\theta_{CH}/\theta_e=1.0$, but less asymmetric $\mu=0.5$ good	
c=computed, o=observed, θ_{CH}/θ_e refers to the average value of this quantity between $\log \zeta_s=-1.0$ and $\log \zeta_s=-2.0$										

c=computed, o=observed, θ_{CH}/θ_e refers to the average value of this quantity between $\log \zeta_s = -1.0$ and $\log \zeta_s = -2.0$

The turbulence model--The radial microturbulent velocity of 1.4 km/sec determined from the equivalent widths of the CH lines is similar to the average value of 1.2 km/sec deduced from curve-of-growth studies (de Jager, 1959). Furthermore, if we assume as a first approximation (Huang, Su-Shu, 1950) that

$$\xi_{\text{tot}}^2 = \xi^2 + s^2$$

where ξ_{tot} is the total turbulent velocity, ξ is the microturbulent velocity, and s is the macroturbulent velocity, then the total turbulent velocities for the CH molecule in the radial and tangential directions are 1.72 km/sec and 2.24 km/sec respectively. These total turbulent velocities compare favorably with the values of 1.8 km/sec radially and 2.0 km/sec tangentially found by Waddell (1960) from the center-limb behavior of the half-width of a moderately strong iron line formed between $\log \tau_0 = -1.0$ and $\log \tau_0 = -2.0$.

In figure 4-13 we have compared the line-of-sight macroturbulent velocity determined from the profile of $\lambda 4248.944$ with the macroturbulent velocities determined from measurements of local Doppler shifts in moderately strong atomic lines. As is apparent the agreement is not very satisfactory. The macroturbulent velocity deduced from the profile of $\lambda 4248.944$ is considerably larger and increases more rapidly toward the limb than the velocities determined from measurements of local Doppler shifts. The lack of agreement between these two types of measurements suggests the existence of significant observational uncertainties. The profiles of $\lambda 4248.944$ are accurate to about ± 4 per cent which means that the velocities determined from these profiles are accurate to only about ± 30 per cent. The velocities determined from measurements of local Doppler shifts may be inaccurate because of the restriction in

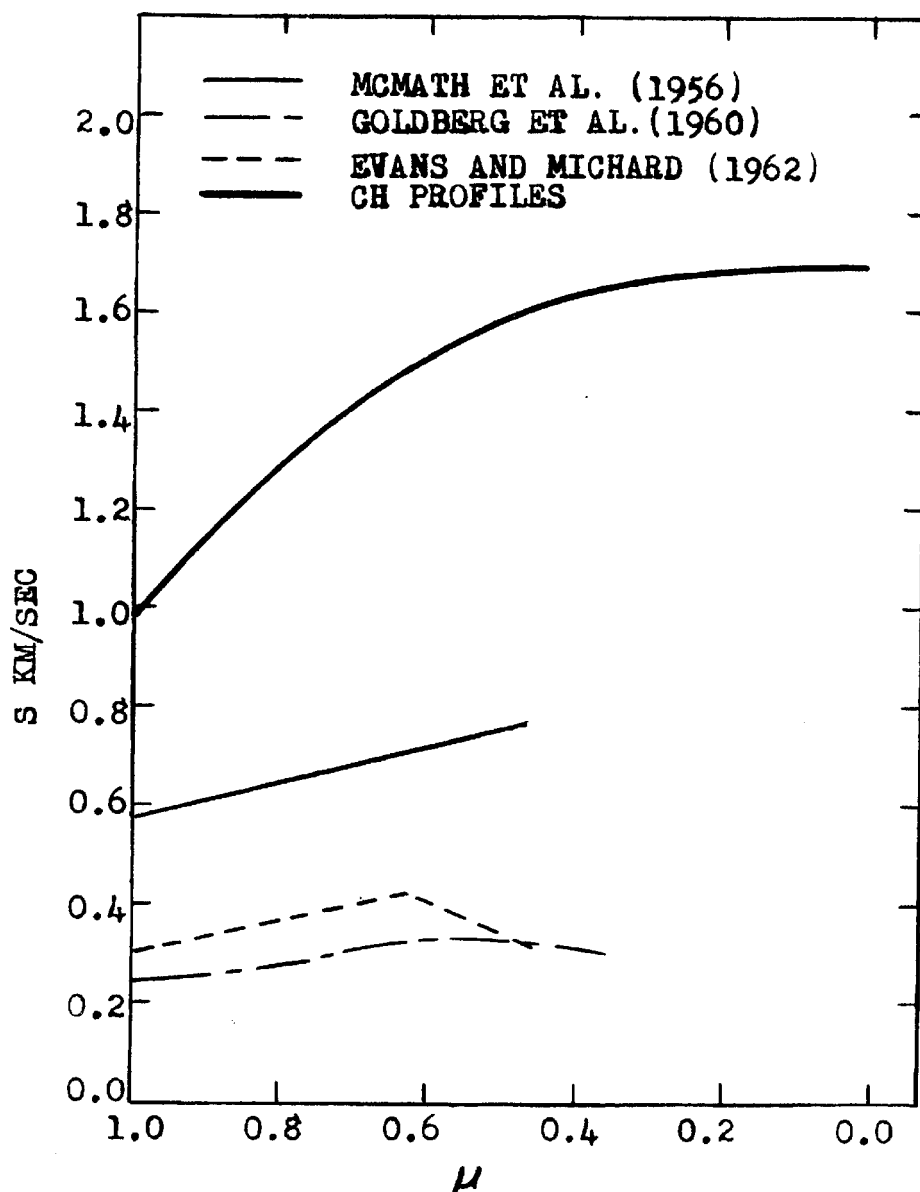


Figure 4-13.--Comparison between macro-turbulent velocities determined from CH profiles and from measurements of local Doppler shifts.

spatial resolving power on the solar disc due to atmospheric seeing and scattered light. The latter velocities are if anything lower limits to the actual photospheric macro-turbulent velocities. It is of interest that theoretical studies of the solar convection zone by Unno (1957) and Böhm (1963) both predict the existence of turbulent motions in the photosphere in which the tangential velocities are greater than the

radial velocities. The macroturbulence model deduced from studies of $\lambda 4248.944$ is consistent with this prediction.

The temperature-pressure model and departures from local thermodynamic equilibrium--In the computations with Elste's homogeneous model we found that departures from local thermodynamic equilibrium appear to be required in order to obtain satisfactory agreement between the computed and observed behavior of the equivalent widths of the CH lines. How significant are these departures? One way of measuring this is to compare the average difference between the computed and observed values of the ratio $R = W_\lambda(\mu)/W_\lambda(1.0)$ for the limb position where this difference is largest. This occurs at $\mu = 0.3$. Here the computed values of R are systematically larger than the observed values by varying amounts which depend upon the assumed microturbulence model. For microturbulence models which are consistent with past studies of photospheric turbulence

$$\bar{R}(\text{computed}) \geq 1.06 \cdot \bar{R}(\text{observed})$$

Where $\bar{R}$ is the mean value of R for the CH lines. If we are going to conclude that we have found significant evidence for departures from local thermodynamic equilibrium, then the probable error in $\bar{R}(\text{observed})$ must be less than 2 per cent.

