Advanced evolution of helium stars and massive close binaries
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II. EVOLUTIONARY CODE AND INPUT PHYSICS.

Summary.

A description is presented of a stellar evolution code for the calculation of the helium- and carbon-burning phases up to neon ignition in intermediate-mass helium stars (~ 2 to 4 M☉). Special attention is given to the input physics and to the conditions for obtaining numerically stable solutions.

Introduction.

In this Chapter we describe a numerical code with which the evolution of intermediate-mass helium stars (~ 2 to 4 M☉) can be calculated up to carbon or neon ignition. A general introduction to the (Newtonian) theory of stellar structure can be found in Schwarzschild (1958); a detailed, more technical, introduction to the construction of evolutionary programs is given by Kippenhahn et al. (1967). Recently, Richardson et al. (1982) described a program for calculating the evolution of a cooling neutron star using general relativistic equations for the thermal structure of the neutron star interior (see also Thorne, 1977). In the course of time technical improvements of the evolutionary codes have been continuously devised, including changes in the input physics; due to this the documentation of most of the existing programs has become spread over several publications which span sometimes more than two decades. This led to several publications for which the precise input physics is very hard to trace, e.g. Barkat et al. (1974) and Delgado and Thomas (1981). This problem has now been recognized: e.g. Nomoto (1982a, b; 1984a) gives more details to the input physics than earlier. In the present work, we give, in section IIc, the input physics to the program as completely as possible. Since the iterative method of solution of the set of mathematical equations describing the internal structure of star is almost standard, we restrict ourselves in section IIb to a description of both this set of equations and to the restrictions set to the code for obtaining numerically stable solutions and reliable results. In section IIa a list of symbols (and, eventually, of their corresponding units) is given.
IIa. List of symbols (and their corresponding units).

stellar structure variables: $T$, $\rho$, $r$, and $L$

- $T$ - temperature (in K)
- $\rho$ - mass density (in g cm$^{-3}$)
- $r$ - radius (in solar radii, $R_\odot$)
- $L$ - (bolometric) luminosity (in solar luminosities, $L_\odot$)
- $L_r$ - luminosity at radius coordinate $r$ (heat flow)
- $\rho^-$ - mass density at the convective side of the convective boundary
- $\rho^+$ - mass density at the radiative side of the convective boundary

compositional variable: $X_I$

- $X$ - mass fraction (or abundance) of hydrogen ($^1$H)
- $X_I$ - mass fraction of chemical element $i$
- $X_I^-$ - mass fraction of the $i$-th chemical element at the convective side of the convective boundary
- $X_I^+$ - mass fraction of the $i$-th chemical element at the radiative side of the convective boundary
- $m$ - mass of the electron ($9.109558 \times 10^{-28}$ g)
- $m_n$, $m^n$ - mass coordinate of mesh point number $n$; the centre has $n = 0$
- $m_r$, $M_r$ - mass interior to a radius $r$ (mass coordinate in the mesh, in $M_\odot$)
- $\dot{M}$ - mass-loss rate in $M_\odot$ yr$^{-1}$
- $M_1$ - mass of the primary (initially more massive) component in a binary
- $M_1^0$ - initial mass of the primary
- $M_1^f$ - final mass of the primary
- $M_\odot$ - solar mass ($1.989 \times 10^{33}$ g)
- $M_{\text{Ch}}$ - Chandrasekhar limiting mass (~ $1.44 M_\odot$)
- $M_{\text{bol}}$ - absolute bolometric luminosity ($\equiv -2.5 \times 10^4 \log (L/L_\odot) + 4.72$)
- $M_{\text{min}}$ - minimum C-O core mass (in $M_\odot$) for a star required to
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_0$</td>
<td>solar bolometric luminosity ($3.826 \times 10^{33}$ erg s$^{-1}$)</td>
</tr>
<tr>
<td>$\rho_C$</td>
<td>mass density in the centre</td>
</tr>
<tr>
<td>$\rho_r$</td>
<td>mass density at distance $r$ from the centre</td>
</tr>
<tr>
<td>$T_C$</td>
<td>temperature in the centre</td>
</tr>
<tr>
<td>$T_r$</td>
<td>temperature at distance $r$ from the centre</td>
</tr>
<tr>
<td>$T_n$</td>
<td>temperature in units of $10^N$ ($= T/10^N$)</td>
</tr>
<tr>
<td>$T_{\text{eff}}$</td>
<td>effective temperature (&quot;surface temperature&quot;)</td>
</tr>
<tr>
<td>$t$</td>
<td>time coordinate (in seconds or years; 1 year = 31556735 seconds)</td>
</tr>
<tr>
<td>$t_{\text{evol}}$</td>
<td>evolutionary time (in years) elapsed since the helium star arrived on the helium main sequence</td>
</tr>
<tr>
<td>$\tau_{\text{evol}}$</td>
<td>duration of certain evolutionary phase (in years)</td>
</tr>
<tr>
<td>$\tau_{\text{He}}$</td>
<td>duration of the convective core-helium burning phase (in years)</td>
</tr>
<tr>
<td>$\tau_C$</td>
<td>duration of the convective core-carbon burning phase (in years)</td>
</tr>
<tr>
<td>$t_{\text{final}}$</td>
<td>evolutionary time of the last calculated model plus 1 year</td>
</tr>
<tr>
<td>$t_h$</td>
<td>time scale of heat diffusion (or of heat conduction or of heat transport)</td>
</tr>
<tr>
<td>$t_h(r)$</td>
<td>$t_h$ at distance $r$ from the centre</td>
</tr>
<tr>
<td>$t_{\text{KH}}$</td>
<td>Kelvin-Helmholtz time scale, time scale for restoring thermal equilibrium or for contraction ($\equiv \frac{G M^2}{LR} = 3.265 \times 10^7 \cdot \left(\frac{N}{M_H}\right)^2 \left(\frac{R}{R_H}\right)^2$, in years)</td>
</tr>
<tr>
<td>$p$</td>
<td>total pressure (in dyn cm$^{-2}$)</td>
</tr>
<tr>
<td>$p_r$</td>
<td>total pressure at distance $r$ from the centre</td>
</tr>
<tr>
<td>$p_n$</td>
<td>total pressure in mesh point $n$</td>
</tr>
<tr>
<td>$p^-$</td>
<td>pressure at the convective side of the convective boundary</td>
</tr>
<tr>
<td>$p^+$</td>
<td>pressure at the radiative side of the convective boundary</td>
</tr>
<tr>
<td>$p_e$</td>
<td>electron pressure</td>
</tr>
<tr>
<td>$p_{\text{ex}}$</td>
<td>excess pressure, correction to the total pressure due to quantum mechanical effects, Coulomb interaction and other effects</td>
</tr>
<tr>
<td>$P_i$</td>
<td>nuclear production rate of chemical element $i$ (per second), a symbol also used for the initial orbital period before a mass-exchange phase in a binary (in days)</td>
</tr>
<tr>
<td>$P_0$</td>
<td>initial orbital period of a binary (in days)</td>
</tr>
</tbody>
</table>
**Pf** - final orbital period after a mass-exchange phase or a supernova explosion in a binary (in days)

**D_i** - nuclear destruction rate of chemical element i (per second)

**D** - diffusion coefficient (in cm$^2$ s$^{-1}$)

**D(r)** - diffusion coefficient at distance r from the centre.

**D_c** - diffusion coefficient in a convective region (see Appendix II of Chapter II)

**D_m** - ion, gas, or molecular diffusion coefficient

**D_r** - radiation diffusion coefficient (or "thermal diffusivity" for non-turbulent matter

**D_r(r)** - D_r at distance r from the centre

**D_rad** - "radiation diffusion coefficient for turbulent matter" or kinematic radiative viscosity (see Appendix II of Chapter II)

**D_S** - "Schwarzschild" diffusion coefficient (see Appendix II of Chapter II for the definition)

**D_tur** - turbulent diffusion coefficient (see Appendix II)

**ε** - (total or net) energy generation rate (in erg g$^{-1}$ s$^{-1}$), unless defined in another way

**ε_V** - energy generation rate in the form of neutrinos

**ε_n** - energy generation rate by thermonuclear reactions

**ε^n** - total energy generation rate in the n-th mesh point

**ε_g** - energy generation rate by gravitational contraction or expansion

**ε_net** - net energy generation rate (defined in equation (30) of Chapter II)

**ε_max** - maximum net energy generation rate (in a shell or in the convective core of the star)

**Q** - "internal heat" of the gas (in erg g$^{-1}$, dQ = T dS)

**QR** - $\frac{\partial S}{\partial \ln p} T$, T times the density gradient of the specific entropy S at constant temperature and composition

**QT** - $\frac{\partial S}{\partial \ln T} \rho$, T times the temperature gradient of the specific entropy S at constant density and composition

**QX_i** - $\frac{\partial S}{\partial \ln X_i} \rho$, T times the composition gradient of the specific entropy S at constant density and temperature

