MODELS FOR SOLAR ABUNDANCE STARS WITH GRAVITATIONAL SETTLING AND RADIATIVE ACCELERATIONS: APPLICATION TO M67 AND NGC 188

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ABSTRACT

Evolutionary models taking into account radiative accelerations, thermal diffusion, and gravitational settling for 28 elements, including all those contributing to OPAL stellar opacities, have been calculated for solar metallicity stars of 0.5–1.4 $M_\odot$. The Sun has been used to calibrate the models. Isochrones are fitted to the observed color-magnitude diagrams (CMDs) of M67 and NGC 188, and ages of 3.7 and 6.4 Gyr are respectively determined. Convective core overshooting is not required to match the turnoff morphology of either cluster, including the luminosity of the gap in M67, because central convective cores are larger when diffusive processes are treated. This is due mainly to the enhanced helium and metal abundances in the central regions of such models. The observation of solar metallicity open clusters with ages in the range of 4.8–5.7 Gyr would further test the calculations of atomic diffusion in central stellar regions: according to nondiffusive isochrones, clusters should not have gaps near their main-sequence turnoffs if they are older than $\approx$4.8 Gyr, whereas diffusive isochrones predict that gaps should persist up to ages of $\approx$5.7 Gyr. Surface abundance isochrones are also calculated. In the case of M67 and NGC 188, surface abundance variations are expected to be small. Abundance differences between stars of very similar $T_{\text{eff}}$ are expected close to the turnoff, especially for elements between P and Ca. Moreover, in comparison to the results obtained for giants, small generalized underabundances are expected in main-sequence stars. The Li/Be ratio is discussed briefly and compared with observations. The inclusion of a turbulent transport parameterization that reduces surface abundance variations does not significantly modify the computed isochrones.

Subject headings: convection — diffusion — Hertzsprung-Russell diagram — open clusters and associations: general — open clusters and associations: individual (M67, NGC 188) — stars: evolution

1. ASTROPHYSICAL CONTEXT

The open clusters M67 and NGC 188 have about the solar metallicity, bracket the solar age, and have turnoff stars only a few hundred degrees hotter than the Sun. As such, they are interesting testing grounds for the effects of atomic diffusion on age determinations and surface abundances, since, in the case of the Sun, there is now ample evidence from helioseismology that atomic diffusion has reduced the surface He abundance (Guzik & Cox 1992, 1993; Christensen-Dalsgaard, Proffitt, & Thompson 1993; Proffitt 1994; Bahcall, Pinsonneault, & Wasserburg 1995; Guenther, Kim, & Demarque 1996; Richard et al. 1996; Brun, Turek-Chieze, & Zahn 1999). Indeed, diffusive processes presumably also cause small underabundances of metals in the Sun: these are caused mainly by gravitational settling but are also modified by radiative accelerations ($\gamma_{\text{rad}}$), which are predicted to be especially important at the end of the main-sequence phases of solar-type stars (Tucotte et al. 1998). What abundance anomalies are then to be expected in the turnoff stars of M67, which are $\sim$400 K hotter than the Sun (Hobbs & Thorburn 1991), and in those of NGC 188, which are $\sim$100 K hotter (Hobbs, Thorburn, & Rodriguez-Bell 1990)? As the cluster turnoff stars are expected to have smaller surface convection zones, they may show larger effects of atomic diffusion than the Sun. On the other hand, since the radius and age of the Sun are used to calibrate the mixing length and assumed initial He abundance, this normalization may eliminate the effects of diffusion on age determinations. Whereas an $\approx$10% reduction in age at a given turnoff luminosity—compared to the predictions of models that neglect diffusion—was derived by VandenBerg et al. (2002) from the diffusive models for Population II stars computed by Richard et al. (2002), it is not clear that a similar reduction should be expected in the case of Population I stars. In addition, there may be some important differences in the morphologies of the diffusive and nondiffusive isochrones in the age range in which a transition is made between isochrones that have a gap near the main-sequence turnoff and those that do not. One naively expects that both the sizes of convective cores in models for main-sequence stars of a given mass and the predicted mass marking the transition between stars that have convective and radiative cores on the main sequence will depend (to some extent) on whether or not diffusive processes are treated. (For instance, the concomitant increase in opacity with the settling of Fe in the cores of stars would tend to enhance convective instability.)
In this regard, we note that the first studies of NGC 188 (Sandage 1962; Eggen & Sandage 1969) concluded that it has a gap near the top of its main sequence on the \((V, B-V)\) diagram reminiscent of that seen in M67. McClure & Twarog (1977) carried out a statistical test of the photographic photometry that they obtained for the same cluster and confirmed the existence of the gap in the color-magnitude diagram (CMD) that was constructed for stars within ring I on Sandage’s original finder chart. Curiously, no statistically significant evidence for a gap was found if their CMD included stars in Sandage’s ring II, but McClure & Twarog concluded that contamination by field stars was almost certainly much more severe in the outer ring and that, if it were possible to remove the field stars, “the gap would be obvious.” The proper-motion membership study of Dinescu et al. (1996) does not shed any light on this problem (because of the very large scatter in their CMD fainter than \(V = 15\); the gap is located at \(V \approx 15.5\) according to McClure & Twarog [1977]). However Platais et al. (2003) provide a well-defined CMD down to \(V = 20\), with no indication of a turnoff gap.