As an estimate for the error in an individual measurement of R we define

$$\begin{aligned} \Delta R &= \sqrt{\left[\frac{\delta R}{\delta W_\lambda(1.0)} \right]^2 [\Delta W_\lambda(1.0)]^2 + \left[\frac{\delta R}{\delta W_\lambda(\mu)} \right]^2 [\Delta W_\lambda(\mu)]^2} \\ &= R \sqrt{\left[\frac{\Delta W_\lambda(1.0)}{W_\lambda(1.0)} \right]^2 + \left[\frac{\Delta W_\lambda(\mu)}{W_\lambda(\mu)} \right]^2} \end{aligned}$$

where we have assumed that the errors in $W_\lambda(1.0)$ and $W_\lambda(\mu)$ are independent. We also define $\Delta W_\lambda(1.0) = \epsilon_1 \cdot W_\lambda(1.0)$ and $\Delta W_\lambda(\mu) = \epsilon_\mu \cdot W_\lambda(\mu)$.

Therefore,

$$\frac{\Delta R}{R} = \sqrt{\epsilon_1^2 + \epsilon_\mu^2} \quad 4-2$$

Now if we consider each observed value of R for the 23 lines used in this analysis as an independent measurement and assume $\epsilon_1 = \epsilon_\mu = 6.3$ per cent (Chapter II), we obtain

$$\frac{\Delta \bar{R}}{\bar{R}} = \frac{1}{\sqrt{23}} \sqrt{\epsilon_1^2 + \epsilon_\mu^2} = 1.9 \text{ per cent.} \quad 4-3$$

Actually the errors in $W_\lambda(1.0)$ and $W_\lambda(\mu)$ are correlated, since the errors in the intensity of the local continuum and in the blending correction should be as a first approximation identical at $\mu = 1.0$ and $\mu = 0.3$. Hence these errors should tend to cancel in the ratio R making the error expressed by equation 4-3 an upper limit. These results indicate that the evidence of departures from local thermodynamic equilibrium in the CH lines appear to be significant--providing that we accept Elste's homogeneous temperature-pressure model as accurately representing conditions in the upper photosphere.

How accurate is this temperature-pressure model? The dependence of temperature on depth in the upper layers of this model, $\log \tau_0 < -0.8$, is based on observations of limb darkening made near the edge of the solar disc. Such observations are difficult to interpret because of problems of seeing and scattered light; hence we may expect that the temperature model may be inaccurate for $\log \tau_0 < -0.8$.

In order to see what effect a change in the assumed temperature-pressure model would have, an empirical model for the upper photosphere

was derived from the CH observations assuming local thermodynamic equilibrium. For simplicity we neglected the effects of CO formation and assumed that the photospheric microturbulence is isotropic and independent of depth. It was possible to obtain satisfactory agreement between the computations and observations by modifying Elste's temperature-pressure model slightly in the upper layers. The temperature variation of the modified model is given as a function of $\log \tau_0$ in figure 4-14. In the derivation of the corresponding pressure model we used a computer program kindly furnished by G. Elste.

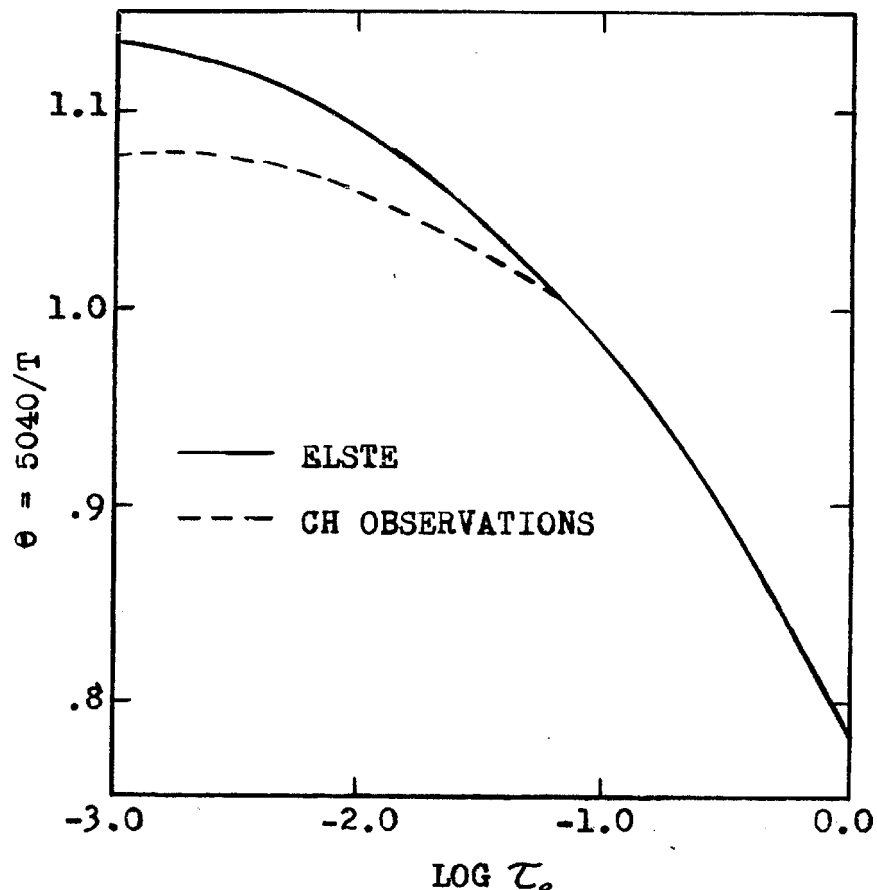


Figure 4-14.--The depth-dependence of the electron temperature determined from CH observations assuming local thermodynamic equilibrium.

As is apparent in figure 4-14, the temperatures in this model

fall fairly close to those in Elste's model. Since the differences between the two models are small, only 130 °K at $\log \tau_0 = -2.0$, the model derived from the CH observations will probably predict limb darkening within the accuracy of existing observations. On the basis of these results we conclude that there is no significant evidence that the local excitation and dissociation temperatures of the CH molecule deviate from the local electron temperature. There is some evidence that the local dissociation temperature may be higher than the local electron temperature, but this evidence depends upon the assumption that Elste's homogeneous temperature-pressure model accurately represents conditions in the upper photosphere.