**Q_m** - energy generated in the form of nuclear binding energy in
the m-th thermonuclear reaction (in erg or Mev)

\[ R_m \]

reaction rate of the m-th thermonuclear reaction (in \( \text{s}^{-1} \))

\[ R_0 \]
solar radius \((6.9599 \times 10^{10} \text{ cm})\)

\[ R_1, R_2 \]
radius (in \( R_0 \)) of the primary or secondary component in a binary, respectively

\[ R \]
universal gas constant, \( R = N_A \cdot k (8.3143 \times 10^7 \text{ erg K}^{-1} \text{ moles}^{-1}) \)

\[ R_e^* \]
critical Reynolds number (see Appendix II of Chapter II)

\[ S \]
- specific entropy of the gas per gram (in \( \text{erg g}^{-1} \text{K}^{-1} \)),
- \( dS = \frac{dQ}{T} = \frac{dU}{T} - P \cdot \rho^{-2} \cdot dp \); the symbol \( S \) is also defined else (paragraph 5 of section IIIA)

\[ U \]
total internal energy per gram of the gas excluding stored thermonuclear energy (in \( \text{erg g}^{-1} \))

\[ U_{qm} \]
correction to the internal energy \( U \) due to quantum mechanical effects (in \( \text{erg g}^{-1} \))

\[ U_{Coul} \]
correction to the internal energy \( U \) due to Coulomb interactions in the liquid phase of the gas

\[ U_{lattice} \]
correction to the internal energy \( U \) due to Coulomb interactions in the solid phase of the gas

\[ U_{ex} \]
excess internal energy \( U \): correction to the total internal energy for quantum mechanical effects, Coulomb interaction, and other effects

\[ F \]
Helmholtz free energy per gram (\( = U - TS \), in \( \text{erg g}^{-1} \))

\[ F_{ideal gas} \]
ideal gas contribution to the Helmholtz free energy

\[ F_{liquid} \]
Helmholtz free energy per gram of the ions in the liquid state

\[ F_{solid} \]
Helmholtz free energy per gram of the ions in the solid (crystalline) state

\[ F_{phonon} \]
Helmholtz free energy per gram of the ions due to lattice vibrations

\[ F_{phonon i} \]
\( F_{phonon} \) for the i-th chemical element

\[ F_{Coul} \]
correction to the Helmholtz free energy due to Coulomb interactions of the ions in the liquid state (\( \text{erg g}^{-1} \))

\[ F_{Coul_s} \]
correction to the Helmholtz free energy due to Coulomb interactions of the ions in the solid state

\[ F_{qm} \]
correction to the Helmholtz free energy due to quantum
mechanical effects

\( \Gamma_i \) - dimensionless Coulomb coupling parameter of the \( i \)-th chemical element (defined in equation (25), Chapter II)

\( \Gamma \) - composition-weighted mean Coulomb coupling constant, mean of the \( \Gamma_i \)'s (defined in equation (26), Chapter II)

\( \kappa \) - total opacity (in \( \text{cm}^2 \text{s}^{-1} \))

\( \kappa^{-1} \) - total conductivity (in \( \text{cm}^{-2} \text{s} \)) defined in equation (21) of Chapter II

\( \kappa_r \) - total opacity at radius \( r \) from the centre

\( \kappa_0 \) - classical low-temperature, low-density opacity for photons scattering off electrons

\( \kappa_{es} \) - Thomson electron scattering opacity (equation (16), Chapter II)

\( \kappa_{rad} \) - radiative opacity (see e.g. equation (15), Chapter II)

\( \kappa_{cond} \) - conductive electron opacity

\( a \) - radiation constant in Stefan's law (\( = \frac{4 \sigma}{c^2}, 7.5645 \times 10^{-15} \text{erg cm}^{-3} \text{K}^{-4} \))

\( a_o, a_{orb} \) - initial orbital separation in a binary (in \( R_0 \))

\( a_f \) - final orbital separation in a binary (in \( R_0 \))

\( c \) - speed of light (\( 2.9979250 \times 10^{10} \text{cm s}^{-1} \)), unless defined in another way

\( c_p \) - specific heat (\( \equiv \frac{\partial Q}{\partial T} \)) at constant pressure

\( c_v \) - specific heat (\( \equiv \frac{\partial Q}{\partial T} \)) at constant volume

\( e \) - electron charge (\( 4.80288 \times 10^{-10} \text{esu} \))

\( e_f \) - final orbital eccentricity in a binary system

\( k \) - Boltzmann's constant (\( 1.380622 \times 10^{-16} \text{erg K}^{-1} \))

\( K \) - adjustment parameter in the diffusion constant \( \sigma_D \)

(see Appendix II of Chapter II)

\( N_A \) - Avogadro's number (\( 6.022169 \times 10^{23} \text{moles}^{-1} \))

\( h \) - Planck's constant (\( 6.6261963 \times 10^{-27} \text{erg s} \))

\( G \) - gravitational constant (\( 6.6732 \times 10^{-8} \text{dyn cm}^{-2} \text{g}^{-2} \text{or cm}^3 \text{g}^{-1} \text{s}^{-2} \))

\( \sigma \) - Stefan-Boltzmann's constant (\( 5.67032 \times 10^{-5} \text{erg s}^{-1} \text{cm}^{-2} \text{K}^{-4} \))

\( \sigma_D \) - diffusion constant (in \( M_\odot^{-2} \text{s}^{-1} \))

\( \sigma_T \) - Thomson electron scattering cross section (\( 6.652 \times 10^{-23} \text{cm}^2 \))
\( q_r \) - dimensionless adjustment parameter in the definition of \( D_s \)
(see Appendix II of Chapter II)

\( \alpha \) - dimensionless mixing-length parameter \( (\equiv \frac{1}{H_p}) \)

\( l \) - mixing length (in cm)

\( H_p \) - pressure scale height \( (\equiv -\frac{\ln p}{\ln r})^{-1}, \text{in cm} \)

\( H_p(r) \) - \( H_p \) at distance \( r \) from the centre

\( v_c \) - average velocity of a convective element (in \( \text{cm s}^{-1} \))

\( v_{es} \) - escape velocity from the surface (of the companion, in \( \text{km s}^{-1} \))

\( v_{im} \) - velocity of impact of the supernova shell onto the companion (in \( \text{km s}^{-1} \))

\( v^0 \) - relative velocity in the initial circular orbit of the binary (in \( \text{km s}^{-1} \))

\( v_{SNshell} \) - ejection velocity of the supernova shell at the supernova explosion (in \( \text{km s}^{-1} \))

\( v_{kick} \) - kick velocity in an asymmetric supernova explosion (in \( \text{km s}^{-1} \))

\( Z \) - either total chemical abundance of heavy elements with atomic number > 2 or ionic charge for a chemical element

\( Z_i \) - ionic charge of the \( i \)-th chemical element

\( A_i \) - atomic mass number of the \( i \)-th chemical element

\( Y \) - mass fraction of helium \((= \text{He})\)

\( Y_i \) - mass (weight) fraction of the \( i \)-th chemical element \((\equiv X_i/A_i)\)

\( \varepsilon \) - electron degeneracy parameter (dimensionless, equation (20), Chapter II)

\( \mu \) - chemical potential not including the rest mass of the electron \((\equiv -\frac{\Delta U}{\Delta \mu S}, \rho \), where \( N \) is the number of particles; measured in erg)

\( \mu_0 \) - mean molecular weight per free electron

\( \mu_1 \) - mean molecular weight excluding electrons

\( \mu_0 \) - mean of the molecular weight times \( Z \) per free electron

\( \mu_f \) - final total mass of a binary system in units of the initial total mass

\( \Delta \) - evolutionary change in a quantity .. in a time step \( \Delta t \)

\( \text{Be star} \) - standard abbreviation for B-emission star, i.e. a star of spectral type B with hydrogen lines in emission

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\( \Omega \) - angular velocity of a rotating star

\( \tau \) - temperature gradient defined as \( \frac{\partial \ln T}{\partial \ln P} \)

\( \tau_{\text{rad}} \) - radiative temperature gradient at constant radius \( r \)

\[
(\equiv \tau_{\text{rad}}(r) \equiv \left| \frac{\partial \ln T}{\partial \ln P} \right|_r = \frac{3 \kappa P L}{16 \pi c G T^4 r^4 m r}, \text{ fictitious gradient assuming no convection and assuming energy transport purely by radiation and conduction only}
\]

\( \tau_{\text{rad}}^- \) - \( \tau_{\text{rad}} \) at the convective side of the convective boundary

\( \tau_{\text{ad}} \) - adiabatic temperature gradient, i.e. at constant specific entropy \( S \), \( (\equiv \left| \frac{\partial \ln T}{\partial \ln P} \right|_S) \)

\( \tau_{\text{ad}}^- \) - \( \tau_{\text{ad}} \) at the convective side of the convective boundary

---

In order to indicate the value of a parameter of the \( n \)-th mesh point in the thesis we used a superscript \( n \). Whenever a subscript \( n \) is used for this purpose, this is mentioned.

IIa. Evolutionary program - implicit code - numerical techniques.

The computations of the evolutionary sequences of helium stars were started with a program originally based on a scheme described by Paczynski (1970a), which was considerably modified by Savonije and Takens (1976) and subsequently by Van der Linden (1982, 1984).

In the original Paczynski version the compositional changes are calculated analytically by employing the solution of the four structure equations (equations (2) - (5), see below) which describe the hydrostatic evolution of a spherically symmetric star. This explicit solution for the composition is suitable only in stellar evolution when small time steps are chosen. In the following we describe an implicit method to calculate compositional changes.

In our version the composition is determined from the diffusion equation given by:

\[ \frac{d}{d\tau_r} \left( \sigma_D \frac{dX_i}{d\tau_r} \right) = \frac{dX_i}{dt} - P_i + D_i, \]

where \( \sigma_D = 0 \) in radiative regions and \( \sigma_D = 10^{-8} \ M_\odot^2 \ s^{-1} \) in regions which are convectively unstable according to the Schwarzschild criterion (i.e. in regions in which \( V_{\text{rad}} > V_{\text{ad}} \), see the list of symbols in section IIa), \( X_i \) is the abundance by mass of element \( i \), \( P_i \) and \( D_i \) are its production and destruction rates [for the precise definition see Van der Linden (1982, 1984) and Fowler et al. (1975)], \( m_r \) is the mass coordinate of the shell at distance \( r \) from the centre, i.e. the star is divided into a large number of mass shells (up to 800 if necessary) by means of a grid of mesh points. In this way semi-convective is neglected and the value \( 10^{-8} \) of \( \sigma_D \) provides complete mixing of convective regions. Lower values of \( \sigma_D \) (\( 10^{-9} \) or less) do not give complete mixing and higher values (\( 10^{-7} \) or more) do not give acceptable, if any, solutions. Whenever a point becomes convective during the first iteration, it is mixed even if it becomes radiative before convergence is reached. If a point becomes convective after the first iteration it will not be mixed. Such a procedure is required in order to ensure convergence (see also Appendix II).

