STUDIES IN STELLAR EVOLUTION. III. THE CALCULATION OF MODEL ENVELOPES

LOUIS HENYEY, M. S. VARDYA,* AND PETER BODENHEIMER
Berkeley Astronomical Department, University of California
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ABSTRACT

The formal theory underlying existing techniques for representing the superadiabatic layers in convective envelopes is re-examined. Particular emphasis is placed on the discussion of points of uncertainty and possible controversy. The analysis has been carried out in a form which permits the formulation of certain constants, the arbitrariness of whose values represents the inherent uncertainty in the theory. Parallel calculations based on different values of these constants lead to a quantitative evaluation of their effect upon evolutionary tracks in the Hertzsprung-Russell diagram. Marked effects result from uncertainties in the ratio of mixing length to scale height and possibly from inadequate knowledge concerning opacities at low temperatures.

I. INTRODUCTION

In an earlier paper (Henyey, Forbes, and Gould 1964) an elaboration of a technique for the calculation of evolutionary sequences was presented. That paper described the formal method of coupling the surface boundary conditions to the over-all solution for the stellar interior. However, the physical theory and method of calculation involved in obtaining these boundary conditions, through construction of model atmospheres, was not treated in detail. The present paper reviews the equations that are in use in the atmosphere calculation, discusses the approximations that are involved, and examines the influence of various numerical assumptions that are made in the theory.

Recent developments in the theory of stellar evolution have indicated that the structure of late-type giants and pre–main-sequence stars, which have deep convective envelopes, is strongly affected by the surface boundary conditions. Hence it is particularly important to have an understanding of the structure of the atmospheric layers of such stars. The work of Mrs. Böhm-Vitense and others has emphasized the importance of superadiabatic regions in convective envelopes, and it is the theoretical treatment of these regions that turns out to influence the entire structure of theoretical models so sensitively. Unfortunately, since this is also the region where modern atmospheric theory is far from satisfactory, the only available method of treating turbulent convection in superadiabatic layers is, at best, a rough approximation. The difficulty of the treatment of the convection zone occurs simultaneously with other problems affecting the atmosphere as a whole. Line blanketing, sphericity—which is important in the extended atmospheres of late-type stars—and sources of opacity, particularly at low temperatures, are examples of effects that require further approximations and, in some instances, *ad hoc* assumptions in the theory. A more rigorous and complete theory of the outer layers of stars is, of course, highly desirable, and it is hoped that vigorous research activities in the near future will greatly improve the situation. The use of the present theory in stellar-evolution calculations can be justified to some extent, however, if it is clearly understood to what degree the assumptions involved in the atmospheric calculation influence the evolutionary tracks. Therefore, in the following outline of the atmospheric equations we indicate where arbitrary parameters have been introduced, and in the final section we present the results of some calculations of evolutionary sequences that have been designed to test how critical these assumptions are in the evolutionary phases that involve deep convection zones.

* Presently at Joint Institute for Laboratory Astrophysics, Boulder, Colorado.

II. DISCUSSION OF THE METHOD

The model atmospheres that we construct are divided into two types of regions, radiative layers, and superadiabatic convection zones, which require considerably different approaches. However, the equation of state, thermodynamic quantities, and the radiative opacity can be calculated in the same manner in both types of zones. The calculation of these quantities is carried out in some detail. The equation of state and the adiabatic gradient are treated along the lines of Vardya's (1965) work. Hydrogen has been considered in five states, H_2, H_2^+, H^-, H, and H^+; helium has been considered in all of its ionization states; and eight representative metallic elements have been included in the neutral and first ionization states, with provision for including higher states. Molecular hydrogen is not considered if the surface temperature T_f (defined below) exceeds 6000° K. When H_2 is considered, it is cut off below a given depth in the atmosphere if any one of the following conditions is satisfied at that depth: (1) the temperature exceeds 20000° K; (2) $n \leqq 10^{-5}$, where n is the fraction of hydrogen nuclei in the form of H_2; (3) n shows a spurious inward increase, for optical depths $\tau \geqq 0.09$. H^- and H_2^+ are cut off at the same point as H_2. All effects arising from radiation are included in the pressure and internal-energy equations.

A program for computing atmospheric Rosseland mean opacities (Vardya 1964) has been prepared. The sources of opacity included are H_2^-, H^-, H, H_2^+, He, and He^+ in the form of continuous absorption, and H, H_2 and e^- in the form of scattering. A two-dimensional table in temperature T and electron pressure P_e of atmospheric Rosseland mean opacity is read into the electronic computer for use in the computation of model envelopes. Because the opacity program for the interior calculation (cf. Bodenheimer, Forbes, Gould, and Henyey 1965, Appendix B) is slightly incompatible with that for the atmosphere, we interpolate between 75000° and 100000° K such that we pass linearly in T between complete atmospheric opacities at the lower temperature to complete interior opacities at the upper value.

a) *The Outer Radiative Layers*

Regardless of the extent of the convective regions, the very outermost layers are invariably stable against convection. It is true that convection is present in some cases as a result of overshooting (cf. Böhm 1963), but it is also an unfortunate fact that allowance for this effect is extremely difficult on the present level of treatment. The simplest possibility is to consider these layers as being in strict radiative equilibrium. Indeed it is likely that in many cases the effect of overshooting may not be important. Furthermore, in the outermost superadiabatic regions the efficiency of convective transport is so low that the actual gradient is close to the radiative.