The oscillator strength of the $\Sigma^z - \Pi^z$ band system--In order to compute theoretical profiles and equivalent widths for the CH lines it was necessary to assume a value of the quantity $N_C/N_H \cdot f_{CH}$ where N_C/N_H is the solar abundance of carbon with respect to hydrogen and f_{CH} is the oscillator strength of the $\Sigma^z - \Pi^z$ band system (see Chapter III). Since neither of these quantities is precisely known, the equivalent widths of the CH lines observed at the center of the solar disc were used to determine an empirical value for $\log(N_C/N_H \cdot f_{CH})$. The value found is -6.39. If we assume that $\log(N_C/N_H) = -3.35$ (obtained from solar CI lines by Baschek, 1961), then $\log f_{CH} = -3.04$. Various other determinations for the f-value of the $\Sigma^z - \Pi^z$ band system of the CH molecule are:

Bennett (1960, lab)	$\log f_{CH} = -2.31$
Stephenson (1951, theory)	$\log f_{CH} = -2.10$
Lyddane et al. (1941, combination theory, lab; corrected by Dwyer, 1944)	$\log f_{CH} = -2.72$

Eugene-Praderie (1960, solar) $\log f_{\text{CH}} = -3.35$

and

Baschek (1962, solar) $\log f_{\text{CH}} = -3.29$

The Eugene-Praderie value is not exactly the same as is quoted in that paper, since we have allowed for the difference between the carbon abundance used there and the abundance assumed here. Note that the laboratory and theoretical f-values are systematically larger than our value while the other recent solar determinations are smaller. Thus while our f-value is fairly consistent with past solar determinations, it is closer to the laboratory values.

An Analysis of the CH Observations Based
on a Three Stream Model

Introduction

The presence of granular structure on the solar disc implies that there are temperature-pressure inhomogeneities in the solar photosphere. This suggests that it might be worthwhile to investigate the influence of inhomogeneities on the center-limb behavior of the CH lines.

The granulation observed on the solar disc is generally assumed to be produced by the upward flow of hot material which cools and falls back into the lower layers of the photosphere. A simple model which can be used to represent this phenomenon is the three stream model. In the typical three stream model there is an upward moving hot column, a warm stationary column, and a downward moving cool column. Multicolumn models have been used in the past to explain such phenomena as the center-limb behavior of the wavelengths and asymmetries of spectral lines (e.g. Schröter, 1956; Voigt, 1956, 1959; de Jager and Neven, 1964). They do

not, however, account for the oscillatory motions that have been observed in the solar photosphere (e.g. Leighton, 1963).

Since the derivation of multicolumn photospheric models has been described elsewhere (e.g. Voigt, 1956; Schröter, 1956; David, 1961), we will not discuss it in any detail here. The major problem in constructing such models is the reliable estimation of the depth-dependence of the photospheric temperature fluctuations. These estimates depend on observations of the variation of granular contrast across the solar disc. Since solar granules are small, of the order of one second of arc in diameter, it is difficult to obtain satisfactory observations of them because of problems of seeing and scattered light. Even the excellent Stratoscope photographs of granulation have proved difficult to interpret because of uncertainties in the photometric calibration (Leighton, 1963). Since existing observations are of low quality, multicolumn models based on them are likely to be inaccurate. For this reason we must be careful in interpretation of results derived from such models.

The Adopted Three Stream Model

The three stream model used in this investigation was developed by G. Elste and is based on the results of Edmonds' analysis (Edmonds, 1961) of photographs of granulation obtained from Stratoscope. According to Edmonds the granular contrast on the solar disc increases away from the center, reaches a maximum at $\mu \approx 0.6$, and decreases near the limb. Elste's three stream model reproduces the initial rise in contrast but not the diminution near the limb. A possible explanation for the decrease in contrast at the limb is that the observer's line-of-sight may pass through more than one granule for $\mu < 0.6$. This effect was not taken

into consideration in computing the center-limb variation of the surface contrast in Elste's model. This model was derived from the homogeneous model used in the first part of this analysis. The temperatures in the three columns of the three stream model are plotted as a function of $\log \tau_0$ in figure 4-15.

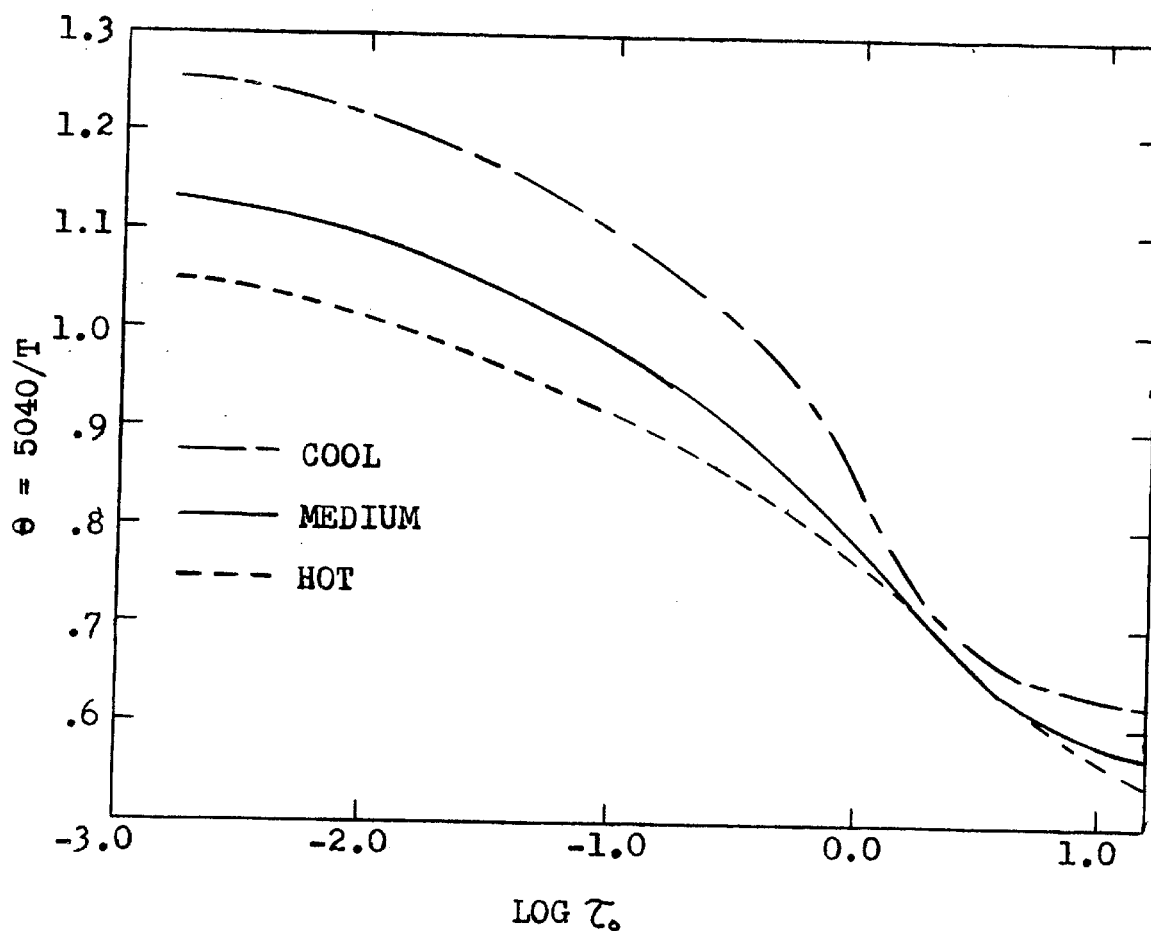


Figure 4-15.--The depth-dependence of temperature in the three columns of Elste's three stream model.