Simultaneously with equation (1) we solve the following four structure equations for hydrodynamic evolution:

\[ \frac{d\ln P}{dm_r} = -\left( \frac{G m_r}{r^2} + \frac{d^2 r}{dt^2} \right)/4\pi r^2 P \]
(3) \[
\frac{\ln T}{\ln P} = \nabla; \quad \nabla = \nabla_{\text{rad}} \quad \text{in radiative areas}
\]
\[
= \nabla_{\text{ad}} \quad \text{in adiabatic areas}
\]

(4) \[
\frac{d\ln r}{dm} = \frac{1}{4\pi r^3 \rho}
\]

(5) \[
\frac{dL}{dm} = \epsilon_n - \epsilon_v - \frac{dQ}{dt}, \quad \text{see equation (30) for a comment.}
\]

As described by Savonije and Takens (1976) the helium-burning convective core of a helium star in the mass range 2 - 8 M_\odot grows in mass in the course of time. These authors succeeded in calculating self-consistently the growth of the convective core by using the implicit mesh point technique, with which they could solve for the precise boundary of the convective core. Whenever we used their technique we solved equations (1) - (5) together with the equation:

(6) \[
p^- = p^+,
\]

which describes the continuity of pressure at a convective boundary or at a compositional discontinuity (see the list of symbols).

If the convective core grows, the mass-value at the convective boundary is determined by solving equations (1) - (6) together with the equation:

(7) \[
\nabla_{\text{rad}}^- = \nabla_{\text{ad}}^-,
\]

which demands that the convective side of the boundary is precisely convectively neutral (see the list of symbols). In the implicit mesh point technique, a movable double mesh point is inserted at the convective boundary, see also below. The mass coordinate of this point is obtained by solving equation (7).

To facilitate the computation single mesh points can be made movable in our program by adding the mass coordinate m_r to the set of unknowns and by solving equations (1) - (5) together with:

(8) \[
m_r = \frac{(m_n-1 + m_{n+1})}{2},
\]

where m_r is the mass at the n-th mesh point in the grid, m_n-1 and m_{n+1} are the masses at mesh points n-1 and n+1.
Equations (2) - (7) were all discretized and linearized with a two-point difference equation. A differential equation of the form:

\begin{equation}
\frac{dy}{dx} = f(x,y),
\end{equation}

was discretized into:

\begin{equation}
y^{n+1} - y^n = \frac{1}{2} (f(x^{n+1}, y^{n+1}) + f(x^n, y^n)) \cdot (x^{n+1} - x^n),
\end{equation}

or:

\begin{equation}
y^{n+1} - y^n = (\sqrt{f(x^{n+1}, y^{n+1}) \cdot f(x^n, y^n)}) \cdot (x^{n+1} - x^n) \text{ if } f(x,y) > 0
\end{equation}

for all \( x \) and \( y \).

The \( y^i \) are the values of the variables of the new model at \( (t + \Delta t) \) in mesh point numbers \( i = n \), and \( i = n + 1 \).

The second-order diffusion equation (1) is discretized stably by the three-point difference equation given by Van der Linden (1982). His expression for the mesh points \( j = n-1, n, n+1 \) for chemical element \( i \) is:

\begin{equation}
\frac{2\alpha}{m^{n+1} - m^n - m^{n-1}} \cdot \left( \frac{x_i^{n+1} - x_i^n}{m^{n+1} - m^n} - \frac{x_i^n - x_i^{n-1}}{m^n - m^{n-1}} \right) \cdot \Delta x = \Delta x_i^n + (D_i^n - p_i^n) \cdot \Delta t.
\end{equation}

In the linearization of equation (11) we took care that conservation of particles was guaranteed. The discretization in equation (11) is stable, also for small time steps, but the two-point difference equation (10a) does not give numerically stable solutions if the time steps are small or if \( f(x,y) \) is large compared with \( y \). In the latter case the solution tends to give:

\[ f(x^{n+1}, y^{n+1}) = -f(x^n, y^n); f(x^{n+2}, y^{n+2}) = -f(x^{n+3}, y^{n+3}), \]

but \[ f(x^{n+2}, y^{n+2}) \neq -f(x^{n+1}, y^{n+1}). \]

Thus, this solution decouples adjacent mesh points. Sugimoto (1970a, 1981) already pointed this out and he gave another two-point discretization for the four structure equations which ensures coupling of adjacent points and which he found to be always stable for stellar evolution calculations. However, his method is less accurate in the stable regime where equation (10a) is still applicable. Furthermore, it is possible to derive three-point difference equations which are stable for the evolution considered here and which are even more accurate than the two point equations. Normal three-point difference equations are based on equidistant mesh point distributions. However, such a distribution does not occur in our grid. Takens derived a three-point
expression which is applicable to any mesh points division and which is given in Appendix I. In order to fit this formula into the program, equation (3a) was rewritten with the help of equation (2) into:

\[
(3b) \quad \frac{\mathrm{d} \ln T}{\mathrm{d} r} = \frac{\mathrm{d} \ln P}{\mathrm{d} r} \cdot \frac{\mathrm{d} \ln \rho}{\mathrm{d} r} = - \nabla \cdot \left( \frac{G m}{r^2} + \frac{d^2 r}{d t^2} \right) / 4 \pi r^2 P ,
\]

where \( \nabla = \nabla_{\text{rad}} \) in radiative areas
\[ = \nabla_{\text{ad}} \] in adiabatic areas

Further details of the implantation of the three-point expressions into our code can be found in the Appendix I.

The inner boundary conditions as described by Savonije and Takens (1976) are used in our program. The outer boundary conditions used are the same as given by Savonije (1978). The mixing-length parameter \( \alpha \) which enters in the envelope integrations is taken to be unity, i.e. the mixing length is one pressure scale height, as in Paczynski's version. For a convective region two special boundary conditions for the diffusion equation (1) are needed, one for the inner boundary and one for the outer boundary. At each boundary the composition variables of the two innermost and the two outermost convective mesh points, respectively, have to be equated in order to ensure element conservation, see also paragraph 3 of Appendix II.

Although the solution obtained from equations (1) - (5), method I, does not give a smooth growth of the mass of the convective helium-burning core, the maximum extent of the core found for a 2.5 M\(_\odot\) helium star was the same (within 1\%) as the extent given by applying equations (1) - (7) and by inserting a movable, double, mesh point, method II. In order to mimic method II with method I the mesh point distribution has to be fine at the convective boundary. If semi-convection does not occur at the convective boundary (see Chapter IV and Savonije and Takens (1976)) method II uniquely determines whether a point should be mixed or not during the iterations, because mixing is determined by the position of the movable implicit point. Whenever the movable point has to jump over an adjacent fixed point in the grid to reach convergence, this fixed point has to be deleted before starting the iterations. To postpone this action, it is easier to make this adjacent point movable by adding equation (8) to the set of equations to be solved. The double mesh point also describes very well the duality of the convective boundary in the model. This double point has separate densities and
compositions for the radiative and convective sides of the boundary. The mass coordinate of this movable point is found implicitly from solving equation (7) together with equations (1) - (6). For a compositional discontinuity, which is not a convective boundary, the mass coordinate is fixed, and the densities and compositions in this point are found by solving equations (1) - (6).

The mass zoning is chosen such that the maximum differences between two adjacent mesh points give:

$$\Delta m_r = f'(T, \rho, r, L_r, X_i) < \varepsilon,$$

where \( f' \) is the partial derivative of the left hand side with respect to \( \ln T \), \( \ln \rho \) or \( \ln r \) for equations (2), (3a) or (3b), and 4, respectively. The value of \( \varepsilon \) is arbitrarily chosen, but such that the number of mesh points does not increase too much. No special restrictions are set to the other unknowns. The zoning can be as fine as one wishes, but redistribution of the zones is only allowed before the start of the calculations. The number of grid points is limited by the largest matrix which fits into the computer.

The time step is allowed to vary only between \( 10/7 \) and \( 5/7 \) times the previous step, but if the evolutionary changes are too large, due to sudden ignition or mixing of fuel, a smaller time step is chosen.

The unknowns in our model are for a single mesh point: \( \ln T, \ln \rho, \ln r, L_r, \ln X_i \), and for a double mesh point: \( \ln T, \ln \rho^-, \ln r, L_r, L^-_X, \ln \rho^+, \ln X^+_i \).

For a movable mesh point the mass coordinate \( m_r \) is an extra unknown. The unknowns are solved with the tri-diagonal block matrix system as described in appendix 2 of Savonije and Takens using a Newton-Rhapson iterative method. As criterion for convergence of the iterations we use that the iterative corrections to \( \Delta T/T, \Delta \rho/\rho, \Delta r/r, \) and \( \Delta L_r/L_r \) should be less than \( 5 \times 10^{-4} \). (In the case of rapid convergence this value was lowered to smaller than \( 1 \times 10^{-4} \)). As soon as the heat flow \( L_r \) becomes negative in a mesh point, the iterative corrections to \( L \) are no more restricted.