Because there is no obvious indication of a gap in subsequent CMDs for NGC 188 (e.g., Kaluzny 1990; Caputo et al. 1990; Sarajedini et al. 1999), and because the best-fitting isochrones for current best estimates of the cluster distance and reddening do not predict a gap at the turnoff \(M_V\), the gap is located at \(V \approx 15.5\) according to McClure & Twarog [1977]).

In NGC 188, the surface Li abundance in solar-type stars appears to be consistent with a single-valued function of \(T_{\text{eff}}\), just as in the Hyades (see Randich, Sestito, & Pallavicini 2003). Furthermore, even though NGC 188 is older than M67 by \((2 - 3) \times 10^9\) yr (e.g., Sarajedini et al. 1999), the Li abundance in its G-type stars is comparable to the largest abundances measured in M67 stars with similar colors/temperatures. Could a simpler model account for the Li observations in the Hyades and NGC 188 than that for M67? Pre-main-sequence evolution could be largely responsible for the Li destruction in the Hyades and NGC 188 (see, e.g., Proffitt & Michaud 1989; Piau & Turck-Chièze 2002). Finally, we note that the relative abundances of Li and Be along the subgiant branch of M67 have been evaluated in models including gravitational settling by Sills & Deliyannis (2000). However, what are the ratios of the Li and Be abundances to be expected from diffusion if \(g_{\text{grad}}\) is also taken into account?

In this paper, after a very brief description of the calculations in § 2, the chemical composition expected on the surfaces of stars of M67 and NGC 188 is discussed in § 3.1, and Li/Be ratios in § 3.2. The effect of atomic diffusion on central convective cores is analyzed in detail in § 3.3. The effect of diffusion on isochrones is discussed in § 4, and these results are applied to M67 and NGC 188 in § 5. The main conclusions are summarized in § 6. Throughout this paper the emphasis is on calculations in the presence of atomic diffusion and, in some cases, of turbulent transport with the same parameterization as used for Population II stars by Richard et al. (2002). The discussion of potential star-to-star variations of turbulent transport to explain Li abundance spread at a given \(T_{\text{eff}}\) is left to a paper in preparation.

2. Calculations

The models were calculated as described by Turcotte et al. (1998) and Richard, Michaud, & Richer (2001). They were assumed to be chemically homogeneous on the pre-main sequence with a solar abundance mix and relative concentrations as defined in Table 1 of Turcotte et al. (1998). The radiative accelerations are from Richer et al. (1998), with the correction for redistribution from Gonzalez et al. (1995) and LeBlanc, Michaud, & Richer (2000). The atomic diffusion coefficients were taken from Paquette et al. (1986) (see also Michaud & Proffitt 1993). In all cases, the Krishna Swamy \(T-\tau\) relation (Krishna Swamy 1966) was used to derive the outer boundary condition for the pressure that is needed to construct stellar models. Semiconvection was included as described in Richard et al. (2001), following Kato (1966), Langer, El Eid, & Frick (1985), and Maeder (1997).

In Turcotte et al. (1998), the solar luminosity and radius at the solar age were used to determine the value of \(\alpha\), the ratio of the mixing length to the pressure scale height in the usual mixing-length theory (MLT) of convection, and of \(Y_0\), the He concentration in the zero-age Sun. The value of \(Y_0\) mainly affects the luminosity, while \(\alpha\) primarily determines the radius, through the depth of the surface convection zone. The required value of \(\alpha\) was found to be slightly larger in the diffusive than in the nondiffusive models, because an increased value of \(\alpha\) is needed to compensate for the settling of He and the metals from the surface convection zone. The increase in \(\alpha\) in the diffusion models of the Sun is thus determined by the settling that occurs immediately below the surface convection zone.

The value of \(\alpha\) and the initial values of \(Y_0\) and \(Z_0\) that were adopted in each of the three series of models computed for this study are given in Table 1, together with the accuracy with which they represent the solar properties at the solar age. We did not force convergence as precisely as in Turcotte et al. (1998), but the convergence should suffice for the purposes of this paper. The model with atomic diffusion only is calculated using the same values of \(Y_0\), \(Z_0\), and \(\alpha\) as in Turcotte et al. (1998), even though small changes have since been made to the code, such as a better treatment of some interaction terms in the diffusion equations for the various species. (This is what has caused a slight degradation of the convergence criteria.) For the nondiffusive case, the values of \(Y_0\), \(Z_0\), and \(\alpha\) tabulated...
by Turcotte et al. (1998) (model B of their Table 2) were calculated using tables of mean opacities, while here the monochromatic opacities were used even for models without diffusion. This causes small differences in the central regions of the solar model where CNO abundance variations modify the opacity, leading to slight differences in our value of \( \delta/C_{11} \) (see Table 1) compared to that used in model B of Turcotte et al. (1998).

One series of models was calculated with the same turbulent transport parameterization, labeled T6.09, that was found to minimize the surface Li abundance changes in Population II field stars (see Richard et al. 2002 for both the definition of this turbulent transport parameterization and its justification). As can be seen from Figure 6 of Richard et al. (2002), that turbulent transport coefficient approximately equals the He atomic diffusion coefficient at \( \log T = 6.3 \) and diminishes rapidly as \( T \) increases further. Because this is the temperature close to the bottom of the solar surface convection zone, this level of turbulent transport does not affect solar models significantly. We have, in fact, verified that the same values of \( Y_0 \), \( Z_0 \), and \( \alpha \) are obtained for the calibrated solar models that allow for only atomic diffusion, on the one hand, and atomic diffusion plus T6.09 turbulence, on the other. Since, furthermore, it is the effect of adding turbulence to models with atomic diffusion that we wish to study, the models with turbulence must have the same \( Y_0 \) and \( \alpha \) as those with atomic diffusion only.