In the event that such an equilibrium prevails to great depths one may use the temperature distribution given by Böhm-Vitense (1958):

$$T^4 = \tfrac{3}{4} T_e^4 (\tau + 0.727 - 0.1406 e^{-2.54\tau}) . \tag{1}$$

In her work she has modified this expression to take account of the blanketing by spectral lines. This is done by replacing the effective temperature by a quantity T_e' given by (Baker and Kippenhahn 1962)

$$\left(\frac{T_e'}{T_e}\right)^4 = 1.17(10^{-4} T_e - 1.1)^4 + 1.047 \tag{2}$$

and by adding a term

$$- B e^{-30\tau} , \tag{3}$$

where the coefficient B is given by

$$B = 0.4398(T_e')^4 - (T^0)^4 \tag{4}$$

with

$$\left(\frac{T_e}{T^0}\right)^4 = \begin{cases} -2.087T_e \cdot 10^{-4} + 5.465 & \text{for} \quad T_e < 9800^\circ \text{ K} \\ 2.68T_e \cdot 10^{-4} + 0.79 & \text{for} \quad T_e \geqq 9800^\circ \text{ K}\,. \end{cases} \tag{5}$$

We feel that these formulae need modifications for several reasons. In the first place the linear term in τ in equation (1) should not be modified for arbitrarily large depths in the manner indicated. Its coefficient must approach no other than $\frac{3}{4}T_e^4$ itself. Line effects, if present, must at large depths be included only in the opacity used to calculate τ. The principal effect of blanketing on the form of the right-hand side of equation (1) is to modify the term arising from 0.727. Thus we feel that a preferable expression is obtained by allowing the blanketing corrections to taper off over unit optical depth as follows:

$$T^4 = \tfrac{3}{4}T_e^4(\tau - 0.1406e^{-2\ 54\tau}) + \tfrac{3}{4} \times 0.727(T_e')^4 - Be^{-30\tau}\,. \tag{6}$$

However, further modifications are essential. The expressions (2) and (5) cannot be valid for arbitrarily high effective temperatures. For $T_e > 15000^\circ$ K we have chosen to keep the values of T_e' and T^0 equal to their values at $T_e = 15000^\circ$ K.

Another significant alteration must be made to include the effect of sphericity, which becomes increasingly important as a star passes over to the red-giant phase. The theory of extended photospheres has been considered by Kosirev (1934) and by Chandrasekhar (1934, 1950). The results for the two-stream approximation of Chandrasekhar may be summarized by the statement that the true optical depth must be replaced by the effective optical depth

$$\tau' = \int_0^\tau \left(\frac{R_0}{r}\right)^2 d\tau = \int_{R_0}^r \left(\frac{R_0}{r}\right)^2 d\tau\,. \tag{7}$$

In this expression R_0 is the radius at which we regard the depth to be effectively zero. While it is true that the level of approximation implied by equation (1) is strictly speaking beyond the scope of the theory underlying equation (7), we adopt it since it correctly allows for the variation of the radiative flux with the inverse square of the radius. The substitution of τ' for τ in equation (6) must also be accompanied by a replacement of T_e by a temperature which measures the radiative flux at radius R_0 in accordance with the definition

$$T_f^4 = \frac{L}{4\pi\sigma R_0^2}\,. \tag{8}$$

The allowance for blanketing is based on calculations using solar abundances for the heavy elements. In order to take into account the variation of blanketing with chemical composition we assume that a considerable amount of saturation is present in the features affecting the temperature distribution, and that therefore the deviations from the non-blanketing case vary as the square root of the metal-to-hydrogen ratio in the star $(M/\text{Hy})_*$ (by number). Let

$$\zeta = \left[\frac{(M/\text{Hy})_*}{(M/\text{Hy})_\odot}\right]^{1/2}. \tag{9}$$

The final expression, incorporating all the modifications and replacing equation (6), is therefore

$$T^4 = \tfrac{3}{4}T_f^4(\tau' + 0.727 - 0.1406e^{-2\ 54\tau'}) + \zeta(A - Be^{-30\tau'})\,, \tag{10}$$

where

$$A = [0.6379(10^{-4}T_f - 1.1)^4 + 0.02565]T_f^4\,,$$
$$B = [0.5146(10^{-4}T_f - 1.1)^4 + 0.4605 - C]T_f^4\,. \tag{11}$$

As before we regard the parenthetical expressions as reaching a limiting value of 0.4 at temperatures above 15000° K. The last term in the second equation is a modification of equation (5):

$$C = \begin{cases} (-2.087\times 10^{-4}T_f + 5.465)^{-1} & \text{for} \quad T_f < 9800^\circ\,\mathrm{K} \\ (2.68\times 10^{-4}T_f + 0.79)^{-1} & \text{for} \quad T_f \geqq 9800^\circ\,\mathrm{K}\,. \end{cases} \tag{12}$$

As indicated above, the formulae which we have devised strictly apply to a semi-infinite atmosphere. Although previous investigations have used them in the presence of an underlying convective region it must be emphasized that the temperature gradient as modified by convection must alter, to some extent, the properties of the radiative layer.

The complete treatment of the radiative layer must, of course, also include application of the equation of hydrostatic equilibrium:

$$\frac{dP}{dr} = -g\rho\,. \tag{13}$$

As discussed later the position of the photosphere is defined as the layer where $\tau = \frac{2}{3}$ using the true optical depth. It is necessary to integrate the relation, supplementary to equation (7) for τ':

$$\frac{d\tau}{dr} = -\kappa\,, \tag{14}$$

where κ is the volume Rosseland mean opacity. In order to provide for the eventuality of a deep envelope, we integrate for mass and radius, and thus allow for a variable value of the acceleration of gravity g.