**IIc. Input physics.**

Special effort was taken to use analytical expressions for the calculation of the thermodynamic quantities and their partial derivatives, but without losing precision. This resulted into a program which is applicable to all stages from hydrogen through neon burning without replacing subroutines or
tables for these evolutionary phases. Furthermore, all effort was made to obtain partial derivatives for all thermodynamic variables in the linearization of the set of difference equations. Much convenience gives the following set of expressions for the compositional dependence:

\[
\mu_e^{-1} = \sum_{j} \frac{Z_j X_j}{A_j}; \quad \mu_1^{-1} = \sum_{j} \frac{X_j}{A_j}; \quad \mu_s^{-1} = \sum_{j} \frac{Z_j^2 X_j}{A_j}.
\]

The use of tables in the program is restricted to the calculation of the radiative opacities (in \(\text{cm}^2\text{ g}^{-1}\)) for hydrogen burning and for helium burning if \(Y > 0.5\). For hydrogen-rich mixtures the radiative opacities (including line opacities) are derived from Lagrangian interpolation into a table constructed by Van der Linden (1982) from the tables of Cox and Stewart (1969), and of Cox and Tabor (1976). Van der Linden's (1982) formula for the radiative opacities for \(Y < 0.5\) (including line opacity) is employed and is given in \(\text{cm}^2\text{ s}^{-1}\) by:

\[
\kappa_{\text{rad}}^1 = 2.88 \times 10^{17} \mu_s^{-1} \rho 0.655 T^{-2.665}.
\]

A smooth transition to this formula and to the interpolation in opacity tables for \(Y > 0.5\) (\(\kappa_{\text{rad}}^2\)) was made and the final expression (in \(\text{cm}^2\text{ s}^{-1}\)) is:

\[
\kappa_{\text{rad}} = a \cdot \kappa_{\text{rad}}^2 + (1-a) \cdot (\kappa_{\text{rad}}^1 + \kappa_{\text{es}}),
\]

where \(a\) is the maximum of 0 and \(2 \cdot (Y + Z - 0.5)\). Note that \(Z\) is now the metal content. The Compton scattering opacity \(\kappa_{\text{es}}\) is given by:

\[
\kappa_{\text{es}} = \kappa_o \cdot f_r^{-1} \cdot f_d^{-1},
\]

where \(\kappa_o\) is the classical low-temperature, low-density opacity for photons scattering off electrons:

\[
\kappa_o = \sigma_T N_A \mu_e^{-1} (= 0.4 \mu_e^{-1} \text{ in cgs units}),
\]

where \(\sigma_T\) is the Thomson electron scattering cross section, \(N_A\) is Avogadro's number, \(f_r\) is the correction factor for relativistic effects at temperatures above \(10^3\) K, \(f_d\) corrects for electron degeneracy in the density range \(\rho = 10^3 \text{ g cm}^{-3}\) to \(\rho = 10^6 \text{ g cm}^{-3}\). The numerical fit to \(f_r\) by Van der Linden is:
(18) \[ f_r = 1 + 2.235 \cdot 10^{-9} T - 0.255 \cdot 10^{-18} T^2. \]

The factor \( f_d \) as fitted by Weaver et al. (1978) to the opacity calculations of Buchler and Yueh (1976) is:

(19) \[ f_d = 1 + \exp(0.522 \xi - 1.563), \]

where \( \xi \) is the electron degeneracy parameter defined by:

(20) \[ \xi = \mu/kT, \]

with \( \mu \) the chemical potential not including the rest mass of the electron, and \( k \) the Boltzmann constant. Both fits are good for \(-\infty < \xi < 4 \) and \( 2 \cdot 10^6 \text{ K} < T < 2 \cdot 10^9 \text{ K}. \) However, expression (19) is used only for the regime \(-2 < \xi < 5\), where Compton scattering dominates significantly over other contributors to the opacity or in which it is not negligible, see Chin's (1965) figure 1. The interpolation formula (19) is only good to < 5% and for \( \xi < -2 \) the factor \( f_d \) has to be \( = 1 \). Inclusion of the factor \( f_d \) for \( \xi < -2 \) results in a change of \( \eta_{\text{rad}} \) by \( \sim 5\% \) and into \( \sim 10\% \) uncertainty in the mass of the convective helium-burning cores of 2 to 4 \( M_\odot \) helium stars, which have, generally, \( \xi < -2 \) during core-helium burning. The conductive electron opacities are calculated from the analytical expressions given by Iben (1975), which fit to the tables of Hubbard and Lampe (1969) and to the modified results of Canuto (1970) for relativistic electrons. The total conductivity (\( \kappa^{-1} \)) is obtained from:

(21) \[ \kappa^{-1} = \kappa_{\text{rad}}^{-1} + \kappa_{\text{cond}}^{-1}, \]

where \( \kappa_{\text{rad}} = \) radiative opacity and \( \kappa_{\text{cond}} = \) conductive opacity.

When the percentage of doubly ionized helium is less than 99.9\% (equation (43) of Paczynski, 1969), the Saha ionization equation is solved iteratively by a Newton-Rhapson method in order to take into account the ionization of both hydrogen and helium [for the expressions used see Van der Linden (1982, 1984)]. The dissociation of the \( \text{H}_2 \) molecule is not included in the calculations, cf. Paczynski (1969). In other cases the equation of state relations are evaluated with the approximate solution of Divine (1965b) which is reliable to better than 0.3\% in both relativistic and electron degenerate
regimes as well as in the limits of these regimes for an electron gas, see e.g. Divine or Chiu (1968). The electron pressure obtained from Divine's approach agrees within the cited accuracy with the electron pressure as obtained from the approximate solutions of Kippenhahn and Thomas (1964), whose accuracy can be improved for large electron degeneracy if a series expansion of the f-function (see Kippenhahn and Thomas) is used. In the original version of Paczynski's (1970a) program the electron pressure and the internal energy of the electrons and their first and second partial derivatives to the thermodynamic variables are obtained by interpolation in a table (only good for \( T < 10^9 \) K, and not used for \( T < 10^5 \) K). The interpolated values of the electron pressure and internal energy of the electrons were found to be in good agreement with the values derived analytically from Divine's expressions. However, the first and second numerical partial derivatives of the tabulated quantities to the thermodynamic variables do not always agree with the analytical derivatives. In the approximations of Divine, Paczynski, and Kippenhahn and Thomas the ions are assumed to obey the perfect gas law and no allowance was made for the effects of radiation. Unfortunately, the solution of Divine (1965b) does not give the electron degeneracy parameter \( \xi \) [except for large electron degeneracy (\( \xi > 600 \))], which enters in the Coulomb screening factors of Graboske et al. (1973). For the non-degenerate and non-relativistic regime \( \xi \) is found from the expression given in Chiu (1968, equation 3.236) and for the transition region up to the electron degenerate and relativistic regime \( \xi \) is evaluated using the method of Kippenhahn and Thomas (1964) [which for large electron degeneracy agrees good with the \( \xi \)-value obtained from Divine (1965b)]. If \( \xi \) is obtained from the approximate relation \( \xi = E_f/(kT) \), where \( E_f \) is the Fermi-energy for large electron degeneracy of the electron gas as given by:

\[
E_f = mc^2 \left\{ \left[ 1 + \frac{\sigma}{\mu_e} \cdot N_A \cdot \left( \frac{3}{\sqrt{\pi}} \right) \cdot \left( \frac{\hbar}{m c} \right)^3 \frac{2}{3} \right]^{1/2} - 1 \right\},
\]

it does not yield an as accurate approximation of the electron pressure as the \( \xi \)-value obtained from the method of Kippenhahn and Thomas [1964; a small deviation in \( \xi \) has large effects on the electron pressure].

The total pressure is given by

\[
P = P_e(\rho, \mu_e, T) + \frac{R}{\mu_1} \rho T + \frac{4}{3} \frac{\sigma}{c} T^4 + P_{ex}(\rho, \mu_e, \mu_1, T),
\]

(22)
where the electron pressure $P_e$ is obtained either from Divine's solution or from the solution of Saha's ionization equation, the second term is the ideal gas pressure of the ions, the third term describes the radiation part of the pressure, the last term (the excess pressure) corrects the ideal gas pressure of the ions for the effects of Coulomb interactions of the ions if the gas is in a liquid or solid state (the compositional dependency is strong) and for quantum mechanical effects, and $R$ is $N_A \cdot k$. Similarly, an expression with four components can be derived for the internal energy per gram of the gas, $U$, excluding stored nuclear energy (or binding energy). In this way $P$, $U$, and the first and second order partial derivatives of $P$ and $U$ with respect to the thermodynamic variables, are computed analytically. The expressions for the specific heat at constant pressure, $c_p$, the specific heat at constant volume, $c_V$, $V_{ad}$, the thermodynamic functions $P$ and $U$, and the partial derivatives of these functions to the thermodynamic variables, can be obtained from formulae (40) given by Paczynski (1969) and from Landau and Lifshitz (1970).

The effects of Coulomb interaction of nuclei are not always taken into account in our computations. As soon as the ions behave like a liquid, Coulomb corrections to the equations of state of ions have to be included. For carbon and neon burning this occurs for densities larger than about $10^6 \text{ g cm}^{-3}$. Coulomb corrections result into a density and temperature increase by a few percent, and a pressure decrease for each model. Major changes to the evolutionary tracks for carbon and neon burning are not expected. However, in most cases the evolutionary tracks have been calculated without correcting for Coulomb interaction and other effects (see section IIIB). Our equations of state for hydrogen, helium, or carbon mixes agree perfectly with those tabulated by Fontaine et al. (1977) or those derived from the formulae of Eggleton et al. (1973), but not in the regions where hydrogen dissociation, pressure ionization, and most cases of carbon ionization contribute dominantly to the equation of state, or the Coulomb corrections are non-negligible, or the effect of electron degeneracy has to be accounted for in the partial ionization zone, see figure 1 and chapters III and V in Fontaine et al. However, in the evolutionary code of Eggleton (1971, 1972, 1973) a treatment of carbon ionization is not included.