### 3. EVOLUTIONARY MODELS

In Figure 1 is shown, for a few of the calculated models, the time dependence of \( T_{\text{eff}} \), as well as of the depth of the surface and central convection zones. The data were taken from some of the models without diffusion (top panels) and from some with atomic diffusion (bottom panels). The surface convection zone mixes to the surface the abundances that are modified by atomic diffusion below the fully mixed outer layers. The time dependence of the depth of the surface convection zone determines the time dependence of the depth of the region where element separation occurs. In these models, the smallest convection zones (in terms of the amount

| \( Z_0 \) | \( Y_0 \) | \( \alpha_{\text{MLT}} \) | Atomic Diffusion | Turbulence | \( L/L_0 \) | \( R/R_0 \) |
|---|---|---|---|---|---|---|
| 0.01750 | 0.26811 | 1.94646 | No | No | 0.999 | 0.996 |
| 0.01999 | 0.27769 | 2.09635 | Yes | No | 1.002 | 1.002 |
| 0.01999 | 0.27769 | 2.09635 | Yes | T6.09 | 1.001 | 1.002 |

Note.—A Krishna Swamy boundary condition is used for all computations shown here.

* For \( L/C_{12} = 3.86 \times 10^{33} \) ergs s\(^{-1} \).

b For \( R/C_{12} = 6.9599 \times 10^{10} \) cm.

c See Richard et al. 2002.
of mass that they contain) occur early in the evolution and for a brief period just past the turnoff. This is different from the stars in low-metallicity Population II globular clusters, in which the mass in the surface convection zone decreases throughout the main-sequence phase (see Richard et al. 2002, Fig. 1).

3.1. Chemical Composition

Figure 2 illustrates the variation in the surface abundances of several species as a function of $T_{\text{eff}}$ at 3.7 Gyr, which is our estimate of the age of M67 (see §5 below). These "surface abundance isochrones" were calculated for an additional 19 species, but only representative ones are shown; the other loci bear considerable similarity to those that have been plotted. The corresponding $g_{\text{rad}}$ values are illustrated in Figure 3 for B, Mg, P, Ti, Fe, and Ni. (The $g_{\text{rad}}$ values of He, Li, and Be are negligible in 1.3 $M_\odot$ models.)

The surface abundances of $^3$He and LiBeB are affected by both diffusion processes and nuclear reactions. The effect of nuclear reactions on the surface abundances of these elements becomes evident during the evolution of a star on the subgiant branch, when dredge-up occurs. Overabundances of $^3$He are predicted to appear as the star reaches $T_{\text{eff}} \approx 5400$ K (the temperature at which the surface abundance isochrone becomes nearly vertical in Fig. 2). At this point in the star’s evolution, the bottom of the surface convection zone reaches down to regions where $^3$He has a concentration maximum produced during the main-sequence stage (Iben 1965). For LiBeB, underabundances are expected at $T_{\text{eff}} \approx 5800$ K for Li and Be and $\lesssim 5600$ K for B (see Fig. 2); this occurs as the bottom of the surface convection zone reaches the regions where Li, Be, and B burn. The other abundance variations are caused by atomic diffusion.

In the model with atomic diffusion only, the surface abundance variations as a function of time are directly related to the depth of the surface convection zone (see Fig. 1); overabundances normally appear when $g_{\text{rad}} \geq g$ immediately below the surface convection zone. When the reverse is true, underabundances generally appear at the surface. The detailed results can be understood by remembering that, for those elements whose $g_{\text{rad}}$ is small, the surface abundance decreases approximately as

$$\exp(-t/\theta),$$

(1)
where

\[ \theta \simeq 2.3 \times 10^{11} (\Delta M/M_\odot)^{0.545} \text{ yr} \]  

\( (2) \)

(for helium, with similar expressions for other species; see Michaud 1977). The precise value of the multiplying constant varies slightly with stellar mass, but more so with the atomic weight of each element and its charge. When \( \theta \) is smaller than the age of the star, the abundance reached is a very sensitive function of the mixed mass.

The \( g_{\text{rad}} \) for B below the surface convection zone (see Fig. 3) is always smaller than gravity by at least a factor of 2. Consequently, it has no more than a small effect (if any) on the B concentration, which is mainly determined by gravitational settling until the bottom of the surface convection zone reaches the temperature at which B burns.

The Mg abundance has a \( T_{\text{eff}} \) variation typical of species from O to Si: it is caused by \( g_{\text{rad}} \) (see Fig. 3) being much smaller than gravity below the surface convection zone, throughout the evolution of the stars in the relevant mass range. Elements from O to Si have \( g_{\text{rad}} \) with a similar \( \log (\Delta M/M_\odot) \) dependence. All of these elements settle by gravitation below the surface convection zone, and they have the largest underabundances at the end of the main-sequence phase. The underabundances are larger in the more massive stars because they have smaller surface convection zones (see Fig. 1).

P and Ti represent all elements between P and Ti (except for S, which is more like Mg). Their \( g_{\text{rad}} \) values are slightly larger than gravity for a significant mass interval below the convection zone (see Fig. 3). The mass interval in which \( g_{\text{rad}} \) is large varies from P to Ti. As the atomic number of the species increases, the larger values of \( g_{\text{rad}} \) shift to a greater depth. Very small overabundances may appear at the turnoff, but at a later epoch in only the more massive stars considered here. For most species, the effect of \( g_{\text{rad}} \) is merely to reduce the expected underabundances in the hotter stars.

