# COMPOSITION CHANGES DURING STELLAR EVOLUTION

# Peter P. Eggleton

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#### SUMMARY

This paper presents an algorithm by means of which composition changes in stars due to nuclear reactions, convection and semiconvection can be relatively simply calculated. The algorithm is based on a simple physical picture of convective mixing as a diffusion of convective cells throughout a region of a star; however it is not essential to the method that this physical picture be exact. We attempt to show that the method tends, in a limiting sense, to give results which are identical with the 'standard' treatment of mixing by convection or semiconvection, for a wide range of possible physical models of convective mixing. The essence of the method is the simultaneous solution, in an implicit difference scheme, of equations governing both the structure and the composition changes in a star. One defect of the method as it was employed here is discussed, and some solutions suggested. Qualitative results are presented for a 14  $M_{\odot}$  main sequence star and a 0.775  $M_{\odot}$ horizontal branch star.

# I. INTRODUCTION

During the lifetime of a star, its composition, i.e. the relative abundances of different elements and isotopes, changes basically because of nuclear reactions in the deep interior. However, at a given point in a star, for instance at a given mass coordinate, the changes in composition with time may be due either to nuclear reactions or to convective mixing; and in certain circumstances it may be necessary to invoke the concept of semiconvective mixing (Schwarzschild & Härm 1958; Paczyński 1970). The purpose of this paper is to describe a numerical procedure by which these three composition-changing processes can be included rather simply in an evolutionary calculation. The method is based on a highly qualitative physical picture of convection and semiconvection as a diffusion mechanism. Although such a diffusion mechanism may be capable of giving quite an accurate description of mixing, given a reasonable theory regarding the velocity and mean free path of convective elements, we seek to show that numerical results of quite sufficient accuracy can be obtained using expressions for the rate of diffusion of composition which have no relation to physics but are chosen only for numerical convenience.

Let us define s and c to be sets of functions which describe the structure and composition distribution respectively in a star. Notionally, we can write differential equations of the form

$$\frac{dc}{dt} = f[s, c] \tag{1}$$

$$\frac{ds}{dt} = g[s, c] \tag{2}$$

for the composition and structure distributions, where f, g are functionals (which cannot, of course, be written explicitly as functions of s, c). For a finite time-step  $\Delta t$  we can approximate equations (1) and (2) in an 'explicit' fashion

$$\Delta c = f[s, c] \,\Delta t \tag{3}$$

$$\Delta s = g[s, c] \,\Delta t, \tag{4}$$

where s, c, are the structure and composition at the beginning of the interval. However, the nature of nuclear burning, of hydrostatic equilibrium and of diffusion processes including the diffusion of heat through the star and the diffusion of composition through convection regions, is such that we would expect an ' implicit ' method, i.e. the simultaneous solution for  $\Delta c$ ,  $\Delta s$  of the equations

$$\Delta c = f[s + \Delta s, c + \Delta c] \,\Delta t \tag{5}$$

$$\Delta s = g[s + \Delta s, c + \Delta c] \Delta t, \tag{6}$$

to be more reliable. For sufficiently small  $\Delta t$ , both the implicit and explicit formulations give much the same accuracy, but in the explicit scheme errors tend to grow exponentially with time, unless  $\Delta t$  is taken unreasonably small, whereas in the implicit scheme errors tend to be damped exponentially.

Computational methods of which we are aware tend to be a mixture of implicit and explicit treatments. For instance, the scheme

$$\Delta c = f[s, c] \,\Delta t \tag{7}$$

$$\Delta s = g[s + \Delta s, c + \Delta c] \Delta t \tag{8}$$

gives the composition changes explicitly, while solving for the structure implicitly. A more reliable procedure is to iterate towards a solution of equations (5), (6), for instance thus:

$$\Delta c_n = f[s + \Delta s_{n-1}, c + \Delta c_{n-1}] \Delta t \tag{9}$$

$$\Delta s_n = g[s + \Delta s_n, c + \Delta c_n] \Delta t. \tag{10}$$

This scheme will be started with an initial guess  $\Delta s_0$ ,  $\Delta c_0$ , which might be zero, for instance. If such a scheme converges at all, we would expect it to converge to the solution of equations (5) and (6). However, even if a solution of the implicit equations exist, there is no guarantee that equations (9) and (10) will converge to it; and while they generally do converge when semiconvection is absent, there appears to be some difficulty, or a complete lack of convergence, when semiconvection arises (Paczyński 1970). On the other hand, solving the fully implicit scheme, equations (5) and (6), should not have this difficulty, since no iteration is involved at this level (but note that an internal iteration is normally involved, since equations such as (5) and (6) together, or (8) by itself, are usually transcendental and have to be solved by some such iterative procedure as Newton-Raphson). It is our experience that a totally implicit scheme, which involves solving simultaneously for both the structure and the composition, can be very effective, particularly when semiconvection arises.