The following relations for the excess pressure of the ions, $P_{ex}$, and the excess internal energy, $U_{ex}$, for a liquid and a solid have been adopted:

- 29 -
\[ P_{ex} = N_A \cdot k \cdot \rho \left( \frac{1}{2} U_{qm} + \frac{1}{3} U_{Coul} \right) \]  
\( (23) \)

\[ U_{ex} = N_A \cdot k \left( U_{qm} + U_{Coul} \right) \]

and in the solid state (in which the ions are arranged as in a lattice):

\[ P_{ex} = N_A \cdot k \cdot \rho \left( \frac{1}{2} U_{qm} + \frac{1}{3} U_{lattice} \right) \]  
\( (24) \)

\[ U_{ex} = N_A \cdot k \left( U_{qm} + U_{lattice} \right) . \]

In order to define \( U_{qm} \), \( U_{Coul} \), and \( U_{lattice} \) we introduce the dimensionless Coulomb coupling parameter \( \Gamma_i \) of the \( i \)-th chemical element by:

\[ \Gamma_i = \frac{Z_i^{5/3}}{3} \cdot \left( \frac{4\pi}{3} N_A \right)^{1/3} \cdot \frac{\rho}{k} \cdot \left( \frac{\rho}{\mu} \right)^{1/3} \cdot T^{-1} \]

\[ = 2.2745 \cdot 10^5 \cdot Z_i^{5/3} \cdot \left( \frac{\rho}{\mu} \right)^{1/3} \cdot T^{-1} \text{ (in cgs units)} . \]

The mean Coulomb coupling constant \( \Gamma \) is defined as:

\[ \Gamma = \mu_1 \cdot \sum \frac{Y_i}{A_j} \cdot \Gamma_j , \text{ with } Y_j = \frac{X_i}{A_j} , \text{ see (13) and Ichimaru (1982)} . \]

Recent Monte Carlo calculations (see below, for \( \Gamma \) in the range 1 to 300) resulted in approximations of the ion liquid and ion solid Helmholtz free energy \( F \) per gram (\( F \equiv U - TS \), with \( U \) the internal energy per gram and \( S \) the entropy of the system of ions). From this thermodynamic potential the pressure and internal energy of the ions can be deduced (see Landau and Lifshitz, 1970). The Helmholtz free energy per gram in the liquid state of the \( i \)-th element in an one-component-plasma is given by (see e.g. Richardson et al., 1982):

\[ F_{liquid \ i} = F_{ideal \ gas \ i} + F_{qm \ i} + F_{Coul \ i} , \]

where \( F_{ideal \ gas} \) is the ideal gas contribution, \( F_{qm} \) is the first order correction for quantum mechanical effects to the classical statistical mechanics (in the Wigner expansion), and \( F_{Coul} \) is the Helmholtz free energy of the ions due to the interaction of particles in the Coulomb potential in a
liquid. These components are given as follows (with $R = N_A \cdot k$ and $h$ is Planck's constant) for the $i$-th element by:

$$F_{\text{ideal gas } i} = -1 - \ln \left( \frac{(2\pi kT)^{3/2}}{h^2 N_A} \right) Y_1^{-1} \cdot \left( A_1 T \right)^{3/2},$$

$$= -1 - \ln (3.1204 \cdot 10^{-4} \cdot \rho^{-1} \cdot Y_1^{-1} \cdot \left( A_1 T \right)^{3/2}), \text{ in cgs units;}$$

$$F_{\text{qm } i} = \frac{h^2}{24} \cdot \frac{\rho}{Z_i \mu_e} \left( \frac{Z_i}{T} \right)^2 (\frac{1}{N_A})^2,$n \text{ cgs units;}$$

$$F_{\text{Coul } i} = a_1 \Gamma_1 + 4(b \Gamma_1^{1/4} - c \Gamma_1^{-1/4}) + d \ln \Gamma_1 - (a_1 + 4(b - c) + 0.420).$$

The expression for $F_{\text{Coul } i}$ is derived from a fit to the excess internal energy of a one-component-plasma in a liquid state as derived from a Monte Carlo method by Slattery et al. (1980). The values adopted for the constants $a_1$, $b$, $c$, and $d$ are $-0.89752$, $0.94544$, $0.17954$, and $-0.80049$, respectively. The Helmholtz free energy per gram of the $i$-th chemical element in a one-component-plasma in the crystalline state is given by Pollock and Hansen (1973) by:

$$F_{\text{solid } i} = F_{\text{phonon } i} + F_{\text{Coul } i},$$

where the component of lattice vibrations (phonons), $F_{\text{phonon } i}$, is approximated in the classical statistical mechanical limit (see Pollock and Hansen) as given by:

$$F_{\text{phonon } i} = 1.5 \cdot \ln \left( \frac{24 R T}{Z_i} \right) - 2.4938.$$

The solid state component of the Helmholtz free energy, $F_{\text{Coul } i}$, is derived from the excess internal energy (also) as fitted to Monte Carlo computations of a one-component-plasma (by Slattery et al., see also Hansen (1973)):

$$F_{\text{Coul } i} = a_2 \Gamma_1 - \frac{h}{2} \Gamma_1^{-2}, \text{ where } a_2 = -0.895929 \text{ and } h = 2980.$$

We adopted the following expression for the various components of the Helmholtz free energy in a multi-components-plasma, which is a generalization.
of the expression for a binary mixture (see Ichimaru (1982) and Mochkovitch (1983)):

\[ F_x = \mu_x \cdot \sum_j F_{x_j}, \]

where the index \( x \) is \( \text{qm, ideal gas, liquid or solid} \).

The expressions for the Helmholtz free energy used by us differ from the one used by Slattery et al. to determine the solid-liquid transition, because the latter authors evaluated that transition at \( kT = 1 \) ionic Rydberg unit (\( = N_A \hbar^2 kT(Ze)^{-4}/(2\pi^2) = 3.4755 \times 10^{-9} \ T/Z^4 \)). The solid-liquid transition occurs at the value of \( \Gamma = \Gamma_m \) for which \( (F_{\text{liquid}} - F_{\text{qm}}) \) is equal to \( F_{\text{solid}} \) (see Slattery et al.). The most recent value of \( \Gamma_m \) for a one-component-plasma is 171 ± 3. [As we never reach the melting point of any chemical element in our calculations of the evolution of helium stars, we need not worry about a different approach in case freezing in a multi-components-plasma gives rise to a separation of elements as suggested by Stevenson (1980, see also Mochkovitch (1983)).]

Finally, the expressions for \( U_{\text{qm}}, U_{\text{Coul}}, \) and \( U_{\text{lattice}} \) are obtained from:

\[
\begin{align*}
U_{\text{qm}} &= 2 \sum_i F_{\text{qm}i}; \\
U_{\text{Coul}} &= \sum_i Y_i (a_1 \Gamma_1 + b \Gamma_1^{1/4} + c \Gamma_1^{1/4} + d); \\
U_{\text{lattice}} &= \sum_i Y_i (-a_2 + 1.5 + h \Gamma_1^{-2}),
\end{align*}
\]

where the constants \( a_1, a_2, b, c, d, \) and \( h \) are the same as before. The phonon component to \( P \) \( \equiv [\rho \frac{\partial P}{\partial \mu} \Gamma_j] \) and \( U \) \( \equiv [T \frac{\partial U}{\partial \mu} \Gamma_j] \) in a solid is 3/2 and 1 times the ideal gas component to the total pressure and total internal energy in a fluid, respectively. Hence, the total pressure (and total energy) for a solid can be derived from equations (22), (24) and (29).

The quantum correction breaks the following relation of classical statistical mechanics:

\[
\frac{P_{\text{ex}}}{\rho} = \frac{U_{\text{ex}}}{3}.
\]

The first order quantum corrections to the classical statistical mechanics are not applicable to the low-temperature domain in a non-relativistic electron gas and the high-temperature domain (see Pollock and Hansen, 1973). The \( \rho - T \) condition for a one-component-gas to be classical is:

\[
\frac{6 \cdot 10^{-4}}{AZ^{2/3}} < 180 \cdot Z^{-2} \rho^{2/3} T^{-1} < 14.
\]
The total energy generation rate per gram is given by

\[ (30) \quad \varepsilon = \varepsilon_n - \varepsilon_v - \frac{dQ}{dt}, \]

where \( \varepsilon_n \) is the nuclear energy generation rate, \( \varepsilon_v \) is the neutrino loss rate (excluding neutrino losses by electron captures), and \(- \frac{dQ}{dt}\) is the gravitational energy generation rate (per gram) and according to the second law of thermodynamics (see Cox and Giuli, 1968) given by:

\[ (31) \quad \frac{dQ}{dt} = \frac{dU}{dt} - \frac{P}{\rho^2} \cdot \frac{dp}{dt} = T \cdot \frac{dS}{dt}, \]

where \( S \) is the specific entropy per gram.

The nuclear energy term \( \varepsilon_n \) per gram is given by

\[ (32) \quad \varepsilon_n = \sum \frac{Q_m}{R_m}, \]

where the summation is over all involved nuclear reactions. The energy generated in a single reaction \( Q_m \) (corrected for possibly created neutrino's), or binding energy, for each reaction is taken from Wapstra and Bos (1977). The reaction rates, \( R_m \), are given by Fowler et al. (1975) and are corrected for electrostatic Coulomb screening by the factors given by the prescription of Graboske et al. (1973) and DeWitt et al. (1973); the factor (0 to 1) which appears in some of the reaction rate expressions of Fowler et al. (for example in the triple-alpha rate) was set equal to 0.1. The nuclear partition functions for reverse reactions which enter into the reverse reaction rates are adopted from Bahcall and Fowler (1970). For the envelope integrations the energy generation rate \( \varepsilon \) is taken to be \( \varepsilon_n \) alone (which is very small in the envelope).

The neutrino loss rate \( \varepsilon_v \) is derived from an expression given by Beaudet et al. (1967), which includes pair, photo, and plasma-neutrino losses in the ordinary theory of weak interactions. Using the correction factors ofDicus (1972) and the recent values of the constants \( c_A \) (0.5) and \( c_v \) (0.96) these rates are evaluated in Weinberg's theory (1967, 1971). Furthermore, the neutrino-pair Bremsstrahlung emission rate for a degenerate electron gas (in Weinberg's theory according to Dicus et al., 1976) is included using the formulae of Festa and Ruderman (1969) as corrected for a typographical error by Richardson et al. (1982, see also Lamb and Van Horn (1975) for other expressions). This latter corrected rate can be very important for the
evolutionary stages studied in this thesis, especially for low mass helium stars of 2 to 2.5 $M_\odot$, see also sections IIIA and IIIB.

Usually, the mass in the envelope was to be taken to be 1% - 2%, but sometimes $10^{-3}$ of the total mass of the star. The model calculations are started with a stationary Schwarzschild model, i.e. assuming hydrostatic as well as thermal equilibrium (or simply $\varepsilon = \varepsilon^\ast$) and a homogeneous composition of 97% $^4$He, .75% $^{12}$C, .75% $^{16}$O, and 1.5% $^{20}$Ne. If $^20$Ne is included in the initial model we replaced .75% $^{16}$O by .6% $^{16}$O and .15% $^{20}$Ne. Thus $Z = 0.03$ always. The integration procedure is described in detail by Schwarzschild (1958, chapter III, section 13). The first model does not give evolutionary corrections to the unknowns.