Fe is representative of species of the Cr, Mn, Fe group. For all of them, \( g_{\text{rad}} \) is continuously smaller than gravity below the surface convection zone, but not by as large a factor as for Mg. Consequently, the predicted underabundances are not as large either. Finally, Ni is supported below the convection zone in the hotter stars considered.

In the presence of T6.09 turbulence, one expects underabundances of the metals at the \( \sim 6\% \) level in stars between 4000 and 5000 K, progressively increasing to \( \sim 12\% \) in stars of 6000 K. Only underabundances are predicted, because the T6.09 turbulence mixes deep enough in the star (down to \( \log (\Delta M/M_\odot) \approx -2 \)) for \( g_{\text{rad}} \) to never play a dominant role. The \( g_{\text{rad}} \) still limits the underabundances of a number of species, and in particular of Ti, as can be seen in Figure 2.

\[^2\] In this paper, \( \Delta M \) always represents the mass of the spherical shell outside a certain radius. Furthermore, in the above equation, this mass is assumed to be mixed (for instance, by convection).

\[^3\] To see the variation of all \( g_{\text{rad}} \) values with \( T \), reference can be made to Fig. 1 in the study by Richer et al. 1998.

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**Fig. 3.**—Radiative accelerations in a 1.3 \( M_\odot \) solar metallicity star at 1.4, 2.4, and 3.7 Gyr. The bottom of the surface convection zone at each epoch is indicated by a vertical line of the same type. Gravity (\( g \)) is plotted in each panel of the figure. The \( g_{\text{rad}} \) values of Li and Be are not shown because they are always smaller than that of B below the surface convection zone, and so do not have a significant impact on Li and Be abundances.
3.2. The Li/Be Ratio in M67

Sills & Deliyannis (2000) calculated the Li/Be abundance ratio with a number of evolutionary models that included either turbulent transport, atomic diffusion, or no transport process (dubbed "standard models") and presented a comparison of the different results in their Fig. 5. They used these results to determine the relative importance of those transport processes. In their models with atomic diffusion only, they obtain a factor of \(100\) reduction of the Be abundance at the same time as a factor of \(30\) reduction of the Li abundance, or \(X(\text{Be}) \approx [X(\text{Li})]^{1/3}\). This is to be compared with the results shown in Figure 5 of this paper. On the leg of the isochrone corresponding to main-sequence stars, one has \(X(\text{Be}) \approx [X(\text{Li})]^{1/3}\), while on the leg corresponding to subgiants, one has \(X(\text{Be}) \approx X(\text{Li})\). Combining the two segments would give approximately \(X(\text{Be}) \approx [X(\text{Li})]^{1/2}\), but with a large dispersion that is in agreement with the Li/Be ratios observed in field stars and discussed by Sills & Deliyannis (2000). Our results for the diffusion models are very different from theirs, probably because of our more complete description of atomic diffusion processes.

Observations of Li and Be in M67 were recently made by Randich et al. (2002), and their Li/Be ratios are also plotted in Figure 5. Some of their stars have \(V\) magnitudes that correspond to stars just before turnoff, while others are slightly above it. Four of the five observed points are compatible with the model that includes only atomic diffusion processes. Given the error bars, the agreement could be considered satisfactory; however, the star with the smallest Be abundance (S988) has a magnitude corresponding to pre-turnoff stars and so should not be on that segment of the curve.

One can also note that the original Li abundance used in these calculations (see Fig. 5) is smaller than usually believed to be appropriate in young solar metallicity clusters. However, this may be affected by pre-main-sequence burning (see, e.g., Proffitt & Michaud 1989; Piau & Turck-Chièze 2002), which was neglected in this paper. Explaining the range of Li abundances observed in cluster and field stars requires a
3.3. Central Convective Cores and Semiconvection

One of the consequences of the use of diffusive models is to modify the size of the central convective core (see Fig. 1), which is seen in §4 to have a significant impact on the shape of temperature-luminosity isochrones. The convective core is larger in the diffusive models of a given mass than in those that neglect diffusion: 10% larger at 1.3 $M_\odot$ and 20% at 1.2 $M_\odot$. Moreover, while the lowest mass nondiffusive model with a convective core is that for 1.14 $M_\odot$, the lowest mass diffusive model with a convective core has a mass of 1.097 $M_\odot$. This difference can be understood by studying the central properties of 1.1 $M_\odot$ models. Three different models are compared in Figure 6: (1) our standard model with diffusion, (2) that without diffusion, and (3) one with the diffusion of He but without the diffusion of metals.4

The difference between the models with and without diffusion originates from metallicity and He abundance variations. Because of the normalization to the current properties of the Sun (see Turcotte et al. 1998), the initial $Y$ ($Y_0$) is 3% larger in the solar model with diffusion than in the one without diffusion. On the other hand, in order to have the observed value of the ratio of surface metals to hydrogen ($Z_\odot/X_\odot$) at the solar age, the initial value of $Z$ ($Z_0$) must be about 13% larger in the original solar model with diffusion than in the one without diffusion, in order to compensate appropriately for the effects of atomic diffusion during solar evolution (see Turcotte et al. 1998, Tables 2 and 6). Consequently, our series of nondiffusive models have smaller $Y_0$ and $Z_0$ than our series of diffusive models (see Table 1). During the evolution, the central values of $Y$ and $Z$ are further increased by 3%–4% by diffusion processes. At an age of 3.76 Gyr, the central values of $Y$ and $Z$ are consequently larger by about 7% and 18%, respectively, in the diffusive compared to nondiffusive models of the same age.