In a previous paper (Eggleton 1971) hereafter referred to as Paper I, the author has outlined a method for computing stellar evolution in which composition changes are calculated implicitly. In Paper I this technique was used only for a star in which there was little or no convective or semi-convective mixing, and

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it was shown that in this simple case the method was very effective in dealing with thin shell sources of nuclear energy in low mass red giants. Paper I also outlined a possible modification to the method which would allow both convection and semiconvection to be incorporated very simply. In the present paper we show that this modification does in fact work in some circumstances, and probably would have worked in all circumstances had we not made an unfortunate error which will be described in due course. The method is applied here to two stars: one is a massive star (14  $M_{\odot}$ ), in which a linked convection/semiconvection zone appears for a short time during the rapid collapse of the helium core towards helium burning; the other is a putative horizontal branch star of 0.775  $M_{\odot}$ , in which a substantial semiconvection region surrounds the fully convective helium burning core during much of the star's lifetime on the horizontal branch. The evolution of the chemical composition of these stars is crudely illustrated in Figs 1 and 4.

#### 2. CONVECTIVE AND SEMICONVECTIVE MIXING

We have already outlined in Paper I the method used here, and so we begin by elaborating on the treatment of convection and semiconvection as a diffusion process. Let us define, in the standard way, three temperature gradients  $\nabla_a$ ,  $\nabla_r$ and  $\nabla$  (each being a gradient of log T against log P):

$$\nabla_a = \left(\frac{\partial \log T}{\partial \log P}\right)_{s, \text{ composition}} \tag{11}$$

$$\nabla_r = \frac{3\chi PL}{16\pi a c Gm T^4} \tag{12}$$

$$\begin{aligned} \nabla &= \nabla_r & \text{if } \nabla_r \le \nabla_a \\ &= \nabla_a + F(\nabla_r - \nabla_a) & \text{if } \nabla_r \ge \nabla_a. \end{aligned}$$
(13)

 $\nabla_a$ , which generally lies in the range 0.05  $\leq \nabla_a \leq$  0.4, is the adiabatic temperature gradient;  $\nabla_r$ , the 'radiative gradient', is the temperature gradient which would be necessary to carry all the heat flux if convection were incapable of carrying heat; and  $\nabla$  is the actual gradient that the star adopts, assuming (in convection zones) that the flux of heat carried by convection is given by some local formula such as the mixing length theory of Böhm-Vitense (1958) provides. We shall refer to the quantity  $\nabla_r - \nabla_a$ , which determines whether the region is stable or unstable to convection, as the 'superadiabaticity'. The function F in equation (13) is in principle known, given some local theory of convective heat transport.

We suppose that the mixing of composition by convection is given by an equation of the form

$$\frac{d}{dm}\left(\sigma \frac{dX}{dm}\right) = \frac{DX}{Dt} + XR_X - S_X \tag{14}$$

where X is the fraction by mass of a particular nuclear species,  $XR_X$  is the rate at which it is being burnt,  $S_X$  is the rate at which it is being produced by other reactions (if any), and  $\sigma$  is a diffusion coefficient depending on the superadiabaticity of the material. Ordinary derivatives are used for derivatives with respect to a space variable such as the mass coordinate *m*, and D/Dt implies a Lagrangian time derivative, i.e. a derivative following the motion (we assume spherical symmetry

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throughout). Equation (14) clearly also applies in radiative zones provided we take

$$\sigma = 0 \quad \text{if } \nabla_r < \nabla_a. \tag{15}$$

We shall shortly attempt to show that equation (14) also can be made to apply in semiconvection zones, provided the function  $\sigma$  is suitably chosen.