The above equations have been written in difference form for the purpose of numerical integration. Let us divide the whole envelope into spherical shells, and let the subscripts j and $j+1$ designate physical quantities evaluated at the outer and inner edge, respectively, of the jth shell. The mean value of a quantity over the width of the shell is designated by the subscript $j+\frac{1}{2}$. These means are linear unless noted otherwise. Note that m_j represents the total mass of the star interior to point j and that the radius r_j is measured from the center of the star. We write

$$\Delta r = r_{j+1} - r_j\,, \tag{15}$$

$$\Delta\tau' = \tau'_{j+1} - \tau_j'\,, \tag{16}$$

$$m_{j+1} = m_j + 4\pi\rho_{j+1/2}r^2_{j+1/2}\Delta r\,, \tag{17}$$

$$g_{j+1/2} = Gm_{j+1/2}/r^2_{j+1/2}\,. \tag{18}$$

Then the difference form of equations (13) and (14) is

$$P_{j+1} = P_j - g_{j+1/2}\rho_{j+1/2}\Delta r\,, \tag{19}$$

$$\Delta\tau' = \frac{2R_0^2\,\kappa_{j+1/2}\Delta r}{r^2_{j+1} + r_j^2}\,. \tag{20}$$

The solution of these equations is carried out through iteration of the electron pressure $P_{e,j+1}$ for the forward mesh point $j+1$. To proceed from point j to point $j+1$ we first increase τ' by an arbitrary small increment to define the location of $j+1$. The temperature T_{j+1} then is fixed by equation (10) and need not be iterated. The first guess for $P_{e,j+1}$ is obtained by extrapolation from the converged values of this quantity at points j and $j-1$, if available. Using the temperature and the provisional electron pressure, we enter the equation-of-state and opacity calculations to obtain P, ρ, and κ for $j+1$. We then obtain r_{j+1} from equation (20), treated as a quadratic equation in that variable, after which it is possible to calculate $m_{j+1/2}$ and $g_{j+1/2}$ from equations (17) and (18), respectively. The pressure P_{j+1} is recalculated from equation (19) and the procedure is repeated, after modification of P_e, until the pressures obtained from the equation of state and from expression (19) agree to within a given tolerance.

b) Convective Layers

Our treatment of convective regions is based on the formalism developed by Mrs. Böhm-Vitense (1958; also Vitense 1953). For completeness we list all of the important equations but describe in detail only the modifications which we have introduced. If no explanation or derivation accompanies an expression, it may be found in her papers.

The pressure scale height is

$$H=\frac{P}{g\rho}. \tag{21}$$

In our calculation P is the sum of the thermodynamic pressure P_{th} (gas plus radiation) and the turbulent pressure, given as a function of density, ρ, and mean turbulent speed, v:

$$P_{\text{turb}}=\beta\rho v^2=\rho\langle v^2\rangle . \tag{22}$$

This expression is based upon the assumption of isotropic turbulence. Here $\langle v^2\rangle^{1/2}$ is the rms speed; we consider only the radial component of the motion. Unsöld (1955) recommends a value of $\frac{1}{2}$ for the constant β, a value used by most investigators. However, the mean value of the square of the speed is invariably larger than the square of the mean speed, so β must be larger than unity. For example, a normal distribution of velocity leads to

$$\beta=\left(\frac{2}{\sqrt{\pi}}\int_0^\infty x^2 e^{-x^2}dx\right)\Big/\left(\frac{2}{\sqrt{\pi}}\int_0^\infty x\, e^{-x^2}dx\right)^2=\frac{\pi}{2}. \tag{23}$$

A rectangular distribution gives $\beta=\frac{4}{3}$, while a two-stream model gives precisely $\beta=1$. Although we prefer the value $\pi/2$, we will consider various test calculations devised to verify the importance of the value of β.

To describe the actual temperature versus pressure gradient in a given layer of the atmosphere, we use the usual notation

$$\nabla=\frac{d\ \ln T}{d\ \ln P}. \tag{24}$$

Various other aspects of this derivative are designated by subscripts or superscripts. The radiative net flux is

$$F_{\text{rad}}=16\sigma T^4\nabla/3\kappa Hf . \tag{25}$$

This expression contains a factor f devised to represent the same type of correction to the radiative diffusion approximation which appears in the radiative T–τ relation (6). As a matter of fact, we calculate f as if radiative transport prevails in order to eliminate an annoying discontinuity in the condition for radiative instability which might otherwise appear at the radiative-convective boundary, particularly when it appears at a shallow depth. The factor f, which is close to unity for optical depths greater than 1, is given by

$$f = \frac{4}{3T_f^4} \frac{d}{d\tau'} (T^4) \tag{26}$$

and is calculated by differentiation of equation (10).

In terms of the total net flux F, the definition of the so-called radiative gradient ∇_{rad} is

$$F = 16\sigma T^4 \nabla_{\text{rad}}/3\kappa H \,. \tag{27}$$

The convective net flux, F_{conv}, is

$$F_{\text{conv}} = \tfrac{1}{2} C_p \rho v \alpha T (\nabla - \nabla') \,, \tag{28}$$

where C_p is the specific heat per unit mass at constant pressure, ∇' is the gradient describing the internal changes in convective bubbles as they move, and

$$\alpha = l/H \tag{29}$$

is the ratio of mixing length to scale height.

The mean speed can be written in terms of the difference of the gradients $\nabla - \nabla'$ as

$$v^2 = gHQ\alpha^2 (\nabla - \nabla')/\nu \tag{30}$$

with

$$Q = -\frac{T}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p , \tag{31}$$

the derivative taken at constant thermodynamic pressure. Following Biermann (1948), Mrs. Böhm-Vitense uses a value of 8 for the constant ν. It is possible to argue that its value is somewhat larger if more than half of the acquired kinetic energy is dissipated by turbulent viscosity. Test calculations, which verify the sensitivity of the results on the value used for ν, are discussed later in the report.