As can be seen from Figure 7, Fe contributes as much to the Rosseland opacity as H or He, so that an 18% increase in the abundance of Fe leads to about a 6% increase in Rosseland opacity at a given $T$ and $\rho$. Furthermore, a given mass of He contributes less to the opacity than the same mass of H (because H and He contributions to the opacity come mainly from their free electrons), with the result that, as $Y$ increases, the opacity decreases. The increase of He abundance reduces from 6% to 5% the increase in opacity, at a given $T$ and $\rho$, caused by the 18% increase of Fe abundance. The effect can be seen just before the appearance of convective cores in the left panel of Figure 6 in which the opacity per gram is approximately 4% larger in the diffusive than in the nondiffusive models (at $m_r/M_\odot = 0.038$).5 After the appearance of the convective core (Fig. 6, right panels), the opacity outside the core is still larger in the diffusive than in the nondiffusive models, but structural changes wipe out the opacity differences inside the core itself.

The differences in chemical composition, and hence in opacity, appear to be the main cause of the structural differences between the models with and without diffusion. The most evident difference is the convective core that appears shortly after 3.76 Gyr in the diffusive models but not in the nondiffusive one. In the bottom panels in Figure 6 is plotted, as a function of the fractional mass, $\nabla_{\text{rad}} - \nabla_{\text{ad}}$, where (from Cox & Giuli 1968, eq. [23.171])

$$\nabla_{\text{rad}} = \frac{d \ln T}{d \ln P} = \frac{3}{16 \pi c G T^4} \frac{P}{m_r} \kappa L_r. \quad (3)$$

According to equations (2.5) and (2.8) of Stein (1966), one can expect the product $T^3/\rho$ to be approximately constant: this is seen in Figure 8 to hold reasonably well in both the diffusive and nondiffusive models. The $P/T^4$ term then varies as $\mu^{-1}$, and so decreases as $Y$ increases. (For instance, $Y$ increases over time from 0.53 to 0.61 at $m_r/M_\odot = 0.038$ in the nondiffusive model.) The increasing $Y$ also causes a decrease in the opacity, as can be seen in Figure 9. At a given $m_r$, the ratio $L_r/m_r$ increases with time until H is exhausted. Thus, there are two partially cancelling effects in $\kappa L_r/m_r$, which, however, turns out to increase with time (see Fig. 9).

At 3.76 Gyr, the expression $\kappa L_r/m_r$ is 10% larger in the diffusive than in the nondiffusive model, of which 4% comes from the larger $\kappa$ and 6% from the larger value of $L_r/m_r$ in the diffusive model. At that phase, it is apparent that $\nabla_{\text{rad}} - \nabla_{\text{ad}}$ is close to zero, especially in the case of the diffusive models. For them, $d \ln T/d \ln P$ continues to increase, and a convective core appears. However, the central region of the nondiffusive model remains radiative. The reason for this

4 Note that for this discussion only do we consider a model with the diffusion of He but not of the metals.

5 At a given $m_r/M_\odot$, the $T$ and $\rho$ are not exactly the same in the three models because of structural differences, which explains why the opacity increase is 4% in the models, while it is 5% at a given $T$ and $\rho$.  

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**Figure 5**—Isochrone of the Li/Be abundance ratio in M67 stars with $T_{\text{eff}} \geq 5500$ K from models with atomic diffusion (Li and Be panels in Fig. 2, solid curves). The left segment of the solid curve represents stars starting on the subgiant branch, while the right segment indicates main-sequence stars, and the nearly horizontal one denotes stars at turnoff. The dotted part of the curve was occupied at earlier times by stars that have now evolved to the subgiant or giant evolutionary state. The horizontal and vertical dashed lines indicate the initial values used in the calculations. The data points are from Randich et al. (2002), and their quoted error bars are plotted. For comparison purposes, the long-dashed curve gives the evaluation of Li/Be due to atomic diffusion by Sills & Deliyannis (2000) (adjusted to have the same zero-age main-sequence values as we used), while the dot-dashed curve is their fit to the observed Li/Be ratio in field stars.
difference is, then, that the small metallicity-induced opacity enhancement in the central region of the 1.1 \( M_\odot \) model with diffusion is large enough for a convective core to appear (but not in the model without diffusion) before the opacity is reduced too much by the increasing He abundance. In the preceding discussion, we implicitly used Schwarzschild's stability criterion, although the calculations were done using the Ledoux stability criterion. The use of the latter rather than the former has only a moderate effect on the size of the convective core. The main effect of the Ledoux criterion is to temporarily transform a convection zone into a semiconvection zone. Semiconvection then mixes He, however, thereby eliminating the \( \mu \) gradient, and the Schwarzschild criterion is recovered over most of the convective core (as can be seen in Fig. 6). There remains an extension of about 20% of the convective core, caused by semiconvection. However, the total size of the convective core and its semiconvective extension approximately equals the size of the convective core that would be obtained if the Schwarzschild criterion were used instead of the Ledoux criterion (see the bottom panels of Fig. 6). Note that allowing for the diffusion of the metals leads to another 15%–20% increase in the size of the core (compare the core mass in the model with the diffusion of He only to that obtained when the diffusion of metals is also treated).