A mixing-length theory of convection would suggest that, on dimensional grounds,

$$\sigma \sim v l (4\pi r^2 \rho)^2 \tag{16}$$

where v is the velocity of a typical convective element and l is the mixing length. The Böhm-Vitense mixing length theory, as described by Baker & Temesvary (1966), leads to the following estimates

$$l = \alpha H_p, \tag{17}$$

$$v^3 \sim \alpha. (\nabla_r - \nabla_a). \frac{cP_r}{\chi \rho^2 H_p},$$
 (18)

where  $H_p$  is the pressure scale height, c is the velocity of light,  $P_r$  is the radiation pressure,  $\chi$  is the opacity, and  $\alpha$  is presumed to be a constant of order unity. In surface convection layers this formula should be reasonable except very close to the surface, where supersonic velocities may be indicated, and where radiative heat loss from rising elements to the surrounding medium has to be considered. In central convection zones we need to make the following reservations:

1.  $H_p$  tends to infinity at the centre, so perhaps it should be replaced by something which tends to a finite value at the centre;

2. The entire convective core is anyway only one or two pressure scale heights in depth;

3. Near the boundary of the core, the mixing length is presumably at most the smaller of  $\alpha H_p$  and the distance from the boundary.

Ignoring these considerations for the moment, we can estimate  $\sigma$  in typical stellar cores, and compare it with the dimensional quantity  $m_*^2/t_*$ , where  $m_*$  is the star's mass and  $t_*$  is its life time in the current evolutionary phase. Using equations (16), (17) and (18) with typical values for stellar interiors and with  $\alpha = 1$ , we estimate that

$$10^6 \lesssim \frac{\sigma t_*}{{m_*}^2} \lesssim 10^{10}.$$
 (19)

Higher values are appropriate to stars on the lower main sequence (which, however, do not usually have convective cores), intermediate values to the helium cores of horizontal branch stars, and lower values to upper main sequence stars. These values indicate that the typical mixing time of convective cores is  $\sim 1-10$ years for all these types of model. Further order-of-magnitude arguments applied to equation (14) indicate that the gradient of composition within a convective core is given by

$$m^* \frac{dX}{dm} \sim \frac{{m_*}^2}{{\sigma} t_*} \tag{20}$$

so that the abundance of a species is constant within the convective core to about one part in 10<sup>6</sup> to 10<sup>10</sup>, depending on the type of model. This justifies the usual assumption that the composition is homogeneous within a convective core. Of

course, in a rapid phase of evolution such as a helium flash, this kind of estimate is not applicable.

Typically, then, equations (16), (17) and (18) give

$$\sigma \sim 10^8 \alpha^{4/3} (\nabla_r - \nabla_a)^{1/3} m_*^2 / t_*.$$
(21)

We now note that, despite the large coefficient in this equation,  $\sigma$  can be small and mixing slow provided  $\nabla_r - \nabla_a$  is sufficiently small, i.e.

$$\sigma \sim m_*^2 / t_*$$
 if  $\nabla_r - \nabla_a \sim 10^{-24}$ . (22)

This is a semiconvective type of situation, where mixing can build up rather than wipe out a composition gradient during the star's nuclear life time. For such a situation to occur, it is necessary that the radiative gradient be very closely equal indeed to the adiabatic gradient. However, we must bear in mind that the mixing length theory can hardly be applied directly to semiconvective zones.

Near the boundary of a convective core, it is probable that the value of  $\alpha$ , usually assumed constant and of order unity, drops, in view of the consideration mentioned above that the mixing length should not be greater than the distance to the nearest boundary. We believe it is reasonable to assume that  $\alpha \to 0$  as  $\nabla_r - \nabla_a \to 0$  at the boundary. Such behaviour is mimicked by the simple formula

$$\alpha \sim \alpha_0 \, \frac{\nabla_r - \nabla_a}{\nabla_r} \tag{23}$$

where  $\alpha_0$  is the 'standard' value well inside the core (typically  $(\nabla_r - \nabla_a)/\nabla_r \sim 0.5$  to 0.95 at the centre). If we insert this behaviour into equation (21) we arrive at

$$\sigma \sim 10^8 \left(\frac{\alpha_0}{\overline{\nabla}_r}\right)^{4/3} (\nabla_r - \nabla_a)^{5/3} m_*^2 t_*.$$
 (24)

This naïve formula also allows the possibility of semiconvection, but now it is only necessary that  $\nabla_r - \nabla_a \sim 10^{-5}$  in such a region. We do not pretend to have a formula for  $\sigma$  which will be at all exact, but we suggest that on the one hand there is great uncertainty in this quantity, and on the other hand it is not necessary to have a physically correct expression in order to obtain sensible answers. It is clear that there will be no measurable difference between a semiconvection zone where  $\nabla_r - \nabla_a \sim 10^{-5}$  and one where  $\nabla_r - \nabla_a \sim 10^{-24}$ . In this paper we adopt a value for  $\sigma$  which is chosen for numerical convenience, and which is

$$\sigma = K(\nabla_r - \nabla_a)^2 \, m_*^2 / t_*, \qquad (\nabla_r \ge \nabla_a) \tag{25}$$

where values for K that have been used are  $10^4$ ,  $10^5$  and  $10^6$ . While this gives slower mixing in fully-convective regions than we would expect on physical grounds, the difference between a composition which is constant to one part in  $10^5$ , say, and a more realistic one which is constant to one part in  $10^{10}$  is not significant.\* Equation (25) gives mixing in semiconvective zones which is rather slow: a superadiabaticity of  $10^{-2}$  or  $10^{-3}$  is required to provide the necessary mixing. Even so, this means that the model departs from Schwarzschild's criterion by only one per cent or less, and we do not feel that this is a significant discrepancy.