Since the $\log \tau_0$ scales are different in the three columns, the temperatures at a given optical depth τ_0 in the columns do not refer to the same geometrical level in the photosphere.

The computation of line profiles for a three stream model

proceeds in the following manner. One first computes the center-limb behavior of the line profile for each column exactly as for a homogeneous model. Then these profiles are added together weighted by the relative intensity of the continuum in each column. Thus the mean value of $r(\Delta\lambda, \mu)$ is given by

$$\bar{r}(\Delta\lambda, \mu) = \frac{\sum_{i=1}^3 A_i \cdot I_i(\mu) \cdot r_i(\Delta\lambda, \mu)}{\sum_{i=1}^3 A_i \cdot I_i(\mu)} \quad 4-4$$

where A_i is the area of stream i , $I_i(\mu)$ is the emergent continuum intensity at limb position μ in stream i , and $r_i(\Delta\lambda, \mu)$ is the line depth at limb position μ in stream i corresponding to a distance $\Delta\lambda$ from the center of the undisplaced line. In Elste's three stream model the relative areas of the three columns are 1:2:1 for the hot, warm, and cool columns respectively.

In computing the value of $\bar{r}(\Delta\lambda, \mu)$ by equation 4-4 it is assumed that each contribution $r_i(\Delta\lambda, \mu)$ to the mean value $\bar{r}(\Delta\lambda, \mu)$ is formed only in column i . Near the limb this assumption will not be valid because the observer's line-of-sight will pass through more than one column. If our interpretation of the cause of the decrease in granular contrast for $\mu < 0.6$ is correct, then the above assumption is valid only for $\mu \geq 0.6$. However, we have extended this limit to $\mu = 0.5$, since the surface contrast predicted by Elste's model agrees satisfactorily with that observed for $\mu \geq 0.45$.

The Turbulence Model

In the computation of CH equivalent widths with the three stream model the microturbulence was assumed for simplicity to be

independent of depth and identical in all three columns. For the macroturbulence model we assumed that the hot column was rising, the cool column falling, and that one-half of the warm column had a tangential macroturbulent velocity directed in one direction and the other half had a tangential macroturbulent velocity directed in the opposite direction. This macroturbulence model is basically a simplification of a model suggested by Unno (1957). He made a theoretical study of the influence of the solar convection zone on turbulent motions in the photosphere. Unno's model is given in figure 4-16a while the simplified model is given in figure 4-16b.

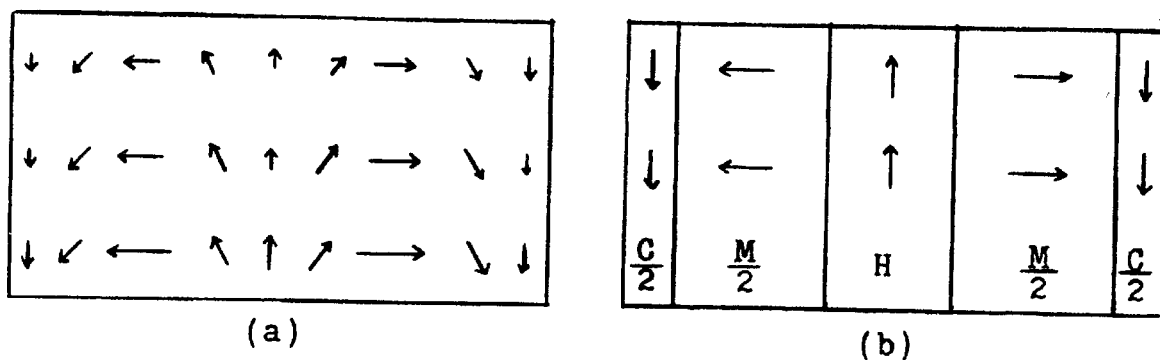


Figure 4-16.--Turbulent motions in the photosphere. (a) Unno's model. (b) Simplified model used in this investigation. The letters C, W, and H refer to the cool, warm, and hot columns respectively. The relative areas of the cool, warm, and hot columns are 1:2:1.

The term "macroturbulence" as it is used above is defined to mean any motions in the photosphere which occur on a scale as large or larger than the scale of the region of line formation (i.e. a few hundred kilometers). The motions do not actually have to be turbulent.

The Results of the Computations

It proved to be relatively easy to explain the center-limb behavior of the CH equivalent widths with Elste's three stream model,

the assumption of local thermodynamic equilibrium, and a variety of microturbulence models. This is in contrast to the computations with the homogeneous model where it was necessary to introduce departures from local thermodynamic equilibrium in order to obtain satisfactory agreement between the computations and observations. For a given microturbulence model the values of $W_{\lambda}(\mu)/W_{\lambda}(1.0)$ computed with the three stream model are smaller than the corresponding values computed with the homogeneous model. Some of the results of the computations are summarized in table 4, page 59. The formation of CO molecules was allowed for in all of the computations with the three stream model, since for inhomogeneous models it influences the relative contributions of the various streams to the mean profile. In particular it weakens the contribution of the cool column with respect to the other two columns.

Although it was relatively easy to explain the center-limb behavior of the CH equivalent widths with the three stream model, it was difficult to obtain satisfactory agreement between the computed and observed profiles of $\lambda 4248.944$. In general the cores of the computed profiles tended to be too broad compared to those observed. The computed profiles were also more asymmetrical than the observed profiles. Neither the three stream model or the observations were of high enough quality to warrant investigating the turbulence model of the upper photosphere in any great detail. When local thermodynamic equilibrium was assumed the best agreement between the computed and observed profiles of $\lambda 4248.944$ was obtained with the macroturbulence model given in figure 4-17 and a depth-independent microturbulence with $\xi_r = 1.0$ km/sec and $\xi_t = 1.4$ km/sec. The resulting profiles are given by the triangles in figure 4-18 for $\mu = 1.0$ and $\mu = 0.5$.