In order to properly solve the diffusion equation (1) with our program the abundances by mass of the elements involved have to be larger than $10^{-20}$. Considering this and the amount of computing time available, the reaction networks for helium and carbon burning as shown in Table 1 are employed for the thermonuclear burning of helium, carbon, and neon; the network for neon burning is recommended for the advanced stages of neon burning. Arnett (1974c) recommended these reaction networks as the minimum necessary, but we suggest to treat neon burning with a more extended network (see also Thielemann and Arnett, 1984). Furthermore, we included the $^{23}$Na($p, \gamma$)$^{24}$Mg reaction for which the reaction rate is changed since Arnett (1972a, b) calculated core-carbon burning and which should be included (Arnett and Thielemann, 1984b). In this way the $^{24}$Mg abundance is not underestimated during carbon and neon burning. Also we do not use the “no sodium” approach (the simplified abundance equations (1-10) of Arnett (1972b)), which neglects the proton channel $^{12}$C + $^{12}$C $\rightarrow$ $^{23}$Na + $^1$H and which does not give realistic energy generation rates for the low-temperature region of carbon burning in 2 to 4 $M_\odot$ helium stars [cf. Endal (1975a, b), but see also Arnett (1973)]. With our network for carbon burning the $^{20}$Ne abundance is obtained more accurately than by the “no-sodium” network of Arnett (1972b, 1973); however, the $^{23}$Na abundance is very much underestimated (the greatest defect of these simple networks). Nevertheless the energy generation rate during carbon burning is correctly represented with our simple network (cf. Endal, 1975b).

The final carbon to oxygen ratio is believed to be very uncertain since Kettner et al. (1982) obtained a 3 to 5 times higher rate for the reaction $^{12}$C($a, \gamma$)$^{16}$O than our adopted rate from Fowler et al. (1975), however a 2 to 4 times higher rate from a re-analysis of experimental data of two laboratories

- 34 -
(Caltech and Münster) is also quoted by Fowler (private communication to Arnett and Thielemann, 1984b), see also Harris et al. (1983) for revised rates for the triple-alpha reaction and for reactions with sodium.

Table 1. Reaction networks used for the various phases of nuclear burning.

<table>
<thead>
<tr>
<th>phase</th>
<th>network</th>
</tr>
</thead>
<tbody>
<tr>
<td>Helium burning</td>
<td>$^3\text{He} + ^{12}\text{C} + \gamma$</td>
</tr>
<tr>
<td></td>
<td>$^{12}\text{C}(\text{He}, \gamma)^{16}\text{O}$</td>
</tr>
<tr>
<td></td>
<td>$^{23}\text{Na}(\text{H}, \gamma)^{24}\text{Mg}$</td>
</tr>
<tr>
<td>Carbon burning</td>
<td>$^{12}\text{C}(\text{C}, \text{H})^{13}\text{N}$</td>
</tr>
<tr>
<td></td>
<td>$^{12}\text{C}(\text{C}, \text{He})^{20}\text{Ne}$</td>
</tr>
<tr>
<td></td>
<td>$^{12}\text{C}(\text{O}, \text{He})^{24}\text{Mg}$</td>
</tr>
<tr>
<td></td>
<td>$^{16}\text{O}(\gamma, \text{He})^{12}\text{C}$</td>
</tr>
<tr>
<td></td>
<td>$^{16}\text{O}(\text{He}, \gamma)^{20}\text{Ne}$</td>
</tr>
<tr>
<td></td>
<td>$^{20}\text{Ne}(\text{He}, \gamma)^{24}\text{Mg}$</td>
</tr>
<tr>
<td>Neon burning</td>
<td>$^{16}\text{O}(\gamma, \text{He})^{20}\text{Ne}$</td>
</tr>
<tr>
<td></td>
<td>$^{12}\text{C}(\text{O}, \text{H})^{27}\text{Al}$</td>
</tr>
<tr>
<td></td>
<td>$^{20}\text{Ne}(\gamma, \text{He})^{16}\text{O}$</td>
</tr>
<tr>
<td></td>
<td>$^{24}\text{Mg}(\gamma, \text{H})^{23}\text{Na}$</td>
</tr>
<tr>
<td></td>
<td>$^{24}\text{Mg}(\gamma, \gamma)^{20}\text{Ne}$</td>
</tr>
<tr>
<td></td>
<td>$^{24}\text{Mg}(\gamma, \text{He})^{28}\text{Si}$</td>
</tr>
<tr>
<td></td>
<td>$^{24}\text{Mg}(\gamma, \text{He})^{27}\text{Al}$</td>
</tr>
<tr>
<td></td>
<td>$^{27}\text{Al}(\gamma, \gamma)^{28}\text{Si}$</td>
</tr>
<tr>
<td></td>
<td>$^{27}\text{Al}(\gamma, \text{He})^{24}\text{Mg}$</td>
</tr>
<tr>
<td></td>
<td>$^{28}\text{Si}(\gamma, \gamma)^{27}\text{Al}$</td>
</tr>
<tr>
<td></td>
<td>$^{28}\text{Si}(\gamma, \text{He})^{24}\text{Mg}$</td>
</tr>
</tbody>
</table>
APPENDIX I

Three-point difference equation.

The ordinary two-point difference equation (10a) does not always give stable solutions: for example it becomes unstable during the carbon-shell burning phase when the neutrino losses are non-negligible. If the time step is of the order or smaller than the time scale of heat diffusion (see section IIIA, paragraph 4a), this instability is due to the averaging of the energy production over two adjacent mesh points in the difference form of the equation of energy conservation: equation (5). If the energy flow $L_r$ is close to zero in two adjacent mesh points $n$ and $n+1$, the solution of the structure equations derived from difference equation (10a) gives $\varepsilon^n \sim -\varepsilon^{n+1}$. If this solution is adopted, further evolution picks up the unstable branch of the differential equation (5). Hence, this solution is physically not realistic. In order to overcome the decoupling of two adjacent mesh points Takens derived a more sophisticated three-point difference expression for any mesh distribution for an equation $\frac{dy}{dx} = p$ as given by:

$$[y_+\xi^3(\xi + 2) - y_0(\xi + 1)^3(\xi - 1) - y_-(2\xi + 1)] + (2\xi + 1)v[y_+\xi - y_0(\xi + 1) + y_-] = \frac{x_+ - x_-}{b} \left[ 3\xi [p_4\xi^2 + p_0(\xi + 1)^2 + p_-] + (2\xi + 1)v \left[ p_+\xi(\xi + 2) - p_0(\xi - 1) - p_- \frac{(2\xi + 1)}{(\xi + 1)} \right] \right] \quad (A1),$$

where $x_-$, $x_0$, and $x_+$ are the $x$-values in three adjacent, not necessarily equidistant, mesh points; $y_-$, $y_0$, and $y_+$ are the corresponding $y$-values, and $p_-$, $p_0$, and $p_+$ are the derivatives of $y$ with respect to $x$ in these mesh points; the expressions for $\xi$ and $v$ are given in the following. The parameter $\xi$ (here not to be confused with the electron degeneracy parameter) is defined as:

$$\xi = \frac{x_+ - x_0}{x_0 - x_-}, \text{ where } 0 < x_- < x_0 < x_+ \text{ and } x = m_r.$$  

This form is used for $\xi$ in the difference expression (A1) applied to the (differential) structure equations (2) and (3b) as given in Chapter II. For use in (A1) applied to the differential equations (4) and (5) of Chapter II we
define $\xi$ as:

$$\xi = \frac{x_0 - x_-}{x_+ - x_0}.$$  

If $A = \left[ \frac{y_0 - y_-}{x_0 - x_-} - \frac{(\xi^2 + 2\xi + 2)p_- + (\xi^3 + 3\xi^2 + 2\xi + 2)p_0 - \xi^3 p_+}{4(\xi^2 + \xi + 1)} \right]^2$

and $B = \left[ \frac{(2\xi^2 + 5\xi + 2)}{12(\xi + 1)(\xi^2 + \xi + 1)} p_- + \frac{(\xi^4 + 3\xi^3 + \xi^2 - 3\xi - 2)}{12(\xi^2 + \xi + 1)} p_0 - \frac{\xi^3(\xi + 2)^2}{12(\xi + 1)(\xi^2 + \xi + 1)} p_+ \right]^2$,

$v$ is given in (Al) by:

$$v = \frac{A}{A + cB + 10^{-14}}$$, where $c$ is a constant.

The three-point expression (Al) derived by Takes is at least of third order, but is at most of fourth order (i.e. a polynomial of degree 3 or 4 can be integrated exactly). If $v = 1$ the three-point expression is of fourth order. The three-point formula reduces to the simple third-order Simpson rule if the grid of mesh points is equidistant (i.e. $\xi = 1$, everywhere in the grid) and if at the same time $v = 0$. The factor $v$ allows a more accurate integration if in the run of $y$-values peaks (or sign changes) occur. With this formula we gain at least one order in accuracy with respect to the second-order ordinary difference equation (e.g. the trapezium rule). By the choice of the constant $c$ $v$ can be set equal to 0 (for a very large value of $c$) or 1 (for a very small value of $c$) and accordingly the three-point formula becomes either of third or fourth order, respectively.

For the two innermost central mesh points of the star and for the two outermost mesh points at the fitting point at the bottom of the envelope the ordinary two-point difference form is used. By the choices of the $\xi$-values (as defined above), by the use of the outer boundary conditions and by the use of the two-point difference expressions at the outer boundaries the structure equations form a closed set.
APPENDIX II

Comparison of the diffusion coefficients used by different authors.