\* The reason for choosing  $K \lesssim 10^6$  is largely the exigencies of using single precision (about seven decimal places), although we are not confident that double precision (about sixteen decimal places) would automatically make it possible to use larger values of K.

In the limit  $K = \infty$ , we can expect to recover the 'standard' formulation, that dX/dm = 0 in convective regions, and that  $\nabla_r = \nabla_a$  in semiconvective regions.

We assume in this paper that Schwarzschild's criterion (Schwarzschild & Härm 1958) for semiconvection is the correct one; evidence for this is outlined by Spiegel (1969). However, the method could presumably be adapted equally to a stability condition such as Ledoux's (1947), which requires that

$$\nabla_r \ge \nabla_a + \frac{\beta}{4 - 3\beta} \frac{d \log \mu}{d \log P},\tag{26}$$

for convective instability ( $\mu$  is the mean molecular weight of the material, and  $\beta$  the ratio of gas pressure to total pressure).

#### 3. EQUATIONS OF STRUCTURE AND EVOLUTION

The four standard equations of stellar structure, along with the equations for change in composition, can be written

$$\frac{d\log P}{dm} = -\frac{Gm}{4\pi r^4 P} \tag{27}$$

$$\frac{d\log T}{dm} = \frac{d\log P}{dm} \cdot \nabla$$
(28)

$$\frac{d\log r}{dm} = \frac{1}{4\pi r^3 \rho} \tag{29}$$

$$\frac{dL}{dm} = -\frac{Du}{Dt} + \frac{P}{\rho^2} \frac{D\rho}{Dt} - \epsilon_v + \epsilon_x$$
(30)

$$\frac{dX}{dm} = \xi \tag{31}$$

$$\frac{d}{dm}\sigma\xi = \frac{DX}{Dt} + XR_X.$$
(32)

Here X represents a composition variable which will be hydrogen in a region where hydrogen burning is important, helium in an inner region where helium burning is important, and carbon or oxygen even further in where their burning is important. Of course, we could in principle write down one pair of equations like (31) and (32) for every nuclear species of interest, but this gives a large number of equations to be solved simultaneously; and in most cases, though not all, it is found that only one nuclear reaction dominates at a given time and a given position in a star. We find that a single variable X whose significance changes between regions of different nuclear burning works well. For more detailed results it would be better to use two sets of equations like (31) and (32), with two composition variables each of which can represent different elements at different positions in the star. But for the present paper, where only qualitative results are obtained, the present approximation is adequate.

In equations (30) and (32)  $\epsilon_X$  is the rate of production of energy from the appropriate X-burning reaction, and  $R_X$  is the rate at which the particles are consumed by this reaction. Generally

$$\epsilon_X = X E_X R_X, \tag{33}$$

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where  $E_X$  is the ergs per gram available from the nuclear reaction. The quantity  $\xi$ , defined by equation (31), is the gradient of composition.  $\nabla$  in equation (28) is the local temperature gradient, determined by equations (11), (12) and (13) in the previous section.

In Paper I we have described in some detail a method for dividing a star up into convenient zones. This method reduces simply to adding a further pair of differential equations to the set (27)-(32). The method leads to a value for the mass coordinate m at a given mesh point which varies with time. Essentially the mesh points are automatically placed at equal intervals of the strange but useful function

$$q \propto -0.02 \log P + 0.1 X + (m/m_*)^{2/3}$$
. (34)

This choice pushes mesh points close together in regions where X changes rapidly (such as thin burning shells) or where P changes rapidly (such as the surface, or the outer layers of an inert, degenerate core). While the method is very effective for its purpose, it is not essential to an understanding of the main burden of this paper, which is the interaction of the four structure equations (27)-(30) with the two composition equations (31) and (32), so we will not refer to it further.