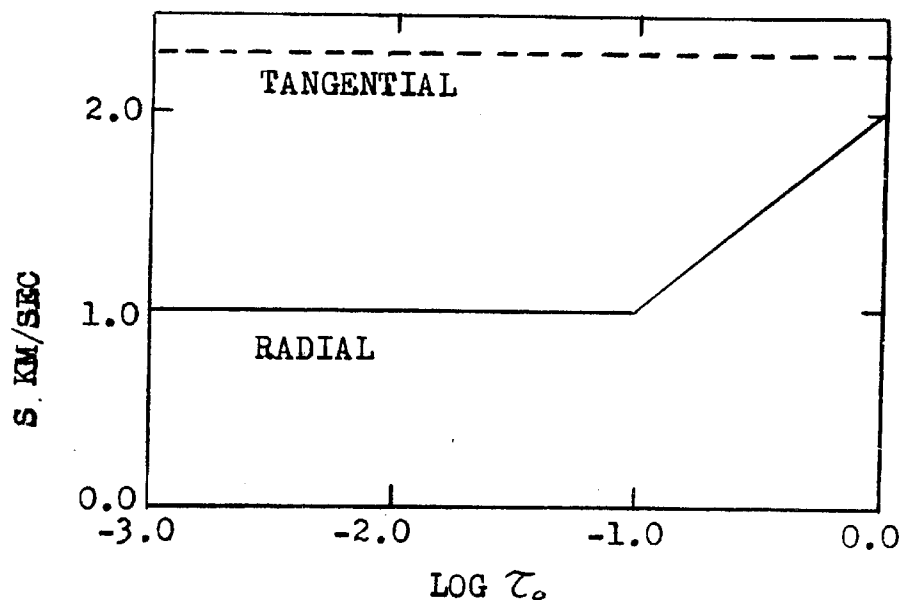


Figure 4-17.--Macroturbulence model for the computations with the three stream model.

If we accept the error limits of ± 4 per cent suggested in Chapter II, then the computed and observed profiles agree. There are some indications that the core of the computed profile at $\mu = 1.0$ is too broad. This profile was computed with $\xi_r = 1.0$ km/sec. The disagreement between the cores of the observed and computed profiles was even worse when radial microturbulent velocities greater than 1.0 km/sec were used. Due to the uncertainties in the observations we did not attempt to determine a precise value for ξ_r from the profile of $\lambda 4248.944$. However, we can suggest that there is some evidence that $\xi_r < 1.0$ km/sec.

If we further examine the profiles in figure 4-18, we note that at $\mu = 1.0$ the profile computed assuming local thermodynamic equilibrium is asymmetrical while the observed profile is very nearly symmetrical. At $\mu = 0.5$ both profiles are symmetrical. The computed profile at $\mu = 1.0$ is asymmetrical because under the assumption of local thermodynamic equilibrium the contribution of the cool column to

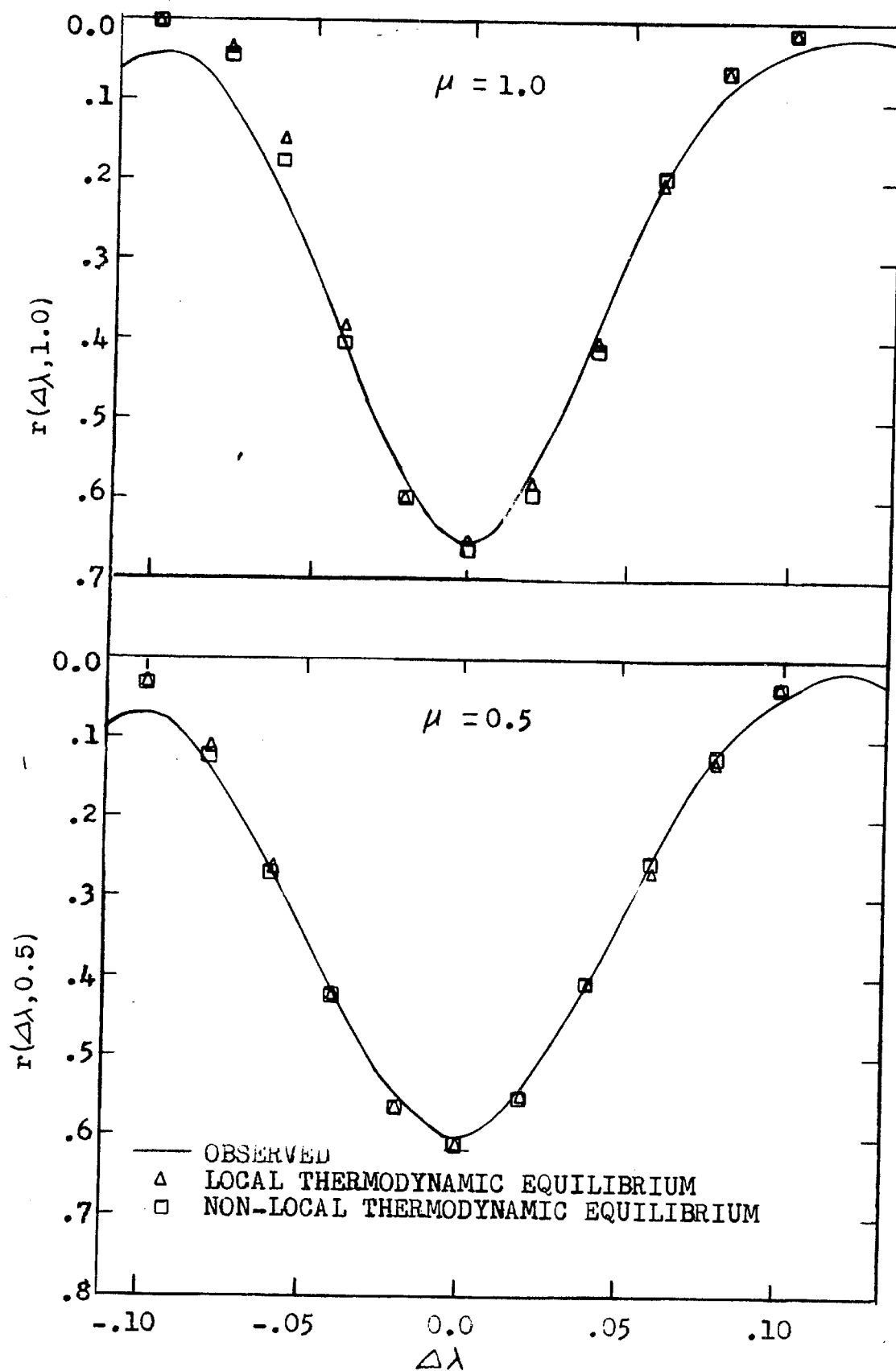


Figure 4-18.--A comparison between the observed profiles of 4248.944 and profiles computed with the three stream model.

the mean profile is larger than that of the hot column. Therefore, since the contributions of the hot and cool columns are Doppler shifted to opposite sides of the line by the streaming motions in the columns, the computed profile becomes asymmetrical. At $\mu = 0.5$ the contributions of the two columns are more in balance and the line is therefore nearly symmetrical. One could remove the asymmetry at $\mu = 1.0$ by setting the radial velocities of the streams to zero or by assuming that the upward and downward directed radial velocities of the streams are not correlated with the hot and cool columns respectively; however, then the three stream model would no longer represent granulation nor would the wavelength shift of spectral lines between the center of the solar disc be explained.