The efficiency factor γ for convection is given by

$$\gamma = \frac{\nabla - \nabla'}{\nabla' - \nabla_{\text{ad}}'} \,. \tag{32}$$

We here depart from the treatment of Mrs. Böhm-Vitense by introducing the modified adiabatic gradient ∇_{ad}':

$$\nabla_{\text{ad}}' = \left(\frac{d \ln T}{d \ln P_{\text{th}}} \right)_{\text{ad}} \left(\frac{d \ln P_{\text{th}}}{d \ln P} \right) = \nabla_{\text{ad}} \cdot \frac{d \ln P_{\text{th}}}{d \ln P} , \tag{33}$$

which involves a conversion to the variation of temperature with total pressure, including P_{turb}. This is necessary since the unmodified adiabatic gradient ∇_{ad} is referred to thermodynamic pressure while all other gradients in equation (32) are referred to the total pressure (however, see below, § II*c*).

For the limiting case of a transparent bubble,

$$\gamma = C_p \rho v / 8\sigma T^3 \omega \,, \tag{34}$$

where

$$\omega = l\kappa \,, \tag{35}$$

the optical thickness of the bubble. Our expression differs from equation (55.37) of Unsöld (1955) in that the factor 16 given by him has been replaced by 8. The point is that the *total* energy emitted is given by $\frac{1}{2}\Delta T$, which is the *average* temperature difference. Therefore his equation (55.36) should contain an extra factor of $\frac{1}{2}$.

The situation for γ in the opaque case is subject to some controversy. This case may be expressed in a general form:

$$\gamma = C_p \rho v \omega y / 8\sigma T^3 , \tag{36}$$

where y is a constant depending on the particular model for a bubble. Mrs. Böhm-Vitense uses $y = \frac{1}{2}$, a value derived from a linear temperature distribution. On the other hand a parabolic law gives $y = \frac{1}{20}$. Perhaps a more plausible model results from the assumption that inside a bubble

$$T^4 = T_1^4 + (T_0^4 - T_1^4) \frac{\sin a r}{a r}, \tag{37}$$

with T_1 the average environmental temperature and T_0 the central temperature. This expression satisfies a diffusion equation for T^4 with a constant diffusion parameter. Here,

$$al = 2\pi \tag{38}$$

since $l/2$ is the radius of the bubble. A similar approach has been considered by Spiegel (1957). For this model $y = 3/4\pi^2$. The effects of the use of different values of y are discussed, using test calculations, in the last section of this report.

A convenient interpolation between the transparent and opaque cases is given by

$$\gamma = (C_p \rho / 8\sigma T^3 \theta) v \equiv \gamma_0 v , \tag{39}$$

where γ_0 is so defined and where

$$\theta = \frac{\omega}{1 + y\omega^2} . \tag{40}$$

The quantities F, v, and ∇' may be eliminated by combining equations (25)–(28), (30), (32), and (39) and by making use of the equation

$$F = F_{\text{conv}} + F_{\text{rad}} \tag{41}$$

to derive the cubic equation in γ:

$$\gamma + \gamma^2 + \phi\gamma^3 = \frac{gHQ(a\gamma_0^2)}{\nu}(f\nabla_{\text{rad}} - \nabla_{\text{ad}}') , \tag{42}$$

where

$$\phi = \tfrac{3}{4}\omega\theta f . \tag{43}$$

In effect this is a cubic equation for v, in view of the outer members of equation (39). Also it should be noted that, in addition to the cubic part, the velocity is also contained in ∇_{ad}' because of the second pair of parentheses in equation (33); however, this is not true if $\nabla_{\text{ad}}' = \nabla_{\text{ad}}$. From equations (30), (32), (39), and (42) we may obtain the true gradient:

$$\nabla = \frac{(1+\gamma) f\nabla_{\text{rad}} + \phi\gamma^2 \nabla_{\text{ad}}'}{1 + \gamma + \phi\gamma^2} . \tag{44}$$

The solution of the equations for the convective region is somewhat more complicated than it is for the radiative region. The scheme of solution is based on an iterative cycle involving three independent variables—the electron pressure P_e, the actual gradient ∇, and the dimensionless quantity γ defined by equation (32). We define the size of the step from point j to point $j + 1$ by fixing T_{j+1} at a value about 3 or 4 per cent higher than T_j. Then first approximations for the variables $P_{e,j+1}$, ∇_{j+1}, and γ_{j+1} are provided by extrapolation. We obtain the total pressure, including gas pressure, radiation pressure, and turbulent pressure, from the estimated gradient by expressing equation (24) in difference form:

$$\nabla_{j+1/2} = (T_{j+1} - T_j)(P_{j+1} + P_j)/(T_{j+1} + T_j)(P_{j+1} - P_j) , \tag{45}$$

and solving for P_{j+1}:

$$P_{j+1} = P_j \left[\frac{1 + (1/\nabla_{j+1/2})(T_{j+1} - T_j)/(T_{j+1} + T_j)}{1 - (1/\nabla_{j+1/2})(T_{j+1} - T_j)/(T_{j+1} + T_j)} \right] . \tag{46}$$