The method we use for replacing equations (27)-(32) by difference equations, and then of solving these difference equations, has already been described in Paper I. In that paper we were only concerned with the situation  $\sigma = 0$  (no convective mixing), so it is rather fortuitous that the method described there for differencing equations (31) and (32) turns out to be suitable for the problem of convective and semiconvective mixing dealt with here, but with one reservation which we discuss shortly. In essence, we write

$$X_k - X_{k-1} = \xi_{k-1} \delta m_{k-1} \tag{35}$$

$$\sigma_k \xi_k - \sigma_{k-1} \xi_{k-1} = \{ (X_k - X_k^{(0)}) / \Delta t + X_k R_{X, k} \} \, \delta m_k.$$
(36)

Here k is an integer which runs from I at the centre to, say, N at the surface;  $\delta m_k$  is the quantity  $h(dm/dq)_k$  of Paper I, equation (26);  $\circ \cdot 5$  ( $\delta m_k + \delta m_{k-1}$ ) is the mass contained in the zone under consideration; and  $X_k^{(0)}$  is the value of  $X_k$  in the previous model, a time step  $\Delta t$  earlier (but if the mesh is non-Lagrangian, allowance must be made for the change of mass-coordinate with time at each mesh point). When  $\sigma$  is non-zero (in which case it is usually large) equations (35) and (36) represent a very stable way of differencing a diffusion equation (Richtmeyer 1957), and lead to a solution with  $\xi$  small so that X is nearly constant, as expected. On the other hand, when  $\sigma$  is zero equation (36) is simply an equation for  $X_k$  with solution

$$X_k = \frac{X_k^{(0)}}{\mathbf{I} + R_{X, k}\Delta t} \tag{37}$$

which is also a very stable way of calculating the new composition; and equation (35) then simply determines the composition gradient  $\xi$ . In a semiconvection zone equations (35) and (36) are too intimately linked with the structure equations to be treated separately, but their effect is partly to determine  $\sigma$ , and hence the slight degree of superadiabaticity. The composition X is then determined partly through  $\nabla_r$ , since it is the dependence of  $\nabla_r$  on composition (via the opacity) which generally is responsible for semiconvection.

It is a pleasant feature of the method that it is not necessary to put a mesh

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point precisely at the boundary of a convective zone. The equations are quite capable of solution even if the boundary  $\nabla_r = \nabla_a$  lies somewhere in the middle of an interval, so that  $\sigma = 0$  at one end of the interval and  $\sigma \neq 0$  at the other. One may of course wonder about the accuracy in such a situation, but we cannot see any reason why an interval which contains a boundary should be substantially less accurate than one which does not. Furthermore, it is not necessary to know in advance whether semiconvection will appear; the method simply puts in semiconvection if it arises.

There is a slight asymmetry in the difference equations (35) and (36), which leads to a problem in connection with the 14  $M_{\odot}$  model. The asymmetry is due to the fact that in equation (36) the composition gradient  $\xi$ , which is an average across one zone, is multiplied by the value of  $\sigma$  at one end of the zone rather than by an average across the zone. We ought to multiply  $\xi_k$  by, say  $(\sigma_k + \sigma_{k+1})/2$ , but in that case the difference equation (36) would no longer have the simple character that we assume for convenience, i.e. that it contains only values at one end or other of the interval. The asymmetry does not matter in a zone which is convective at both ends or radiative at both ends, or which is convective at the inner end and radiative at the outer end, but it can lead to a physically unrealistic situation in a zone which is radiative at the inner end and convective at the outer end. In Section 4 we illustrate this difficulty, and in Section 5 we suggest some means of overcoming it.

The boundary conditions appropriate to equations (35) and (36) have to be considered. These equations, for which k = 2, 3, ..., N, do not contain the value  $\xi_N$ , because of the way they are differenced. Hence,  $\xi_N$  can be given any value we choose, e.g.

$$\xi_N = 0. \tag{38}$$

Now, equation (32) leads to an overall conservation statement

$$\int \frac{DX}{Dt} dm + \int XR_X dm = 0, \qquad (39)$$

since the flux  $\sigma\xi$  of composition clearly vanishes at each end. However, if we sum equation (36) over all values of k, we will only get a good finite difference approximation to equation (39) provided

$$\sigma_1 \xi_1 = \{ (X_1 - X_1^{(0)}) / \Delta t + X_1 R_{X, 1} \} \frac{\delta m_1}{2}.$$
(40)

This single condition essentially contains two conditions, since on the one hand if the centre is radiative ( $\sigma_1 = 0$ ) we have

$$o = (X_1 - X_1^{(0)}) / \Delta t + X_1 R_{X, 1}$$
(41)

which simply gives the change in composition in the absence of convective mixing; while on the other hand if the centre is convective so that  $\sigma$  is large, we have

$$\xi_1 \doteq 0,$$
 (42)

since  $\delta m_1$  is a measure of step size and can in principle be made arbitrarily small. The exact boundary condition for a convective centre would of course be  $\xi = 0$ , since there can be no flux of composition through this boundary, by symmetry. The two boundary conditions (38) and (40) are accompanied by four standard boundary conditions (Paper I) for the structure equations, so that there are three

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boundary conditions at the centre and three at the surface. A numerical procedure for solving the finite difference equations which approximate the differential equations has already been outlined in Paper I. A more detailed description is being prepared, and will be available on request.