The differences between the observed profiles and those computed assuming local thermodynamic equilibrium are not very serious considering the unavoidable limitations in the quality of the observations. However, we did make a few computations to see what effect departures from local thermodynamic equilibrium would have. We assumed that the CH molecules are radiatively dissociated and computed a dissociation temperature model for each column using a method similar to that in Appendix III. When these dissociation temperatures are introduced into the model, there is surprisingly little change in the predicted center-limb behavior of the CH lines. The core of $\lambda 4248.944$ is still too broad at $\mu = 1.0$; however, the asymmetry of the line is reduced slightly. The best agreement between the computations and observations is obtained with the macroturbulence model in figure 4-17 and with a microturbulence which is independent of depth with $\xi_r = 1.0$ km/sec and $\xi_t = 1.5$ km/sec. The profiles at $\mu = 1.0$ and $\mu = 0.5$ for $\lambda 4248.944$ computed using this

set of conditions are given by the squares in figure 4-18.

A Discussion of the Results of the Three Stream Model

In the computations with the three stream model we found that we could explain the center-limb behavior of the CH equivalent widths equally well either by assuming local thermodynamic equilibrium or by assuming that the dissociation of the CH molecules is determined by the radiation field in the upper photosphere. For the profiles of $\lambda 4248.944$ the introduction of radiative dissociation resulted in slightly better agreement between the computed and observed profiles at $\mu = 1.0$. However, since the differences between the profiles computed with and without the assumption of local thermodynamic equilibrium are so small, we conclude that the assumption of local thermodynamic equilibrium in Elste's three stream model is apparently an adequate assumption, at least for analysis of CH lines.

CHAPTER V

SUMMARY AND CONCLUSIONS

Computations were made using a homogeneous temperature-pressure model developed by G. Elste. When local thermodynamic equilibrium was assumed, the agreement between the computations and observations was not entirely satisfactory. In general the computed values of $W_{\lambda}(\mu)/W_{\lambda}(1.0)$ were systematically larger than the observed values. This indicated that the assumed model should be modified.

One way of doing this was the elimination of the assumption of local thermodynamic equilibrium. On the basis of some crude estimates of the importance of different forms of departures from local thermodynamic equilibrium it was concluded that the local dissociation temperature of the CH molecule may be different from the local electron temperature. By assuming that the CH molecules are radiatively dissociated it was possible to compute a dissociation temperature model for the upper photosphere. The introduction of this model into the computations removed the systematic differences between the computed and observed center-limb behavior of the CH lines.

Another way of modifying the assumed set of conditions was to keep the assumption of local thermodynamic equilibrium and to change the temperature-pressure model. By increasing the electron temperatures in the upper layers of Elste's model it was possible to eliminate the systematic differences between the computations and observations.

A series of computations were made with a three stream model

developed by G. Elste. With this model it was possible to explain the CH observations satisfactorily by assuming local thermodynamic equilibrium. The introduction of departures from local thermodynamic equilibrium as predicted by the mechanism of radiative dissociation improved slightly the agreement between the computed and observed profiles of $\lambda 4248.944$.

If we combine the results of the computations made with the homogeneous and three stream models, we may conclude that the evidence of departures from local thermodynamic equilibrium in the CH lines is not significant. There is some evidence of departures in the form predicted by the mechanism of radiative dissociation; however, the uncertainties in the photospheric temperature-pressure model, turbulence model, and in the CH observations do not allow us to conclude that these departures are real.

If we compare the turbulence models resulting from the computations with the three stream and homogeneous models, we find that they are similar. To compare the macroturbulent velocities in the three stream model with those in the homogeneous model it is necessary to divide the former by $\sqrt{2}$. This gives radial and tangential macroturbulent velocities of 0.71 km/sec and 1.56 km/sec respectively. The corresponding velocities in the homogeneous model are 1.0 km/sec radially and 1.75 km/sec tangentially. For both models the tangential component of the microturbulence has a velocity of 1.4 km/sec. However, in the three stream model the radial component has a velocity of 1.0 km/sec compared with the value of 1.4 km/sec in the homogeneous model.

On the basis of the results of this investigation we suggest that the average conditions in the upper layers of the photosphere, $-2.5 \leq \log \tau \leq -0.5$, are fairly well represented by:

1. Elste's homogeneous temperature-pressure model (table 2),
2. a depth-independent microturbulence with a radial velocity of 1.2 ± 0.2 km/sec and with $\xi_t/\xi_r = 1.2 \pm 0.2$,

and

3. a depth-independent macroturbulence with radial and tangential components of 1.0 ± 0.5 km/sec and 1.6 ± 0.5 km/sec respectively.

For an inhomogeneous model we suggest as a first approximation:

1. Elste's three stream temperature-pressure model (temperature variations are given in figure 4-15),
2. the same microturbulence model as above,

and

3. a depth-independent macroturbulence with radial and tangential components of 1.0 ± 0.5 km/sec and 2.3 ± 0.7 km/sec respectively, distributed as in figure 4-16b.

It should be kept in mind that this three stream model, like all multi-column models, is based on observations of low quality and does not account for the influence of photospheric oscillatory motions.

In conclusion we feel that the basic purpose of this investigation has been accomplished: to explain the center-limb behavior of the CH lines and to obtain more information about the conditions in the upper photosphere. On the basis of the results of this study we suggest that the two sets of conditions given above be used to study observations of other spectral lines formed in the upper photosphere.

APPENDIX I

THE COMPUTER PROGRAM

A program for computing theoretical line profiles according to equations 3-9, 3-12, 3-16, 3-17, 3-24, 3-26, 3-31, and 3-36 was written in the FORTRAN language. The program, which was developed in collaboration with G. Elste, made use of a weighting function subroutine, H function subroutine, and an interpolation subroutine made available by him.

All of the integrals used in the program were numerically integrated in steps of $\log \tau_o = 0.2$ using the four point Gauss-Encke procedure for integration. Since the model atmospheres used began at $\log \tau_o = -3.0$, we had to choose some method for integrating equation 3-16 from $\log \tau_o = -\infty$ to $\log \tau_o = -3.0$. The method used is one given in the paper by Aller, Elste, and Jugaku (1957). If one assumes that the logarithm of the integrand, f , of equation 3-16 is a linear function of $x = \log \tau_o$ between $x = -\infty$ and $x = -3.0$, then

$$\log f(x) = \log f(-3.0) + b (x + 3.0)$$

and

$$\int_{-\infty}^{-3.0} f(x) dx = f(-3.0) \cdot \frac{\text{Mod}}{b} = \frac{f(-3.0) \cdot \text{Mod} \cdot 0.2}{\log_e [f(-2.8)/f(-3.0)]}.$$

The overall accuracy of the program is approximately one per cent, which is better than the accuracy of the observed profiles and equivalent widths.