Given the fixed value of T_{j+1} and the provisional value of $P_{e,j+1}$, the equation of state provides ρ_{j+1}, $\nabla_{\mathrm{ad},j+1}$, Q_{j+1}, $C_{p,j+1}$, after which equations (17)–(19) are solved for m_{j+1} and r_{j+1}. The quantities H_{j+1}, θ_{j+1}, ϕ_{j+1}, and $\gamma_{0,j+1}$ follow from equations (21), (40), (43), and (39), respectively. We now find that a Newton-Raphson technique (Henyey, Wilets, Böhm, LeLevier, and Levée 1959) may be used successfully for the simultaneous solution of three equations of condition in the three basic variables P_e, ∇, and γ. One of these is equation (42) and a second is equation (44) with all quantities evaluated at the point $j + 1$. Finally the condition

$$P_{j+1} = P_{\mathrm{th},j+1} + P_{\mathrm{turb},j+1} \tag{47}$$

is applied, with P_{j+1} determined by equation (46), P_{th} calculated from the equation of state, and P_{turb} expressed in terms of γ through equations (22) and (39). The basic variables are adjusted after each iteration, and the whole cycle, starting with equation (46), is repeated until conditions (42), (44), and (47) are all satisfied to within 0.1 per cent. If the atmospheric calculation extends to sufficient depth so that radiative equilibrium is restored, we set $\gamma = 0$, and the equations reduce to the radiative case. The scheme is such that more than one convective zone can be taken into account.

c) Miscellaneous Considerations

A basic result to be derived from the calculations is the radius of the photosphere and, where sphericity is important, the effective temperature. We have adopted the convention that the photosphere occurs at $\tau = \frac{2}{3}$ and that the radius at this depth in conjunction with the luminosity determines the effective temperature:

$$L = 4\pi R_{2/3}^2 \sigma T_e^4 . \tag{48}$$

For thin atmospheric layers the derived values of T_e are insensitive to the value adopted for τ at the photosphere. For extended atmospheres that exist in red giants and supergiants, the value may be more critical. In fact, it is possible that stars exist whose photosphere is not sharply defined. Integrations carried tangentially across the atmosphere would be helpful in clarifying this question.

In starting an integration it is convenient to place $\tau = 0$ at a finite radius R_0 rather than at infinity. The first radiative zone is taken at a small preassigned optical depth. A certain amount of arbitrariness is clearly present in the choice of the exact value adopted, although the effect on the radius at the photosphere and on the physical quantities at the layer of contact with the interior calculation should be negligible.

In addition to the various approximations and *ad hoc* assumptions described above, a serious flaw may exist in our theory because of a complete lack of any reference to the energy in the field of turbulent velocities. It is possible that the energy given to this field is deposited non-locally and that there exists an additional flux term describing the transport of turbulent kinetic energy. We have not succeeded in finding a convincing treatment of this feature, although we attempted one crude scheme based on the velocity gradient, which produced inconclusive results.

In our test calculations of the solution of the equations for the convective region, a substantial numerical, and therefore spurious, instability appeared, which we found to be associated with the second factor in the expression (33) for ∇_{ad}'. This equation depends on the velocity in a manner that seems to cause considerable numerical difficulty for extended atmospheres of red-giant stars. For this reason we have arbitrarily ignored the troublesome factor and have set ∇_{ad}' equal to ∇_{ad} itself. We believe that this approximation does not substantially affect the total structure of the atmosphere since in the layers where ∇_{ad}' differs significantly from ∇_{ad} the actual gradient is generally closer to the radiative than to the adiabatic.

III. COMPUTATIONAL RESULTS

The theory as given in the preceding sections involves several features that are somewhat indeterminate. These enter the calculation in the form of several constants whose values are imperfectly known. Using the techniques described by Henyey *et al.* (1964) in conjunction with investigations of post–main-sequence evolution, we have completed a number of calculations of sequences which are based on variations in the values of these constants. Here we describe only those aspects of the calculations which bear directly on the atmospheric problem and leave the discussion of the detailed structural and evolutionary aspects for a future report. The computational effort has been concentrated on the red-giant phase for a configuration of 5 $M_\odot$ and has been directed toward a study of the quantities β, ν, y, and l/H, which have been defined in the previous section. In addition, the influence of an artificial opacity contribution at low temperatures has been examined. Less detailed calculations are also described for 2.5 $M_\odot$ and 30 $M_\odot$.

The ratio l/H is probably the quantity whose behavior is most mysterious. A constant value causes the mixing length to vary in proportion to the pressure scale height. By properly varying the ratio with depth one can contrive other laws; for example, by so doing one can cause the mixing length to vary in proportion to the density scale height. The physically correct procedure is probably one in which a non-local mixing length is used, as in calculations by Ezer, Stein, and Cameron (1963) and by Hofmeister and Weigert (1964). These investigators detected some differences from the results which are obtained by using a local mixing length, but they concluded that these differences were small insofar as the over-all properties of the configuration are concerned. Since the theory, in more than one aspect, has not reached a high level of refinement, the introduction of the complexities that result from the use of the non-local concept seems to be premature for our purposes.

Figure 1 describes the computed evolutionary track for the configuration of 5 $M_\odot$. We show it here for reference without any intention of discussing the evolutionary aspects. We merely point out that it shows a short pre–main-sequence track (AB) which involves some of the complications discussed by Bodenheimer *et al.* (1965) relating to C^{12} abundance; the main-sequence band (BC); and the post–main-sequence track (CD) which has been carried to a point where the central He^4 concentration has been reduced to 0.56 through conversion to O^{16}. The atmospheric parameters have no influence whatsoever during the greatest portion of this computed curve; only in the extreme red-giant phase, to the right of the point $\log T_e = 3.7$, do the tracks based on different values of the parameters begin to separate. This same region is characterized by a deep convective envelope which, at its greatest extent, covers about two-thirds of the mass of the star. Of particular interest is the value of the lowest effective temperature for the star that can be achieved in the calculations and the corresponding values of the various arbitrary constants.