### 4. Isochrones

The interpolation code described by Bergbusch & VandenBerg (1992) has been used to generate isochrones for ages from 3.5 to 10 Gyr from both the nondiffusive and diffusive grids of evolutionary tracks. Figure 10 illustrates several of the computed isochrones and shows that, at the same age, the diffusive isochrones have cooler turnoffs, fainter subgiant branches, and bluer giant branches than those that neglect gravitational settling and radiative accelerations, even when both sets of models are precisely normalized to the Sun, as indicated. (In order to satisfy the solar constraint, the diffusive models required a higher value of the mixing-length parameter, which is the main cause of the differences between the dashed and solid curves at the base of the red giant branch; see § 2, Table 1.)

A more interesting and informative comparison of the isochrones is given in Figure 11. In this case, the isochrones from the nondiffusive and diffusive grids that resemble each other most closely are plotted; i.e., they predict very similar turnoff
Fig. 7.—Evaluation of the contribution of each element to the Rosseland-averaged opacity in the 1.1 \( M_\odot \) model with diffusion at an age of 4.6 Gyr, just outside of the convective core (near \( m_c/M_\odot \approx 0.02 \); see Fig. 6). The gray line and the scale on the right give the local mass-fraction abundance of each element. Fe contributes to the opacity as much as H or He, and an increase in the Fe abundance leads to a significant increase in the Rosseland opacity. Since Fe contributes about one-third of the opacity, an 18% increase in the Fe abundance leads to a 6% increase in the opacity. For Fe, which has not lost all of its electrons, the main contribution is from bound-bound and bound-free transitions, while for H and He, the main contribution is from free-free transitions.

Fig. 8.—Ratio \( \rho/T \times \rho P/T^4 \), approximately constant in the 1.1 \( M_\odot \) models, both with and without diffusion, and close to the same value in both. See the text for a discussion of its role in the appearance of convective cores.

Fig. 9.—Variation of the ratio \( nL/m_c \) with mass and with age near the centers of the 1.1 \( M_\odot \) models, with and without diffusion. Note that this ratio is larger in the model with diffusion at a given age. See the text for a discussion of its role in the appearance of a central convective core.

Fig. 10.—Comparison of nondiffusive and diffusive isochrones (solid and dashed curves, respectively) for \( [M/H] = 0.0 \) and the indicated ages. The location of the Sun on this diagram is given by the circled dot. To satisfy the solar constraint, the nondiffusive and diffusive isochrones had to be shifted by \( \delta \log T_{\text{eff}} = -0.0022 \) and \( -0.0012 \), respectively.
and subgiant luminosities. Allowance for diffusive processes clearly leads to a 5%–7% reduction in age at a given turnoff luminosity (over the age range considered), which is considerably less than the 10%–12% reduction that is predicted by models for extreme Population II stars (see VandenBerg et al. 2002). However, the latter models were constructed for the same initial He and heavy-element abundances, whereas the present computations have assumed different initial values of $Y$ and $Z$ in order for both the nondiffusive and diffusive models for 1.0 $M_\odot$ to satisfy the solar constraint. It is, in fact, the differences in the assumed chemistry of the respective standard solar models that have compensated for nearly half of the expected effects of diffusion on predicted turnoff luminosity-age relations.

Figure 11 also shows that atomic diffusion has important ramifications for the morphology of isochrones in the vicinity of the turnoff. In particular, the “hook” feature in the youngest isochrones, which traces the rapid contraction phase that occurs at central H exhaustion in those stars that have convective cores during their main-sequence phase, is displaced to somewhat higher luminosities and cooler temperatures when diffusive processes are treated. (Note that the largest differences between the solid and dashed loci occur when they deviate to higher values of $T_{\text{eff}}$ just prior to the beginning of the subgiant stage.) This is very reminiscent of the effects of convective core overshooting. (Indeed, as already mentioned, diffusive models do have enlarged convective cores, and, as shown in § 5, they provide a much improved match to the CMD of the ≈4 Gyr, open cluster M67, as compared to those that neglect diffusion and convective overshooting.)

Moreover, convective cores clearly persist to fainter absolute magnitudes when diffusion is treated: at the same turnoff luminosity, the diffusive isochrone for 5.6 Gyr possesses a small hook feature, while none is present in the 6.0 Gyr nondiffusive isochrone. In fact, the maximum age for which an observed CMD is expected to show a gap near the main-sequence turnoff is ≈5.7 Gyr if diffusion is treated, and ≈4.8 Gyr if diffusion is neglected. Thus, open clusters with ages between approximately 4.8 and 5.7 Gyr have the potential to further test the effects of diffusion physics in the central regions of stars. (This difference in age is a consequence of the fact that the stellar mass marking the transition between tracks that have convective cores throughout the main-sequence phase and those that do not is lower for the diffusive models: 1.097 vs. 1.14 $M_\odot$; see § 3.3.)

As shown in Figures 10 and 11, the blueward hooks in the oldest isochrones that possess such features (in both the diffusive and nondiffusive grids) have small “kinks” at their faint ends. They arise because of the sudden change in the track morphology at the transition mass. Consider, for instance, the tracks plotted in Figure 12 for 1.095 and 1.097 $M_\odot$ stars, for the case in which diffusion is treated. The circles indicate where the predicted age is 5.55 Gyr on both tracks, and it is clear that an isochrone for this age (and similar ages) must undergo a redward jog between these two points.