A simplified flow diagram illustrating the general computing procedure of the program is given in figure A-1. The program runs in the following manner. First the model atmosphere, $\tau_{\lambda}(x)$, and the desired limb positions are read into the computer. Then the weighting functions $g_{\lambda}^{\mu}(x)$ are computed as a function of optical depth for these limb positions. Next the general atomic or molecular information such as partition functions, ionization potentials, etc., are read into the machine and the quantity $U_{CH}(x)$ (or $U_r[x]$) is computed. Then the specific line information is read in and $Z(x)$ is computed. Finally, a turbulence model is read in and the desired points on the line profiles are computed according to equation 3-16.

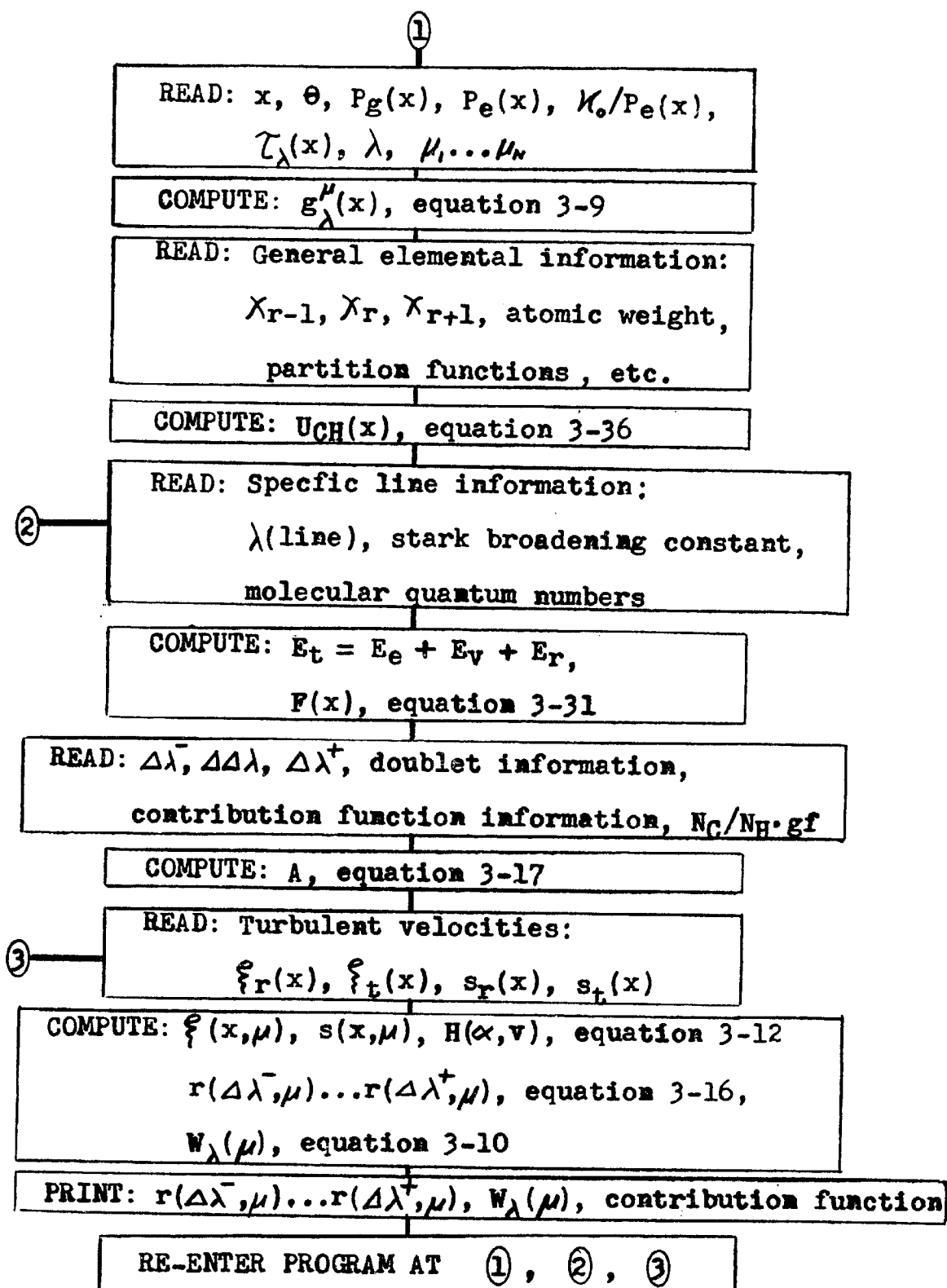


Figure A-1.--Flow diagram of the computer program for calculating line profiles.

APPENDIX II

THE CONSTRUCTION OF THE $W_{\lambda}(\mu)/W_{\lambda}(1.0)$ GRAPHS

If such graphs are to be of value, the CH lines corresponding to the points plotted on them should all be affected by saturation in the same way. A line becomes saturated when there is no longer a linear relationship between its equivalent width and the number of absorbing particles forming it. In general the stronger a line becomes the more saturated it becomes. An important effect of saturation is that lines with different saturations have different center-limb behaviors. For an unsaturated line $W_{\lambda}(\mu)/W_{\lambda}(1.0) = N(\mu)/N(1.0)$ where $N(\mu)$ is the number of absorbers in the line of sight at limb position μ . For saturated lines $W_{\lambda}(\mu)/W_{\lambda}(1.0) < N(\mu)/N(1.0)$. Unfortunately many of the CH lines are doublets. A doublet of a given equivalent width is less saturated than a singlet of the same strength. Therefore, the center-limb behavior of the doublet will differ from that of the singlet.

We allowed for this difference by correcting the observed $W_{\lambda}(1.0)$ of each doublet to that of the corresponding singlet of the same saturation using the simple Schuster-Schwarzchild pure absorption theory (Unsöld, 1938). Then the observed values of $W_{\lambda}(\mu)/W_{\lambda}(1.0)$ for the doublets were plotted as a function of the corrected $W_{\lambda}(1.0)$ values.

The method for obtaining the correction to $W_{\lambda}(1.0)$ is illustrated in figure A-2 where point number 1 represents a doublet and point number 2 represents the corresponding singlet. As a first approximation the center-limb behavior of doublet 1 and singlet 2 will be the same.