Figure 2 shows the effect of varying l/H through the values 1.5, 1.0, and 0.5 in the region of interest. All other constants have the same value as in Figure 1; therefore, the curve marked $l/H = 1.5$ is simply the extreme right-hand portion of Figure 1. The curves for $l/H = 1.5$ and 1.0 include portions of the evolutionary track which return in the direction of the main sequence. The calculation for $l/H = 0.5$ was terminated before the minimum temperature was achieved. It is clear from Figure 2 that changes in l/H produce considerable variation in the effective temperatures of red-giant models. Similar conclusions result from an examination of Figure 3, wherein the red-giant phase for 2.5 $M_\odot$ is displayed for $l/H = 1.5$ and 1.0. As a matter of fact, in this case the effect takes hold even before the abrupt rise in luminosity begins. In the case of the curve for $l/H = 1.0$ only a short portion of the vertical branch is shown. All other constants have the same values as in Figure 1.

The early pre–main-sequence evolution is also characterized by the presence of deep convective envelopes and by a steep vertical track in the H-R diagram, except in this case the star evolves downward and to the left. Portions of the pre–main-sequence evolutionary path for a configuration of 5 $M_\odot$ are illustrated in Figure 4 for $l/H = 1.5$ and

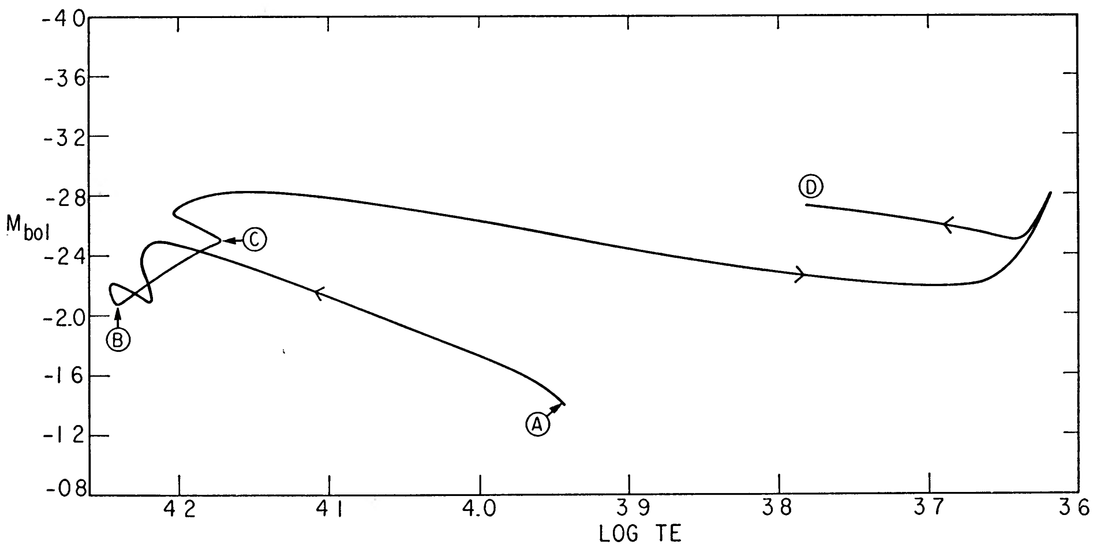

FIG. 1.—The complete evolutionary track in the (log T_e, M_{bol}) plane computed for 5 $M_\odot$. Indicated points are explained in the text. Appropriate parameters are hydrogen content $X = 0.68$; metal content $Z = 0.03$; $l/H = 1.5$; $y = 0.076$; $\beta = 0$ 5; $\nu = 8$.

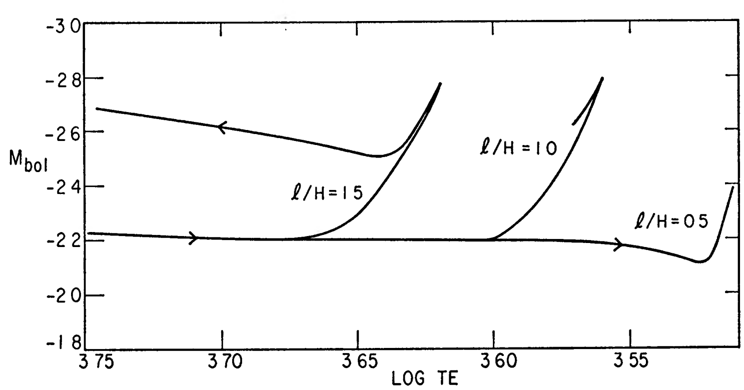

FIG. 2—Portions of the post–main-sequence evolutionary track for 5 $M_\odot$, indicating the influence of l/H upon calculated effective temperatures. The three branches correspond to $l/H = 1.5$, 1.0, and 0.5, respectively; all other parameters have the same values as in Fig 1.

1.0. Internally, there are important differences in the structures of pre– and post–main-sequence models. Yet the influence of l/H on the calculated effective temperatures is approximately the same. To the left of log $T_e = 3.7$ the convective envelope no longer has great influence on the structure of the star, and the curves corresponding to different values of l/H quickly merge.

