On the numerical treatment and dependence of thermohaline mixing in red giants

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ABSTRACT
In recent years much interest has been shown in the process of thermohaline mixing in red giants. In low- and intermediate-mass stars this mechanism first activates at the position of the bump in the luminosity function, and has been identified as a likely candidate for driving the slow mixing inferred to occur in these stars. One particularly important consequence of this process, which is driven by a molecular weight inversion, is the destruction of lithium. We show that the degree of lithium destruction, or in some cases production, is extremely sensitive to the numerical details of the stellar models. Within the standard 1D diffusion approximation to thermohaline mixing, we find that different evolution codes, with their default numerical schemes, can produce lithium abundances that differ from one another by many orders of magnitude. This disagreement is worse for faster mixing. We perform experiments with four independent stellar evolution codes, and derive conditions for the spatial and temporal resolution required for a converged numerical solution. The results are extremely sensitive to the time-steps used. We find that predicted lithium abundances published in the literature until now should be treated with caution.

Key words: diffusion – hydrodynamics – instabilities – stars: abundances – stars: evolution – stars: interiors.

1 INTRODUCTION
Lithium remains an enigmatic element. Because it captures a proton at such low temperatures (about 2 million K) we find that stars are much more efficient at destroying Li than producing it. It is synthesized by cosmic ray spallation and was made only in trace amounts in the big bang. In 1982 it was discovered that there is a baseline minimum Li abundance in old stars in the Galactic halo. This is known as the ‘Spite plateau’ after the discoverers (Spite & Spite 1982), and corresponds to a value of Li/H ≃ 1.1 × 10^{-10} by number. With this background we are able to elucidate a number of so-called ‘lithium problems’.

(i) There remains a significant discrepancy between the predictions for the Li abundance from big bang nucleosynthesis and the Wilkinson Microwave Anisotropy Probe results [Li/H = 5.2 × 10^{-10} or A(Li) = 2.716]1 compared to observations in the oldest Population II stars (essentially the Spite Plateau) which show a consistent Li/H ≃ 1–2 × 10^{-10} or A(Li) = 2.00–2.30 (Cyburt, Fields & Olive 2008).

(ii) There is also a dip in the Spite Plateau appearing over a narrow range of effective temperatures T_{eff} ≃ 6400–6900 (corresponding to dwarf masses in the range ≃ 1.2–1.5 M_☉). This requires some form of mixing to transport the Li to regions where it is destroyed, but which only acts over this narrow range in spectral type or mass [for reviews see Balachandran (1995), Pinsonneault (1997) and Anthony-Twarog et al. (2009)].

(iii) Our Sun has a surface Li abundance about 140 times lower than predicted by the best models for the early evolution of the Sun (e.g. Meléndez et al. 2010).

(iv) In some (Galactic) globular clusters, both populations of stars (usually interpreted as different generations) seem to show the same Li content despite the fact that one population shows the results of hot hydrogen burning, which should efficiently destroy any Li present. This observation thus requires some Li production but, curiously, it must occur at exactly the rate required to match the material that has not undergone burning (D’Orazi & Marino 2010).

1 A(Li) = log ([n(Li)/n(H)]) + 12 where n denotes the number density.
Such longstanding and confounding problems present headaches for stellar physicists, and make it ironic that Li is used to treat depression in humans.

Lithium is involved in the classical pp chains of hydrogen burning, as shown in Fig. 1. The ppII and ppIII chains start with the production of \(^{7}\)Be. At typical hydrogen burning temperatures the \(^{7}\)Be can capture a proton which leads to the completion of the ppIII chain. But one can also produce \(^{7}\)Li through electron capture on \(^{7}\)Be, which occurs at all temperatures. This Li is then destroyed by a proton capture, completing the ppII chain. However, it was pointed out some time ago by Cameron & Fowler (1971) that if one can move the \(^{7}\)Be to a cooler region before it captures a proton, the still rapid electron capture could lead to a net production of \(^{7}\)Li. This is the basis of the ‘Cameron–Fowler beryllium transport mechanism’ which is understood to be active in the more massive AGB stars where we find hot-bottom burning. In these stars the convective envelope extends into the top of the hydrogen burning shell, with the result that nuclear burning happens in a very thin zone at the bottom of a dynamically active convective zone. Models of this phase by Sackmann & Boothroyd (1992) and Mazzitelli, D’Antona & Ventura (1999) seem to explain the observed super-Li-rich AGB stars seen in the Magellanic Clouds (Smith & Lambert 1989a,b).