5. APPLICATION TO M67 AND NGC 188

In their presentation of improved $UBV$ photometry for M67, Meynet, Mermilliod, & Maeder (1993) concluded that “none of the current isochrones fit our data consistently.” The morphology of the main-sequence turnoff and the luminosity of the gap at the turnoff were especially problematic for the models that they considered. Since that study was published, the evidence has become overwhelming that there is significant overshooting beyond the boundaries of convective cores, as determined from the Schwarzschild criterion (e.g., Meynet et al. 1993; Demarque, Sarajedini, & Guo 1994; Nordström, Andersen, & Andersen 1997; Schroder, Pols, & Eggleton...
Finkbeiner & Davis (1998) dust maps, moreover, the reddening that is obtained from the Schlegel, obtained available determinations prior to their paper, and the latest stance, Sarajedini et al. (1999) concluded that M67 has uncertainty of most estimates of the cluster [M/H] value. For in-

The assumption of solar metallicity is within the 1σ uncertainty of most estimates of the cluster [M/H] value. For instance, Sarajedini et al. (1999) concluded that M67 has [M/H] = −0.05 ± 0.08 from their consideration of the best available determinations prior to their paper, and the latest high-resolution spectroscopic study that we are aware of has obtained [M/H] = −0.03 ± 0.03 (Tautvaisiene et al. 2000). Moreover, the reddening that is obtained from the Schlegel, Finkbeiner, & Davis (1998) dust maps, \( E(B-V) = 0.038 \) mag (Schlegel et al. 1998), and the derived distance moduli are \( (m-M)_V = 9.70 \) and 9.67, respectively. Note the differences in the vicinity of the turnoff, which indicate a clear preference for the diffusive isochrone. Our estimate of the luminosity spanned by the gap in M67 is indicated by the vertical line bounded by short horizontal lines; it is used in Fig. 14.

There has also been widespread agreement that the amount of overshooting is less in stars that are just above the mass marking the transition between stars that possess convective cores on the main sequence and those that do not, than in stars of appreciably higher mass. In particular, the extent of core overshooting appears to be equivalent to \( \approx 0.1 \) pressure scale heights in the turnoff stars of M67, whereas something closer to \( 0.25H_P \) is typically found in studies of much younger open clusters (see the aforementioned papers, as well as Sarajedini et al. 1999). However, given the results described in §4, is it possible that diffusive isochrones can provide a good fit to the M67 CMD without requiring any convective overshooting?

To answer this question, we have transposed our isochrones to the observed plane using the semiempirical color-\( T_{\text{eff}} \) relations described by VandenBerg & Clem (2003), and we have performed a main-sequence fit of the Montgomery, Marschall, & Janes (1993) CMD for M67 to the isochrones. The assumption of solar metallicity is within the 1σ uncertainty of most estimates of the cluster [M/H] value. For instance, Sarajedini et al. (1999) concluded that M67 has [M/H] = −0.05 ± 0.08 from their consideration of the best available determinations prior to their paper, and the latest high-resolution spectroscopic study that we are aware of has obtained [M/H] = −0.03 ± 0.03 (Tautvaisiene et al. 2000). Moreover, the reddening that is obtained from the Schlegel, Finkbeiner, & Davis (1998) dust maps, \( E(B-V) = 0.038 \) is, in very good agreement with independent estimates (see the Sarajedini et al. 1999 study). Consequently, the distance modulus that is derived from a main-sequence fit to the isochrones should be quite accurate (under these assumptions).

The left panel of Figure 13 shows how well the nondiffusive isochrones are able to reproduce the M67 CMD. The derived distance modulus is \( (m-M)_V = 9.70 \), and the age of the isochrone that provides the best match to the cluster subgiants is 3.8 Gyr. M67 is known to have a high binary fraction (Montgomery et al. [1993] have estimated that at least 63% of the cluster stars are binaries), which certainly complicates the interpretation of the data. For instance, a large fraction of the group of stars just above the gap (at \( M_V \approx 3.1 \)) are likely to be binaries, given that such a large number of stars at nearly the same color on the subgiant branch is contrary to the predictions of stellar evolutionary theory. The fact that they are displaced by 0.5–0.75 mag above the main-sequence population is consistent with many of them being nearly equal-mass binaries (see the simulated CMDs reported by Carraro et al. 1994).

In most respects, the isochrone fits the observed CMD rather well. However, the predicted location of the termination of the main sequence, and hence of the gap just above it, are somewhat too faint. As illustrated in the right panel of Figure 13, this difficulty can be alleviated to some extent if the observations are fitted to diffusive isochrones. In this case, a slightly smaller distance modulus, \( (m-M)_V = 9.67 \), is obtained from the main-sequence fit, and the inferred age is also slightly less (3.7 Gyr). (If the same distance modulus were adopted as in the left panel of Fig. 13, the inferred age would be closer to 3.6 Gyr.) Although the comparison between theory and observation is still not completely satisfactory (the isochrone appears to be a bit too red at 3.6 \( \approx M_V \approx 4.1 \)), it does represent a significant improvement over that given in the left panel of Figure 13. (Even the predicted location of the base of the red giant branch is much more consistent with that observed.)