The use of a value for l/H that varies according to depth must also be considered. For example, constant proportionality of the mixing length to the density scale height may thus be achieved. In the red-giant phase for very high masses, substantial density gradient inversions are predicted in the hydrogen-ionization region. For example, a calculation of a model atmosphere made for 30 $M_\odot$ in the strongly convective pre–main-sequence phase (with a radius of 700 $R_\odot$) indicated a drop in density by a factor of 4 between temperatures 5000° and 22000° K. It might be argued that the use of the density scale height for l might eliminate the inversion. Our provisional impression, not conclusively demonstrated as yet, is that such is the case, but that the resulting computed value of the mixing length will be inadmissibly long. This conclusion follows primarily from the observation that the pressure scale height is already excessively long

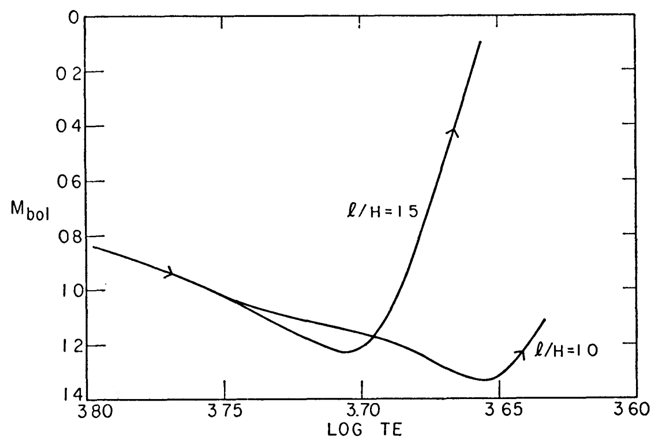

FIG. 3.—Portions of post–main-sequence evolutionary tracks for 2.5 $M_\odot$; $X = 0\ 68$, $Z = 0\ 03$. The effect of l/H in determining the point of turn-up in the H-R diagram is quite similar to that for the case of 5 $M_\odot$.

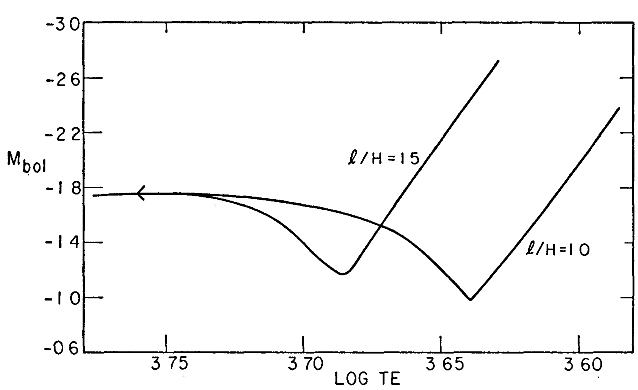

FIG. 4.—Early pre–main-sequence evolutionary tracks for 5 $M_\odot$, covering the region of transition between fully convective and fully radiative configurations. The effect of varying l/H is shown; other parameters have the values $y = 0.375$, $\beta = 0.5$, $\nu = 8$.

in the extreme circumstances which lead to an inverted density gradient. Further work on this point is definitely needed.

The parameter y is apparently directly involved in the degree of adiabaticity within the ascending and descending currents. Surprisingly, varying it over a considerable range produces comparatively little effect on the computed track. For 5 $M_\odot$, with $l/H = 1.0$, the effect of four widely divergent values of y is illustrated in Figure 5. Calculations were also carried out for the same mass but with $l/H = 1.5$ for the cases $y = 0.375$ and

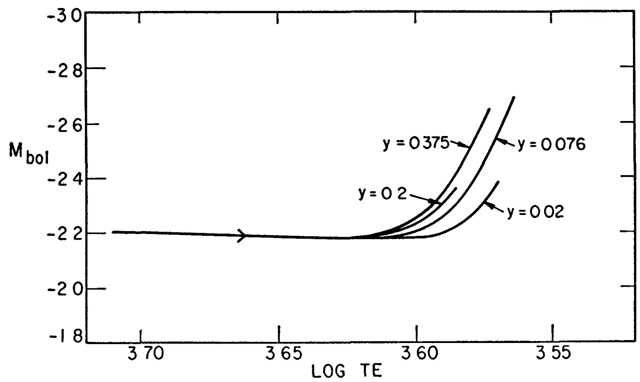

FIG. 5.—Segments of post–main-sequence evolutionary tracks for 5 $M_\odot$, indicating the effect of varying the parameter y through the four values 0.375, 0.2, 0.076, and 0.02; l/H is held fixed at 1.0; all other parameters have the same values as in Fig. 1.

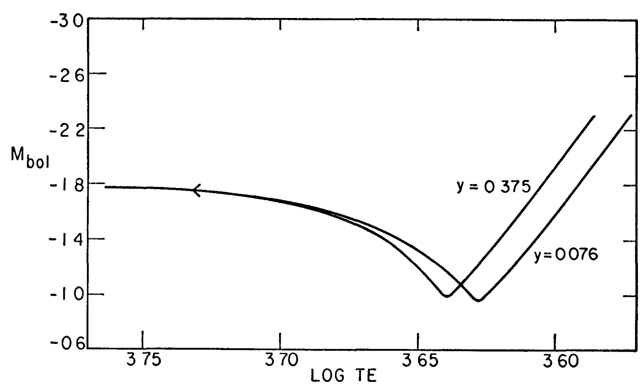

FIG. 6.—Pre–main-sequence evolutionary tracks for 5 $M_\odot$, indicating the effect of changing the parameter y from 0.375 to 0.076; $l/H = 1.0$; all other parameters have the same values as in Fig. 4.

0.076. The separation of the curves for these two values of y was not affected by the change in l/H. Finally, the influence of y in pre–main-sequence computations is shown in Figure 6, for the case of 5 $M_\odot$ and $l/H = 1.0$. As expected, the larger values of y, corresponding to better "insulation" of the moving elements, give the tracks with the higher effective temperatures. Since one might have expected the effect of changing y to be serious, we feel that the relative insensitivity to the value of y is an important result. Although the value of $y = 0.076$ appears to be the most reasonable one, we need not be concerned with the precise value while other larger uncertainties are present.