In recent years it has been realized that during normal evolution along the red-giant branch, low-mass stars will develop an inversion in their molecular weight distribution when the hydrogen shell reaches the maximum interior extent of the convective envelope during the first dredge-up episode (hereafter FDU) (Eggleton, Dearborn & Lattanzio 2006). This mixing is driven by the inversion in mean molecular weight created when the last reaction in the ppI chain takes place. Models of this phase by Sackmann & Boothroyd (1992) and Mazzitelli, D’Antona & Ventura (1999) seem to explain the observed super-Li-rich AGB stars seen in the Magellanic Clouds (Smith & Lambert 1989a,b).

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In this paper, we investigate the sensitivity of Li production and destruction to the numerical details of the calculation of the thermohaline mixing found on the first giant branch. We show that unless great care is taken, the same implementation of the mixing phenomenon in different codes can produce results that differ by orders of magnitude. We concentrate on Li because of its extreme sensitivity to physical conditions in the model. Although this work is done within the framework of the linear theory for thermohaline mixing as developed by Ulrich (1972) and Kippenhahn, Ruschenplatt &
Thomas (1980), the conclusions will apply to any mechanism that determines the abundance of the fragile element Li. This is especially true if that process uses the composition to determine the efficiency of mixing, as we discuss below. This feedback ensures that care must be taken to obtain an accurate solution.

2 THERMOHALINE MIXING ON THE RED-GIANT BRANCH

Eggleton et al. (2006) showed that during the ascent of the first giant branch, red giants would naturally develop a molecular weight inversion when the hydrogen burning shell reached the abundance discontinuity left behind by the maximum inward extent of the convective envelope during FDU. Although this particular application of thermohaline mixing was only recently realized, the process itself has been known for a long time. The linear theory has been developed by Ulrich (1972) and extended to the non-perfect gas case by Kippenhahn et al. (1980). They have cast the theory into a form suitable for a diffusion equation, although we would do well to remember that most forms of mixing are advective, not diffusive. Nevertheless, this is a common approximation in stellar interior studies and it is the one we use here. The thermohaline mixing diffusion coefficient is given by

\[ D_{\text{thm}} = C_t K \left( \frac{\phi}{\delta} \right) \left( \frac{\nabla_T}{\nabla - \nabla_{ad}} \right) \] (1)

where \( K \) is the thermal diffusivity given by

\[ K = \frac{4aC_3 T^3}{3k^3 \rho^3 c_P}, \] (2)

\[ \phi = \left( \frac{\partial \ln \rho}{\partial \ln \mu} \right)_{P,T}, \] (3)

\[ \delta = - \left( \frac{\partial \ln \rho}{\partial \ln T} \right)_{P,\mu}, \] (4)

and all other symbols have their usual meaning. Note that \( \phi = \delta = 1 \) for a perfect gas, and that \( D_{\text{thm}} = 0 \) unless \( \nabla_{ad} < 0 \).

The Ulrich (1972) and Kippenhahn et al. (1980) formulations are equivalent, and depend on one unknown parameter \( C_t \), a non-dimensional coefficient theoretically related to the aspect ratio \( a \) (length/width) of the mixing fingers. Again, we caution that this is a highly idealized formulation, but within this model we have (Charbonnel & Zahn 2007)

\[ C_t = \frac{8}{3} \pi^2 a^2. \] (5)

Comparison with observations has led to the preferred value of \( C_t \approx 1000 \) to match the \( ^{12}\text{C}/^{13}\text{C} \) ratio seen both in field stars and in globular clusters (Charbonnel & Zahn 2007; Eggleton et al. 2008; Charbonnel & Lagarde 2010; Angelou et al. 2011, 2012), and also abundances in CEMP stars (Stanciliffe et al. 2009; Stanciliffe 2010). It is remarkable that a single value produces so much agreement with observations. Yet from a theoretical viewpoint the situation is far from satisfactory.