In equation (1) we have chosen the diffusion constant \( \sigma_D \) rather arbitrarily to be \( 10^{-8} \, M_\odot^2 \, s^{-1} \). In fact, in this way the general diffusion equation degenerates into the heat transport equation. In paragraphs 1, 2, 4 and 5 below we examine all known approaches which treat diffusion of the chemical elements by a diffusion approximation and in some cases convective overshoot at the boundary of a convective region. However, the present ideas on convective overshoot at the boundary of a convective region do not rule out either mixing, partial mixing (on a possible long time scale), or even complete, instantaneous mixing in the overshooted region. In paragraph 3 we comment on the boundary conditions used. In paragraph 6 we give our conclusions and our reasons for the choice of the particular value of \( \sigma_D \).

1. Weaver et al.'s (1978) approach.

We calculate the diffusion constant as defined by Weaver et al. (1978) for the convective regions in the last model of the evolutionary sequence for the 2.2 \( M_\odot \) helium star mass-exchange remnant (see section IIIA). For this calculation the average velocity of a convective element, \( v_c \), has to be determined from standard mixing-length theory. We estimate \( v_c \) to be \( 10^5 \, \text{cm s}^{-1} \) in the convective neon- and helium-burning shells, which is a typical order of magnitude estimate for a burning shell [cf. Couch and Arnett (1972), who find \( v_c \) to be \( 5 \times 10^4 \, \text{cm s}^{-1} \) in the convective helium-burning core of a 8 \( M_\odot \) pure helium star; Arnett (1974b), who derives \( 4 \times 10^5 \, \text{cm s}^{-1} \) for an oxygen- and neon-burning shell; Scalo and Ulrich (1973) who find \( v_c \) to be \( 6 \times 10^4 \, \text{cm s}^{-1} \) in a hydrogen-poor helium shell; Sackmann et al. (1974), who find \( v_c \) to be \( 10^4 \) - \( 10^5 \, \text{cm s}^{-1} \) in helium- or hydrogen-burning shells of red giants of 1, 2 and 5 \( M_\odot \)]. Following Weaver et al. we take the mixing length, 1, to be one pressure scale height, \( H_p \), \( (a = \frac{1}{H_p} = 1) \), which is given by:

\[
H_p(r) = - \left( \frac{d \ln P}{dr} \right)^{-1} = \frac{r^2 P}{G \rho r} = 3.65 \times 10^{-5} \left( \frac{r/R_\odot}{m_r/M_\odot} \right)^2 \rho_r (\text{if } P_r \text{ and } \rho_r \text{ in cgs units, } H_p \text{ in cm}).
\]

Weaver et al. define a diffusion coefficient \( D \) (in \( \text{cm}^2 \, s^{-1} \)) to be given by \( D_c = v_c \cdot H_p / 3 \) if the region is convective according to the
Ledoux criterion [see Ledoux (1947)] and to be \( D_s = q_r \cdot D_C \cdot D_r/(D_r + D_C) \) if the region is convective according to the Schwarzschild criterion [see Schwarzschild (1958)] and not by the Ledoux criterion; \( D \) is zero in radiative regions; \( q_r \) was taken to be 0.1 by Weaver et al. The coefficient \( D_r \) is the radiation diffusion coefficient [or "thermal diffusivity", cf. Mochkovitsch (1983) and references therein] for non-convective and non-turbulent regions which have a slow composition variation with time (\( D_r \) is related to the kinematic radiative viscosity for turbulent regions, see paragraph 5):

\[
D_r(r) = \left( \frac{t_h(r)}{r^2} \right)^{-1},
\]

where \( t_h(r) \) is the time scale of heat diffusion (at radius \( r \)) as given by Sugimoto (1970a) [but see also Henyey and L'Ecuyer (1969), for the simplifications and approximations made in order to derive this time scale]:

\[
2 \cdot \frac{3c \cdot \rho \cdot r}{4acT}.
\]

In the approach of Weaver et al. a few mesh points adjacent to the convective region are treated as overshooted regions which are mixed on the order of the time scale of radiative diffusion (which can be short), however, convective regions are almost entirely mixed on a time scale of the order \( D_r(r) \).

In the 2.2 \( M_\odot \) helium star remnant (see section IIIA) \( t_h(r) \) varies from 3.4 seconds in the centre to \( 1.5 \times 10^5 \) seconds at the bottom of the envelope at the time of off-centre neon ignition. Near and in the convective neon-burning region \( t_h(r) \) varies non-uniformly from 100 s to 700 s (and \( r \) is \( 1.6 \times 10^{-3} \) \( R_\odot \) to \( 2.6 \times 10^{-3} \) \( R_\odot \), \( \rho \) is \( 4.2 \times 10^7 \) g cm\(^{-3} \) to \( 2.6 \times 10^7 \) g cm\(^{-3} \), \( 1nP \) is 57.1 to 56.4, and \( m_r \) is 0.14 \( M_\odot \) to 0.44 \( M_\odot \)). Over this region \( D_r \) varies from \( 4.3 \times 10^{12} \) cm\(^2\) s\(^{-1} \) to \( 9.3 \times 10^{13} \) cm\(^2\) s\(^{-1} \) and \( D_C \) ranges from \( 3.3 \times 10^{12} \) cm\(^2\) s\(^{-1} \) to \( 2.2 \times 10^{13} \) cm\(^2\) s\(^{-1} \); between \( m_r \) is 0.14 \( M_\odot \) and 0.44 \( M_\odot \) (if we assume \( v_c \) to be \( 10^5 \) cm s\(^{-1} \) everywhere in this region).

The value of the diffusion constant \( \sigma_D \) which corresponds to our diffusion constant for convective regions is given by:

\[
\sigma_D = (4\pi r^2)^2 \rho r^2 D(r).
\]

We thus derive \( \sigma_D = 2.6 \times 10^{-6} M_\odot^2 \) s\(^{-1} \) and \( \sigma_D = 3.5 \times 10^{-5} - 6.5 \times 10^{-5} \) in the convective neon-burning shell taking for \( D(r) \) the values of \( D_s \) and \( D_c \).
respectively. Hence, our value \((10^{-8} \, M_\odot \, s^{-1})\) would have been chosen too small; however, nearly complete mixing of the convective neon-burning region is obtained even with this low value.

In the convective helium-burning shell of the \(2.2 \, M_\odot\) helium star remnant (\(m_r\) ranging from 1.543 \(M_\odot\) to 1.590 \(M_\odot\), \(\rho\) ranging from \(10^{-3}\) g cm\(^{-3}\) to 172 g cm\(^{-3}\), \(r\) ranging from 2.74 \(10^{-2}\) \(R_\odot\) to 5.805 \(10^{-2}\) \(R_\odot\), \(\ln P\) from 44.94 to 42.55, \(t_h(r)\) from 100 s to 820 s) we find \(D_r\) is \(3.6 \times 10^{16} \, \text{cm}^2 \, \text{s}^{-1}\) at \(m_r = 1.543 \, M_\odot\) and \(2 \times 10^{16} \, \text{cm}^2 \, \text{s}^{-1}\) at \(m_r = 1.590 \, M_\odot\). However, \(D_c\) ranges from \(1.9 \times 10^{13} \, \text{cm}^2 \, \text{s}^{-1}\) to \(4.5 \times 10^{13} \, \text{cm}^2 \, \text{s}^{-1}\), respectively, and \(\alpha_D = 1.0 - 1.4 \times 10^{-9} \, \frac{M_\odot^2}{\text{s}^{-1}}\) and \(\sigma_D = 1.0 - 1.4 \times 10^{-8} \, \frac{M_\odot^2}{\text{s}^{-1}}\) taking for \(D(r)\) the values of \(D_B\) and \(D_C\), respectively, which agrees reasonably well with our adopted value for \(\alpha_D\).

Already Arnett (1974b) pointed out that during oxygen burning the assumption of instantaneous mixing in a convective neon-burning shell is invalid for helium stars of 4 to 32 \(M_\odot\). Therefore, a time-dependent treatment of convective mixing must be used in that stage. Arnett found that the neon depletion time scale is larger, but of the same order, than the convective "turn-over time scale" for the core, which agrees with our results.

2. Eggleton's approach.

Eggleton (1972, see also 1971, 1973) proposes \(\alpha_D\) to be given by:

\[
\alpha_D = K \left( V_{\text{rad}} - V_{\text{ad}} \right)^2 \frac{m_*^2}{t_*}, \text{where}
\]

\(m_*\) is the stellar mass, \(t_*\) is the life-time of the star in the evolutionary phase considered, and \(K\) is an adjustable parameter chosen to be \(10^4\), \(10^5\) or \(10^6\). In this way Eggleton is able to treat semi-convective regions and superadiabatic regions. Eggleton estimates \(\alpha_D t_*/m_*^2\) to be in the range \(10^6\) to \(10^{10}\), which agrees roughly with the values which we use. If \(K\) is taken to be \(10^4\) we find the diffusion constant \(\alpha_D\) to vary from \(10^{-5} \, \frac{M_\odot^2}{\text{s}^{-1}}\) to \(2 \times 10^{-11} \, \frac{M_\odot^2}{\text{s}^{-1}}\) from the centre to the boundary of the convective core of a 32 \(M_\odot\) hydrogen star (using a version of Eggleton's code in which \(\alpha_P/K\) is not given by the proposed value, but by a function which depends on \((V_{\text{rad}} - V_{\text{ad}})^2\), on \(V\) (i.e. the actual \(\text{dlnT/dlnP}\) gradient), on the mesh point distribution, and on the nuclear time scale of evolution). The value for \(\alpha_D\) in the centre of the 32 \(M_\odot\) star is rather large and would probably give a singular matrix with our diffusion approximation.
In the approach of Eggleton the convective region itself is not completely mixed close to its boundary.

3. Boundary conditions.

The introduction of the diffusion equation (1) requires two boundary conditions for a convective shell and only one for a convective core (due to spherical symmetry). Hence, the change in composition in the first radiative mesh point(s) adjacent to the convective zone must be given (e.g. by local nuclear burning). In order to guarantee conservation of mass in a convective region we require at each boundary that the composition in the two outermost convective mesh points has the same value [A similar approach was adopted by Sackmann et al. (1974), but in case of a turbulent flow or convective overshoot at the convective boundary other boundary conditions are required, see Schatzman (1969)]. However, if nuclear burning is negligible this requirement leads to a singular matrix. In that case we have to set the composition at one convective edge equal to a constant value.