A completely null result followed when β, which measures the departure of the rms speed from the mean speed, was varied. Two tracks based on $\beta = 0.5$ and 1.0, for 5 $M_\odot$ and $l/H = 1.5$, differed by such a small amount that we were not able to construct a diagram that revealed the differences. However, in models characterized by larger turbulent pressures the differences may be more significant.

Changing the value of ν produces the results given in Figure 7. The values 8.0, corresponding to the dissipation of half the turbulent kinetic energy generated, and 16.0, corresponding to dissipation of three-fourths of the energy, are considered. The differences in the computed tracks are significant but not excessive. Since the lower value

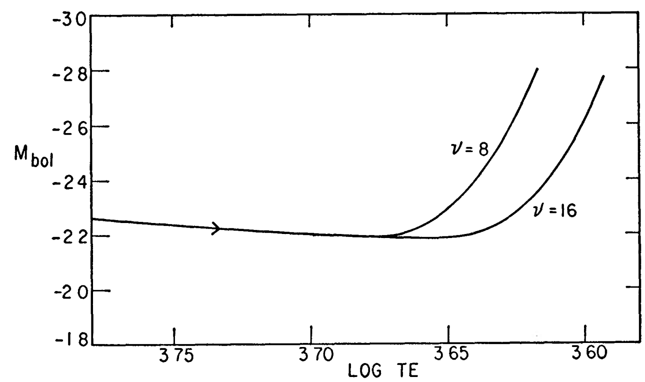

FIG. 7.—Segments of post–main-sequence evolutionary tracks for 5 $M_{\odot}$, indicating the effect of changing the parameter ν from 8 to 16. Other parameters have the same values as in Fig. 1.

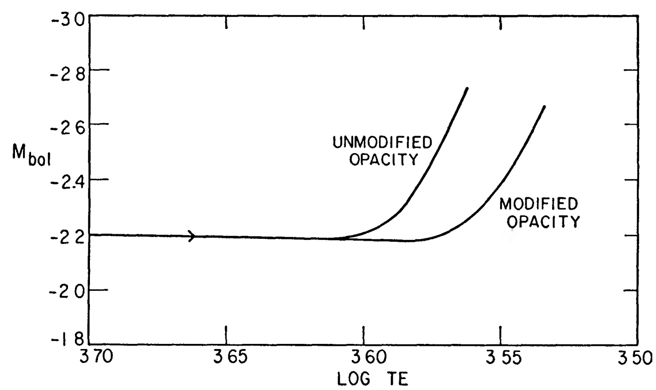

FIG 8.—Segments of post–main-sequence evolutionary tracks for 5 $M_{\odot}$; values of parameters are $l/H = 1\ 0$; $y = 0\ 076$; $\beta = 0.5$; $\nu = 8$. The curve labeled "modified opacity" illustrates the effect of the inclusion of a significant artificial increase in the opacity in the outer layers of the star.

leads to more vigorous convection, it produces the track with the higher effective temperature during the phase of increasing luminosity. The tracks in Figure 7 represent the red-giant phase, again for 5 $M_{\odot}$.

One source of uncertainty in the calculations may result from an inadequate knowledge of atmospheric opacities at low temperatures. Faulkner, Griffiths, and Hoyle (1963) have speculated on this point with reference to the pre–main-sequence Hayashi track for the Sun. We have therefore compared the results obtained with and without the inclusion of an artificial factor which increases the opacity obtained from the table at temperatures below 4500° K. We assume that in this temperature range the artificial factor varies linearly with the temperature, being unity at 4500° K and increasing to a value of 45 at 2500° K. The resulting track is exhibited in Figure 8 where it is compared with the one based on an unmodified opacity; in both cases $l/H = 1.0$. The temperature of 2500° K is the lowest reached in the outermost layers of the atmosphere at the last point given for the modified track. Obviously any result may be obtained by such an *ad hoc* modification; however, that which we give does provide a measure of the importance of the effect.

The general conclusions that may be drawn from these test calculations cannot be definitely stated since they highlight uncertainties rather than verities. Although the ranges of the modifications that have been introduced may be rather larger than acceptable, they are not overly so with reference to our present level of uncertainty in the theory. There seems little doubt that significant variations result.

We hope that comparison with observations may provide a key to the solution of some of these problems. In this connection the occurrence of red supergiants in h and χ Persei should be a fruitful point of departure for calibrating the theory. This cluster possesses the best available data for so doing.

Note added in proof: The relationship between the temperature T and the optical depth τ, which is described in Section II and summarized in equation (10), has proved (Krishna Swamy 1965) to be quite unsatisfactory in accounting for details of various solar absorption lines. The limb-darkening measurements of Pierce (unpublished) as analyzed by Mitchell (1959) have been used to derive a numerical relationship between T and τ by Cayrel and Jugaku (1963). Krishna Swamy has represented these numerical values by the following interpolation formula:

$$T^4 = \tfrac{3}{4} Te^4 (\tau + 1.4 - 0.825 e^{-2.54\tau} - 0.25 e^{-30\tau}) . \tag{49}$$

He has found that the wings of several strong lines can be represented in a satisfactory manner by line-profile calculations based in part on this expression. We have adopted equation (49) in our calculations in place of equation (10) and the auxiliary equations (11) and (12). Also, τ must still be replaced by τ' as defined in equation (7). Moreover, an attempt to derive a general non-gray correction throughout the entire temperature scale from existing published models has proved unsuccessful. It appears that most of these models have not been iterated sufficiently to provide a clear basis for such a program.

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