To reinforce this conclusion, we show in Figure 14 the same isochrones that appear in Figure 13, with crosses plotted along them at 0.01 \( M_V \) intervals. The density of the crosses gives a good indication of the expected variation in the numbers of stars along the two isochrones. For instance, the blueward hook should manifest itself as a gap in the distribution of turnoff stars, and relatively few stars should be found on the subgiant branch, because the rate of evolution is fast, and the variation of mass with evolutionary state is low, in this phase. The vertical line bounded by short horizontal lines just to the right of each isochrone indicates the observed location of the gap in M67 (from Fig. 13). Given that considerably fewer

![Figure 13](image-url)
stars are predicted to be found in the magnitude range encompassed by the observed gap in the right panel than in the left panel, the diffusive isochrone clearly provides the best fit to the observations. (Whether or not the model fit could be further improved by assuming a small amount of convective overshooting is difficult to say in view of the high fraction of binary stars and significant field star contamination.)

It is, of course, very comforting that the diffusive models appear to be the most realistic ones, since it is well known that such calculations are favored from solar oscillation studies (e.g., Christensen-Dalsgaard et al. 1993; Richard et al. 1996). At this time, we can only speculate that errors in the adopted color–$T_{\text{eff}}$ relations or the assumed abundances (perhaps of He) are responsible for the small color offset between the models and observations at $M_V \sim 3.8$.

As noted above, a solar abundance open cluster with an age between 4.8 and 5.7 Gyr would provide a good test of the models, since it is only the diffusive models in this age range that predict the existence of a main-sequence gap. Unfortunately, only a few old open clusters have been identified to date, and it seems unlikely that any of them have the right age to provide such a test. Perhaps the best candidate is NGC 188, but it appears to be too old by ~0.5–1 Gyr. In the left panel of Figure 15, a main-sequence fit of the Sarajedini et al. (1999) CMD for NGC 188 to the nondiffusive isochrones yields $(m - M)_V = 11.40$ and an age of 6.9 Gyr, on the assumption...
of $E(B-V) = 0.087$ (Schlegel et al. 1998). As noted by Sarajedini et al., this reddening estimate is in good agreement with independent determinations, and there is considerable spectroscopic support for a metallicity near solar. They adopted $[M/H] = -0.04 \pm 0.05$, but more recent work (Randich et al. 2003; Worthey & Jowett 2003) favors $[Fe/H] \geq 0.0$. The isochrone provides quite a satisfactory fit to the observations, except at the base of the red giant branch.

If the same reddening is assumed, a main-sequence fit of the photometry to the diffusive isochrones also yields $(m-M)_V = 11.40$, but an age of 6.4 Gyr. As shown in the right panel of Figure 15, this isochrone provides a very good match to the observed CMD, including the lower giant branch. Thus, by treating gravitational settling and radiative accelerations, the inferred age of NGC 188 has been reduced by $\approx 7\%$. There is no indication of a gap in the observed CMD, nor is any predicted, but it is curious that the majority of the stars at $3.8 \leq M_V \leq 4.2$ are redder than the isochrone (in both panels), giving one the impression that the best-fitting isochrone should have a small redward jog in this magnitude range.

6. CONCLUSIONS

Since the Sun is used to normalize convection parameters and initial abundances, one could have imagined that, in solar metallicity clusters with ages similar to that of the Sun, models with diffusion would lead to the same age and the same CMD properties as models without diffusion. The variations of $\alpha$ and initial abundances required to fit the Sun in the diffusion model reproduce the same 1.0 $M_\odot$ star at the same age, and the two sets of models could be expected to do the same for star clusters. Reality turns out to be more complex. For age determinations, partial cancellation effectively occurs, but the shapes of isochrones turn out to be quite different near the turnoff. Both the normalization to solar abundances and the additional gravitational settling in the central regions of stars work together to cause an 18\% increase in the central metallicity. This increases the size of the convective core in stars of 1.09–1.3 $M_\odot$ (see § 3.3), which in turn modifies the morphologies of isochrones (see § 4) around the solar age.

An important consequence of the changes in the shapes of isochrones that arise when diffusive processes are treated is that it is possible to match the CMD of M67 (including the luminosity of the gap near the turnoff) without having to assume an ad hoc amount of convective core overshooting: a diffusive isochrone for 3.7 Gyr does a remarkably good job of matching the cluster observations. The other significant result of this investigation, as far as isochrones are concerned, is that a gap near the turnoff is predicted to persist in open clusters up to an age of $\approx 5.7$ Gyr by the diffusive models, whereas the limiting age is closer to 4.8 Gyr if diffusion is not treated. It would be important to have detailed observations of the fiducial sequences for such clusters as those identified by Friel et al. (2002) to test this prediction. Unfortunately, NGC 188 appears to be too old to do this, given that our best estimate of its age is 6.4 Gyr based on the diffusive isochrones (which, incidentally, provide a superb match to the observed CMD).

The predicted surface abundance variations among near-turnoff stars turn out to be limited to approximately 0.1 dex in M67 and 0.07 dex in NGC 188 (see § 3.1). Most elements heavier than Si have their surface abundances modified by $g_{\text{rad}}$, but no large overabundances are expected. While not negligible, such variations are not easy to detect at the present time. The existing Li/Be measurements in a few stars of M67 (see § 3.2) suggest that another process may be required to reduce the Li abundance (see Sills & Deliyannis 2000), although the Be/Li trend obtained with models including all aspects of atomic diffusion is very different from the trend obtained by these authors. With improved observations, this will become a test of various turbulent models and will be further discussed in a paper in preparation on LiBeB abundances in cluster and field main-sequence stars.

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