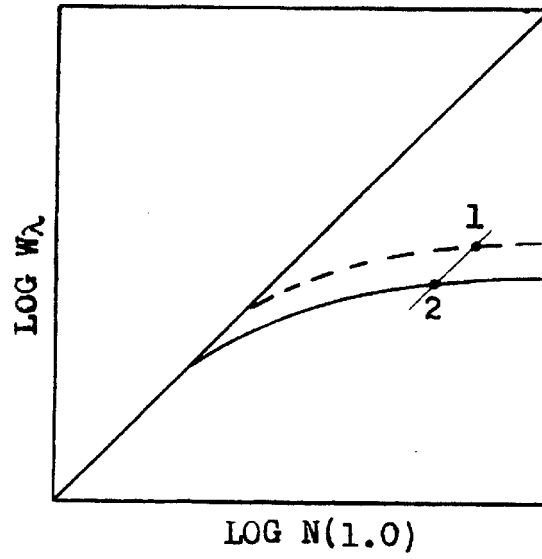


Figure A-2.--Curves of growth of singlet CH lines (solid curve) and of doublet CH lines of a given component separation (dashed curve). Lines corresponding to points 1 and 2 are equally saturated.

APPENDIX III

THEORETICAL DISSOCIATION TEMPERATURES

In order to obtain a first approximation to the magnitude of the deviations from local thermodynamic equilibrium in the upper photosphere we used a method suggested by Böhm (1954, 1960). If we assume that the rate of collisional dissociation is negligible in comparison with the rate of radiative dissociation, then

$$n(\text{dissociations CH}) = \int_0^{\infty} \frac{4\pi J_{\nu}(\tau_{\nu}) \cdot n_{\text{CH}} \alpha_{\nu} d\nu}{h\nu}, \quad \text{A-1}$$

where

$$\begin{aligned} J_{\nu}(\tau_{\nu}) &= \text{mean intensity at optical depth } \tau_{\nu} \\ &= \frac{1}{2} \int_0^{\infty} B_{\nu}(t_{\nu}) E_1(|t_{\nu} - \tau_{\nu}|) dt_{\nu}, \end{aligned}$$

$B_{\nu}(\tau_{\nu})$ = the intensity given by the Planck law,

$E_1(t)$ = the first exponential integral (Aller, 1963),

n_{CH} = the number of CH molecules per cm^3 ,

α_{ν} = the continuous absorption coefficient of CH at frequency ν per CH molecule,

ν = frequency,

and

h = Planck's constant.

The number of recombinations at a given level τ_{ν} is given by:

$$n(\text{recombinations CH}) = n_{\text{C}} n_{\text{H}} R_{\text{CH}}(\tau_{\nu}), \quad \text{A-2}$$

where

n_C = the number of neutral carbon atoms per cm^3 ,

n_H = the number of neutral hydrogen atoms per cm^3 ,

and

$R_{CH}(\tau_\nu)$ = the recombination coefficient at τ_ν .

If we assume dissociation equilibrium, then the number of dissociations per unit time equals the number of recombinations per unit time and

$$n_C n_H R_{CH}(\tau_\nu) = \int_0^\infty \frac{4 \pi J_\nu(\tau_\nu) n_{CH} \alpha_\nu d\nu}{h\nu}, \quad \text{A-3}$$

Similarly under the assumption of local thermodynamic equilibrium the number of radiative dissociations per unit time is given by

$$\begin{aligned} n(\text{dissociations CH}) &= \int_0^\infty \frac{4 \pi B_\nu(\tau_\nu) n_{CH} \alpha_\nu d\nu}{h\nu} \\ &= n_C n_H R_{CH}(\tau_\nu). \end{aligned} \quad \text{A-4}$$

If we assume that the atomic and molecular velocity distributions are independent of differences between the mean and local radiation fields, then the recombination coefficients in equations A-3 and A-4 are identical. Therefore

$$\frac{\left(\frac{n_C n_H}{n_{CH}} \right)_{\text{NLTE}}}{\left(\frac{n_C n_H}{n_{CH}} \right)_{\text{LTE}}} = \frac{\int_0^\infty \frac{4 \pi J_\nu(\tau_\nu) \alpha_\nu d\nu}{h\nu}}{\int_0^\infty \frac{4 \pi B_\nu(\tau_\nu) \alpha_\nu d\nu}{h\nu}}, \quad \text{A-5}$$

where LTE and NLTE refer to the ratios of $\frac{n_C n_H}{n_{CH}}$ under the assumption of local thermodynamic equilibrium and under the assumption that radiative dissociation is important.

Unfortunately the continuous opacity coefficient of the CH molecule is unknown. Since we are only interested in a first order approximation to the magnitude of the departures from local thermodynamic equilibrium, we will assume that α_ν is a delta function about ν_0 where ν_0 is the frequency corresponding to the effective dissociation energy D_{eff} of the CH molecule. Then from equation A-5 we have that

$$\frac{\left(\frac{n_C n_H}{n_{CH}}\right)_{\text{NLTE}}}{\left(\frac{n_C n_H}{n_{CH}}\right)_{\text{LTE}}} \approx \frac{J_{\nu_0}(\tau_0)}{B_{\nu_0}(\tau_0)} \quad \text{A-6}$$

The effective dissociation energy D_{eff} of the CH molecule is defined by

$$D_{\text{eff}} = D_{\text{CH}} - \bar{E}_t, \quad \text{A-7}$$

where D_{CH} is the dissociation energy of the CH molecule. The quantity $\bar{E}_t$ is the mean value of the excitation energy absorbed by the CH molecules in the upper photosphere. The absorption of this energy by the CH molecules reduces the amount of energy necessary to dissociate the molecules. The quantity $\bar{E}_t$ is defined by

$$\bar{E}_t = \frac{\sum_{v,K} (E_v + E_r) e^{-(E_v + E_r)/kT}}{\sum_{v,K} e^{-(E_v + E_r)/kT}}, \quad \text{A-8}$$

where E_v , E_r are the rotational and vibrational energies in the ground electronic state (see equation 3-27) and T is the average value of the

electron temperature in the region where the CH lines are formed.

The dissociation equation for the CH molecule assuming local thermodynamic equilibrium is (equation 3-28)

$$\frac{n_C n_H}{n_{CH}} = \frac{u_C u_H}{u_{CH}} \cdot \left(\frac{2 \pi M k T_1}{h^2} \right)^{3/2} \cdot e^{-D_{CH}/kT_2} \quad A-9$$

Since the temperature T_1 is a kinetic temperature and since the partition functions are relatively temperature insensitive, we have from equations A-6 and A-9 that

$$\begin{aligned} \frac{\left(\frac{n_C n_H}{n_{CH}} \right)_{NLTE}}{\left(\frac{n_C n_H}{n_{CH}} \right)_{LTE}} &= 10^{-(\theta_{NLTE} - \theta_{LTE}) \cdot D_{CH}(\text{volts})} \\ &= \frac{J_{\nu_0}(\tau_0)}{B_{\nu_0}(\tau_0)} \end{aligned} \quad A-10$$

Thus by computing values for $J_{\nu_0}(\tau_0)/B_{\nu_0}(\tau_0)$ as a function of $\log \tau_0$, we can determine dissociation temperatures for each photospheric layer.

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