Various researchers have tried to improve our understanding of the mixing process by producing numerical simulations of one kind or another. Calculations have been performed with the Boussinesq approximation in 2D (Denissenkov 2010) as well as 3D (Denissenkov & Merryfield 2011; Traxler, Garaud & Stellmach 2011); see also Brown, Garaud & Stellmach (2013). These authors agree that the resulting aspect ratio is too small to support the value \( C_t \approx 1000 \) required to match the observations. Nevertheless, that the observations fit this theory so nicely is a compelling fact, also pointed out by Denissenkov (2010). We note that the mechanism naturally starts at the correct place on the giant branch, and there is no freedom in choosing this as it is determined by the extent of first dredge-up and the temperature dependence of the pp chain reactions. So what are we to make of the seeming contradiction between the hydrodynamical simulations and the 1D models? There are three things to consider:

(i) how reliable are the calculations that use the linear theory?
(ii) how reliable are the determinations of \( C_t \) from observations?
(iii) how reliable are the hydrodynamical models?

The first question is the topic of this paper, but let us briefly address the other two questions.

It is true that a value of \( C_t \approx 100 \) seems to be required to match many observational constraints, as listed earlier. However recent work by Angelou et al. (2014) has shown that a value of \( C_t \approx 100 \) is required to match observations of Li in various globular clusters. This is an order of magnitude smaller, and is getting closer to the values preferred by the existing hydrodynamical simulations. So which is correct: is it 100 or 1000? Surely we cannot choose a different value for each species. At this stage we cannot say anything more definite. The thermohaline mechanism is under investigation from many different approaches and much is uncertain. For example, the linear theory assumes that a diffusion equation describes the mixing. But if it is more advective then this may not be appropriate, and the temperature history of a parcel of stellar material may be important. This may reveal itself as different values of \( C_t \) for species with different sensitivities to the temperature. Much work remains to be done; the details are simply unknown at present.

As for the hydrodynamical simulations themselves, these are very difficult calculations. Most are not performed under stellar conditions (Traxler et al. 2011; Brown et al. 2013), and use extrapolations or asymptotic behaviour to try to extend the applicability. This is in contrast to the work of Denissenkov (2010) and Denissenkov & Merryfield (2011) who did simulate stellar conditions. Brown et al. (2013) found that their simulations did not support the linear theory, but agreed with those of Denissenkov (2010) although they believe the latter are under-resolved. We also note that Denissenkov (2010) estimated that a value of \( C_t \approx 800 000 \) would be required to find Li production. We show below that this can be achieved for \( C_t = 10 000 \), indicating again the need for extreme care in performing these calculations.

Finally, we refer to a recent paper by Medrano, Garaud & Stellmach (2014) who investigated the hydrodynamics of thermohaline mixing in the presence of a horizontal inhomogeneity. They found that the efficiency of the mechanism was increased by orders of magnitude over the previous hydrodynamical estimates, and noted that this may bring the hydrodynamical calculations closer to the successes of the linear theory.

Clearly the situation is far from settled. In the rest of this paper we will use the linear theory of Kippenhahn et al. (1980), assuming that \( C_t \) takes values consistent with the observations, and we will look at the resulting predictions from different codes for the same theory. Debate about the correct theory belongs elsewhere – for now we are concerned only with the accurate numerical solution of the existing 1D theory in different stellar evolution codes. We repeat that although \( C_t \) is formally related to the aspect ratio of the expected fingering convection (see equation 5), this association relies on the highly simplified idealized case. We prefer to treat \( C_t \)
as an arbitrary scaling parameter in the theory, much like $\alpha_{\text{MLT}}$ in the mixing-length theory.