#### 4. RESULTS

In an attempt to create a simple stellar model in which semiconvection might occur, we constructed a 14  $M_{\odot}$  star on the zero-age main sequence and evolved it, in the hope that it would develop a semiconvective region of the type described by Schwarzschild & Härm (1958). It did not do so, although we believe it was very close to doing so. This may have been partly due to the fact that notwith-standing the star's high mass we gave it a Population II composition, since tables of opacity for such a composition were readily to hand. However, when the star had exhausted its hydrogen throughout a substantial core, the comparatively rapid collapse of the core led to structural changes which produced convection in the region of composition gradient left behind by the contracting convective core. Such a situation is bound to lead to semiconvection, as we show shortly, and the numerical results did indeed show a convection zone with a semiconvection zone adjacent to it and further out in the star (Fig. 1). Once helium ignited at the centre both zones died out, and the star stabilized at a point in the Hertzsprung-Russell diagram midway between the main sequence and the giant branch.

Hydrogen & Helium Hydrogen & Helium 

FIG. 1. The evolution of a 14  $M_{\odot}$ , Population II star, from the main sequence to the formation of a carbon core. Time steps are plotted horizontally, space steps vertically. The time steps are not equal; the mass steps are not equal, and are not the same at different times. Convective and semiconvective regions are denoted by c and s. Density of dots indicates roughly the steepness of the composition gradient. Diagonally striped regions indicate where nuclear burning principally occurs. The composition profile at the dashed vertical line (model 73) is shown in Fig. 3.

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# Whereas the hydrogen convective core had grown smaller during evolution,

the new helium convective core grew larger, although not rapidly. This might have given rise to a semiconvective situation like that described by Paczyński (1970), but did not. However, this is in accord with Paczyński's conclusion that such semiconvection occurs only in lower mass stars ( $\leq 7 M_{\odot}$ ). When helium was exhausted in the centre, the core contracted rapidly until it became slightly degenerate, and the star moved rapidly to the red giant region. We continued the evolution for part of the phase of growth of the carbon core, but found that our coarse mesh (97 mesh points in the whole star) was becoming inadequate.

Let us consider in more detail the onset of convection in the region of composition gradient left behind by the contracting hydrogen burning core. In most regimes of pressure and temperature (although not all) the opacity coefficient is a function of composition. Because of this, if a star decides to become convectively unstable in a region where there is a composition gradient there is bound to be a semiconvective problem. This is illustrated in Fig. 2.



FIG. 2. A convective region tries to form in the middle of composition gradient: (a) the composition profile is flattened by convection, but no semiconvection is allowed, (b) the resultant superadiabaticity shows that such a picture is not self-consistent. (c) and (d) show two self-consistent pictures (depending on the details of the model) which incorporate semiconvection.

Fig. 2 (a) shows a composition gradient which, we suppose, has been wiped out over some region by convection, producing a discontinuity of composition at each end. In Fig. 2 (b) we attempt to show the resultant superadiabaticity, assuming that opacity (and hence  $\nabla_r$ ) increases with increasing X. Clearly the result is not consistent with the assumed composition profile, since it shows that part of the convective region is subadiabatic. We assume the following propositions:

1. Mixing of some sort occurs whenever  $\nabla_r - \nabla_a > 0$ , and not otherwise.

2. The rate of mixing, and hence the superadiabaticity  $\nabla_r - \nabla_a$ , goes to zero as the boundary of a convective region is approached from inside the region.

3. Mixing can and must continue until a steady state is reached. If these are accepted, we conclude that the only possible steady state is (depending on details of the model) either the dotted or the dashed configuration illustrated in Fig. 2 (c) and (d). The solution may or may not contain a fully convective portion with an almost flat composition profile, but it must contain a semiconvective region towards its outer boundary, where the composition gradient is continuously adjusted as the star evolves to maintain a very small superadiabaticity.