If the centre is convectively unstable we use an expansion for the composition between the centre and the second mesh point at radius \( r \), (which is allowed, because \( \frac{dX}{dr} = 0 \), see Savonije and Takens (1976)):

\[
X(r) = X_0 + \left( \frac{X_1 - X_0}{r} \right)^2, \\
\]

where \( X_0 \) and \( X_1 \) are the composition in the centre and in the adjacent mesh point number 1. Since mixing is in all three dimensions we can rewrite equation (1) with a constant diffusion parameter \( \sigma_D \) into (using a cartesian coordinate system):

\[
6D_0 \sigma_X \frac{(X - X_0)}{m_1^2} \frac{dX}{dt} = P_0 - D_0 + \frac{d}{dt} X_0, \\
\]

where \( m_1 \) is the mass coordinate of mesh point 1, \( \sigma_D \) is the diffusion constant of meshpoint 0, and \( P_0 \) and \( D_0 \) are the production and destruction rates of the element \( X \) evaluated at mesh point 0 (the central mesh point).

4. The use of a molecular diffusion coefficient.

Giannone and Rossi (1981), Prialnik et al. (1981), Stringfellow et al.
applied the diffusion equation of the type as given by Landau and Lifshitz (1966), with a diffusion coefficient $D \neq 0$, also to radiative zones in order to study the effects on thermal pulses and the long-term effects of chemical separation by diffusion (which may be a combination of mass diffusion, thermal diffusion, and pressure diffusion). Prialnik et al. (1981) give an expression for this so-called ion, gas, or molecular, diffusion coefficient $D_m$ for a fully ionized, non-degenerate gas (a mixture of helium and hydrogen):

$$D_m = 4.8 T_6^{2.5} \rho^{-1}, \text{where } T_6 = T/10^6.$$

This coefficient is about $7 \times 10^3 \text{ cm}^2 \text{ s}^{-1}$ in the convective helium-burning shell of the last calculated model of the 2.2 $M_\odot$ helium star remnant at $m_r = 1.543 - 1.590 M_\odot$ which is not sufficiently large to give complete mixing in this shell, i.e. $\sigma \sim 4 \times 10^{-18} M_\odot^2 \text{ s}^{-1}$. A more complex and more general expression for the diffusion coefficient for such a mix is given by Roussel-Dupré (1981, 1982), but see also Stringfellow et al. (1983). Kothari (1932, see Cox and Giuli, 1968) gives an expression for the molecular or gas viscosity coefficient or dynamic viscosity (i.e. in $\text{g cm}^{-1} \text{ s}^{-1}$) for a non-relativistic electron degenerate gas. The kinematic viscosity for this gas (or the diffusion coefficient) is obtained by dividing that expression by the density, which results into:

$$D_m = 4.22 \times 10^{-6} \rho^{2/3} [1/(1 + 3.08 \rho^{2/3}/10^{-3}) + e^{\log(1 + 3.08 \times 10^{-3} \rho^{2/3})}]^{-1}.$$

In the partial electron degenerate, partial relativistic convective neon-burning shell in the last calculated model of the 2.2 $M_\odot$ helium star remnant the gas diffusion coefficient varies from 0.08 to 0.06 $\text{cm}^2 \text{ s}^{-1}$ (with increasing radius) and the corresponding $\sigma_0$ ranges from $1.1 \times 10^{-17} M_\odot^2 \text{ s}^{-1}$ to $2.9 \times 10^{-17} M_\odot^2 \text{ s}^{-1}$.

5. The approaches by Sackmann et al. and by Schatzman and Maeder

Sackmann et al. (1974) adopted a diffusion coefficient $D$ given by:

$$D = v_c \cdot 1,$$

where $v_c$ and 1 are defined as before.
These authors introduced $D$ as a "convective" diffusion constant in deep convective envelopes of red giants. However, Sackmann et al. used a diffusion equation which conserves species of chemical elements only if the density does not change with time.

Finally, Schatzman (1969, 1977) included the effects of turbulence by using the diffusion approximation. In a non-rotating star turbulence can occur only as a consequence of convection or convective overshoot, which can be described with a diffusion approximation in the manner suggested by Weaver et al. (1978, see above). However, a diffusion equation accounting for the effects of convection and of turbulence has to be included in a more-dimensional evolutionary code in order to study the evolution of rotating stars. Schatzman (1977), Schatzman and Maeder (1981), Maeder (1982), Bienaymé et al. (1984), and Michaud et al. (1984) used a one-dimensional code in order to calculate the evolution of 1 to 60 $M_\odot$ hydrogen stars with turbulent mixing. These calculations have to be considered with some caution, because the underlying theory is not firmly founded. In the approach of Schatzman and co-authors a turbulent diffusion coefficient (see below) is introduced. This coefficient is obtained by "blowing up" the molecular diffusion coefficient and the kinematic radiative viscosity (as defined below) by a factor 10 to 200; Michaud et al. obtained the turbulent diffusion coefficient by multiplying only the molecular diffusion coefficient with a constant factor.

In a region in local thermodynamic equilibrium (see Cox and Giuliani, 1968) the kinematic radiative viscosity is given by (see e.g. Van den Horn and Van Weert (1981) and Vaucclair (1983)):

$$D_{\text{rad}} = \frac{16}{15} \frac{\sigma T^4}{\kappa c} \rho^{-2} = 6.728 \times 10^{-26} \frac{4}{4} \kappa^{-1} \rho^{-2},$$

where $\kappa$ is the total opacity. The radiation diffusion coefficient $D_\text{r}$ for non-turbulent matter is related to the kinematic radiative viscosity $D_{\text{rad}}$ by the Prandtl number ($\equiv D_{\text{rad}}/D_\text{r} = c_p T/(5c^2)$). $D_{\text{rad}}$ is largest near the stellar surface (Cox and Giuliani); in the Sun $D_{\text{m}}$ dominates over $D_{\text{rad}}$ at $m_\text{r} = 0.5 \, M_\odot$ and in a 60 $M_\odot$ hydrogen star at $m_\text{r} = 30 \, M_\odot$ (when the central hydrogen abundance is 0.35) $D_{\text{rad}}$ is about $5 \times 10^2$ times as large as $D_{\text{m}}$ and about $10^5$ times as large as in the Sun at $m_\text{r} = 0.5 \, M_\odot$ (Maeder, 1982). $D_{\text{rad}}$ varies from $4.339 \times 10^3 \, \text{cm}^2 \, \text{s}^{-1}$ at $m_\text{r} = 1.590 \, M_\odot$ to $6.950 \times 10^3 \, \text{cm}^2 \, \text{s}^{-1}$ at $m_\text{r} = 1.543 \, M_\odot$ in the convective helium-burning shell in the last calculated model of the 2.2 $M_\odot$ helium star remnant. At the convective neon-burning shell of this model $D_{\text{rad}}$ is about $0.007 \, \text{cm}^2 \, \text{s}^{-1}$.
(for \( m_r \) in the range 0.126 \( M_\odot \) to 0.25 \( M_\odot \)).

The turbulent diffusion coefficient used by Schatzman and co-authors is given by a simple relation (in case of an assumed shear flow instability):

\[
D_{\text{tur}} = R_e^* (D_{\text{rad}} + D_m)
\]

where \( R_e^* \) is a critical Reynolds number (see Schatzman (1977) and Vauclair (1983) for the definition), which is zero for a non-rotating star and which is estimated to be 10 to 200 for 1 to 60 \( M_\odot \) hydrogen stars. Zahn (1983) estimated the value of \( R_e^* \) (for diffusion in the vertical direction) of a rotating star to be:

\[
R_e^* = 5 c^2 T^{-1} c_s^2 \Omega r (G m_r)^{-1} \left( \nabla_{\text{ad}} - \nabla_{\text{rad}} \right)^{-1}
\]

where \( \Omega \) is the angular velocity at radius \( r \) in the star; even though numerous crude approximations have been made in order to derive this expression, the resulting values for \( R_e^* \) for the Sun agree with the estimated values of \( R_e^* \) from a comparison of the observed solar Li and He surface abundances and these abundances derived by Schatzman and Maeder (1981) from stellar evolution calculations including turbulent diffusion, cf. Zahn (1983), Schatzman (1984), and Michaud et al. (1984).

6. Conclusions.

We decided to treat overshooting not in the way as proposed by Weaver et al. (1978), but by inserting new mesh points near the boundary of the convective region or by using the implicit mesh point technique (see Chapters II and IV, and section IIIA). With our methods convective overshoot occurs at the boundary of the convective region and the overshooted regions are mixed almost instantaneously as assumed by us and by Savonije and Takens (1976).

Our choice of \( \sigma_0 \) guarantees complete or nearly complete mixing in convective regions (within at least 3 digits) during helium, carbon, and neon burning in the core. However, during carbon-shell burning or after core-neon burning a larger value of \( \sigma_0 \) (\( \sim 10^{-5} \) to \( 10^{-6} \ M_\odot^2 \text{ s}^{-1} \)) for these shells must be chosen to achieve complete mixing, but that may be no good assumption in these regions which rapidly burn their nuclear fuel (see also Arnett, 1974b). Moreover, we conclude that both a constant and a variable diffusion coefficient may lead to (almost) complete mixing in convective regions depended on the computational method used (for example our or Eggleton's code,
respectively).

The approximation $D(r) = 0$ for radiative regions represents fairly well the actual situation in which either nuclear burning dominates the changes in composition or the time scale of molecular diffusion is very much longer than the evolutionary life-time of a helium star in the mass range $2.0 - 4.0 \, M_\odot$.

It is beyond the scope of our investigation to examine long-term effects of molecular diffusion and it is not correct to treat turbulent mixing with a one-dimensional stellar evolution code with our diffusion approach (Schatzman and Maeder, 1981).