FIG. 3. Details of a computed model where convection occurred in the middle of a composition gradient. See the discussion in the text.

In Fig. 3 we plot an actual model from our evolution of a 14  $M_{\odot}$  star. We observe that there is indeed a semiconvective region in the outer part of the zone. The superadiabaticity  $\nabla_r - \nabla_a$  in this region is of the order of 0.01, which is larger than would probably be the case in an actual star, but we feel that it is still adequately small. However, the inner boundary of the fully convective region is obviously unsatisfactory, for  $\nabla_r - \nabla_a$  does not tend to zero as we approach the inner boundary of the region from inside the convective portion. This would suggest that there should be convective overshooting, mixing material still further inwards. It appears, from a close (though perhaps not conclusive) examination of the difference equations (35) and (36) that the asymmetry referred to above in

the treatment of  $\sigma$  has the following effect: it implies that the inner boundary of a convective region is defined by the condition that  $\nabla_r - \nabla_a \rightarrow 0$  as we approach the inner boundary through the *radiative* region, not through the *convective* region as we would like. It can be seen from Fig. 3 that the computer solution does appear to satisfy this incorrect condition.

This mistake emphasizes, if emphasis is needed, the danger of replacing differential equations of unusual character by difference equations without very careful consideration. Although the mistake is by no means implicit in the method as a whole, it proved rather difficult to remedy within the framework of the specific computational procedure we have been using so far. We outline methods for dealing with it in the next section. Since the main object of this work was to investigate the semiconvective zone which can occur in helium burning cores, and since this mistake is not relevant to that problem (the convective core has no inner boundary) we have chosen to ride rough-shod over it so far.



FIG. 4. The evolution of a 0.775  $M_{\odot}$  star with an initial helium-burning core of 0.502  $M_{\odot}$ . The symbolism is the same as in Fig. 1. The composition profile at the dashed vertical line (model 163) is shown in Fig. 6.

Fig. 4 illustrates the evolution of a star of  $0.775 \ M_{\odot}$  with initially a helium core of  $0.502 \ M_{\odot}$ . Helium burns in the core, producing a central convective region of  $0.11 \ M_{\odot}$  initially. As the helium burns to carbon, the opacity increases (at a given temperature and pressure) because carbon gives greater free-free scattering. The luminosity generated in the core also goes up, and the two effects both act to make the convective core grow in size quite rapidly. The effect of free-free scattering becomes progressively greater as the core boundary moves out to lower temperatures, and beyond a certain point it becomes sufficiently

important that  $\nabla_r - \nabla_a$ , instead of decreasing to zero as it should at the boundary appears to have to increase again. This is illustrated in Fig. 5.

Fig. 5 (a) shows the composition profile near the edge of a convective core which has expanded with age. For a suitable opacity function, it is possible for the superadiabaticity to have the form (see Paczyński 1970) shown in Fig. 5 (b). Since  $\nabla_r - \nabla_a$  is large right at the boundary, we would expect convective overshooting, which would tend to expand the core still further, mixing helium into the carbon-rich core. If once again we make the three postulates mentioned above, we conclude that the situation described by the solid lines in Fig. 5 (a)



FIG. 5. The boundary of a growing convective helium-burning core: (a) the composition profile that would arise in the absence of semiconvection, (b) the resultant superadiabaticity, which increases instead of decreasing to zero near the boundary. (c) and (d) show a self-consistent picture incorporating semiconvection.

and (b) is not permissible, and we appear to be compelled towards the solution illustrated by the dashed line in Fig. 5 (c) and (d). A fractionally superadiabatic semiconvective region extends out far enough to mix in the amount of helium required to reduce the superadiabaticity at the outer edge of the fully convective region to almost zero. In Fig. 6 we show an actual model of our  $0.775 M_{\odot}$  star in this stage of evolution. It has the character suggested, if we make allowance for the coarseness of the mesh. We did not notice any of the fluctuations with time of the size of the convective or semiconvective regions (' breathing ') reported by Demarque & Mengel (to be published).

Although the 14  $M_{\odot}$  star in its central helium-burning phase also has a convective core which expands with age the semiconvective solution does not arise in this case because at the higher temperatures and lower densities that prevail the opacity is almost entirely electron scattering, which is independent of composition so far as a helium/carbon mixture is concerned.

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FIG. 6. Details of a computed model of a growing convective helium-burning core. Allowing for the coarseness of the mesh, this is clearly comparable to Fig. 5 (c) and (d).

#### 5. CONCLUSIONS

It appears that if convection is treated as a diffusion process in which the diffusion coefficient increases with the degree of superadiabaticity, and if further this diffusion equation is solved simultaneously with the structure equations, then a convenient recipe emerges for dealing with both convection and semiconvection. However, the reliability of the method depends, to a somewhat unforeseen extent, on the detailed method by which the composition equation is solved. We believe that if the diffusion equation (14) were replaced by something equivalent to the following properly-centred difference equation

$$\frac{1}{2}(\sigma_{k+1}+\sigma_k)\frac{X_{k+1}-X_k}{\delta m_{k+1/2}} - \frac{1}{2}(\sigma_k+\sigma_{k-1})\frac{X_k-X_{k-1}}{\delta m_{k-1/2}} = \left(\frac{X_k-X_k^{(0)}}{\Delta t} + X_k R_{X,k}\right)\delta m_k \quad (43)$$

then the method would be quite reliable as regards boundaries of convective and semiconvective regions, wherever they might be and however they might move about. Of course, the finiteness of the mesh would lead to inaccuracy, but we see no reason to believe that the inaccuracy would be substantially greater than in any other finite difference problem.

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In our present work we have tried, purely for convenience, to represent all the equations to be solved as first order difference equations. This then allows a general solution scheme of a simple character to be applied to all the equations, giving great programming simplicity. It is not difficult to 'factorize' equation (43) into first order equations giving the correct centring. For instance

$$X_{k} - X_{k-1} = \frac{1}{2} (\xi_{k} + \xi_{k-1}) \, \delta m_{k-1/2}$$

$$\sigma_{k} \xi_{k} - \sigma_{k-1} \xi_{k-1} = \frac{1}{2} \left( \frac{X_{k} - X_{k}^{(0)}}{\Delta t} + X_{k} R_{k} + \frac{X_{k-1} - X_{k-1}^{(0)}}{\Delta t} + X_{k-1} R_{k-1} \right) \, \delta m_{k-1/2}$$
(44)
$$(44)$$

while not exactly equivalent to equation (43) is properly centred. However, we believe that equations (44) and (45) have some instability when applied to a zone where  $\sigma = o$  at one end and  $\sigma > o$  at the other. Also, even when  $\sigma = o$  at both ends, we have shown in Paper I that equation (44) is unstable when applied to thin burning shell, unless very small time steps are used. If, following Paper I, we insist that equation (44) be replaced by equation (35), then equation (45) has to be replaced by equation (36) to obtain correct centring in X; but then the  $\sigma$ 's are not centred the same way as the  $\xi$ 's which they multiply, as we pointed out above. The simplest way (but probably not the cheapest way) that we have found to obtain correct centring is to write equation (36) as two equations:

$$\sigma_k^* \xi_k - \sigma_{k-1}^* \xi_{k-1} = \left( \frac{X_k - X_k^{(0)}}{\Delta t} + X_k R_k \right) \, \delta m_k, \tag{46}$$

and

$$\sigma_k^* = \frac{1}{2}(\sigma_k + \sigma_{k-1}). \tag{47}$$

Equation (47) can also be cast, somewhat awkwardly, into the same form of difference equation as the other eight. However, three simultaneous equations is a rather high price to pay for the simplicity of having them all of the same form, particularly when they can be written as a single equation (43), though of a very different form.

Recently a number of authors (Demarque & Mengel 1971 to be published; Fricke, Stobie & Strittmatter 1971 to be published; Lauterborn, Refsdal & Roth 1971, Paczyński 1970) have pointed to the fact that the behaviour of a star in the H–R diagram, particularly in the region of helium burning where loops through the Cepheid region may or may not occur, is critically dependent on the nature of the composition profile in the star. Since semiconvection is frequently associated with the helium burning phase we feel it is important to have a relatively easy way of dealing with semiconvective mixing, even although at the present time we can only make the simplest possible assumptions about semiconvection. While the method described here, the simultaneous fully implicit solution for both composition and structure changes, may be no better than a standard method when semiconvection is absent, we feel it has substantial advantages of speed, accuracy and simplicity when semiconvection arises; and unfortunately it is not possible to be sure in advance of calculating an evolutionary sequence whether semiconvection will arise or not. Furthermore, the method appears to fit reasonably well with the method described in Paper I for dealing quickly, simply and accurately with thin burning shells. However much further development and

experimentation is still required to be sure that there are no further numerical traps, such as the one described here, in whatever particular numerical method is used to solve the problem.

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# Kellogg Radiation Laboratory, California Institute of Technology, Pasadena California 91109.

On leave of absence from the Institute of Theoretical Astronomy, Madingley Road, Cambridge.

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