It is prudent to note that any competing theory to thermohaline mixing that is intended to produce the required abundance changes in red giant stars must operate over the same physical region in the star and hence its implementation would require the same sort of numerical care that we discuss below. Such stringency is required by the fragility of lithium, rather than any specific mixing mechanism. This is exacerbated if the proposed mixing mechanism is dependent on the composition profile, as is the case in thermohaline mixing. It is the feedback from the composition on the mixing that makes the solution so sensitive to the numerical considerations we discuss below. This is likely to be true for other mechanisms also.

3 THE CODES USED AND THE CASE TESTED

We will compare calculations made with four different evolution codes, and two different versions of the same code, before and after a rewriting of the difference scheme and solution method. All calculations are made initially with each code’s standard criteria for space and time resolution, so that no special demands are enforced. The results thus reflect what one might expect for a naive calculation from each code. Salient features of the codes are described below. We note that the nuclear reactions involved are quite standard pp chains, and that there have been no significant changes in their rates for years, so we do not expect any differences to arise thereby. Convective borders are determined using the normal Schwarzschild criterion, with no overshoot. Any variations from this are discussed in the subsections below, dealing with each code.

3.1 MONSTAR

The first code we will use is MONSTAR, the stellar structure code developed at Monash University. This code began life as the Mt Stromlo code (Wood & Zarro 1981) but has been modified extensively since. We use the OPAL opacity from Iglesias & Rogers (1996) without allowing for changes in the envelope composition, which are small in the cases considered here. We use a mixing-length parameter $\alpha_{\text{MLT}} = 1.75$ from fitting the Sun to the standard mixing-length theory. The solutions for the structure and the chemical composition (as a result of burning and mixing) are separate in this code. However, it is perhaps best to think of them as interleaved, because the latest structure iteration is used for determining the burning rates and mixing regions that are applied at the current iteration. At each iteration during the convergence process we update the composition by calculating the burning and mixing. In this way both structure and composition should converge to a self-consistent solution at the same time.

We will see below that the time-step is crucial to the calculations we are investigating. We note that MONSTAR has multiple criteria that must be met. Broadly speaking these limit the time-step so that changes in dependent physical and composition variables (at each mass shell), and the total luminosity (from various sources), are below specified limits.

3.2 STARS

The STARS code was originally written by Eggleton (1971, 1972), and has been subsequently updated by many authors (e.g. Pols et al. 1995). The version used here is that described in Stancliffe & Eldridge (2009), which is publicly available from the STARS website [see http://www.ast.cam.ac.uk/~stars/]. It also uses the OPAL opacities from Iglesias & Rogers (1996), with a mixing length of 2.00 based on calibration to the Sun. The solution of the compositions of species involved in energetically significant nuclear reactions is solved simultaneously with the structure equations (Stancliffe 2006). The implementation of thermohaline mixing in the code is described in Stancliffe et al. (2009) and Stancliffe (2010). We note that the calculation of the mean molecular weight $\mu$ is, in this code, made with the composition from the previous time-step. This is significant for the problem addressed in this paper, as we will see below. Alongside the main evolution routines, the code has a set of nucleosynthesis subroutines that follow the evolution of 40 nuclear species (Stancliffe et al. 2005). It is these routines that are used to calculate the lithium abundance. The time-step is controlled by restricting the sum of the changes in all variables at all mesh points to be equal to a specified value; there is also a restriction on the maximum change allowed in any dependent variable at any time-step.

3.3 MESA

We also make use of the recently developed MESA suite of stellar evolution codes – http://mesa.sourceforge.net and described in Paxton et al. (2011, 2013); specifically we use MESA version 6208. The formulation for thermohaline mixing in the MESA code is slightly different with (Paxton et al. 2013):

$$D_{\text{th}} = \alpha_{\text{th}} \frac{3k}{2\rho c_P} \frac{B}{\nabla - \nabla_{\text{ad}}}$$

where $k$ is the thermal conductivity given by

$$k = \frac{4\pi T^2}{3k}\rho,$$

and $B$ is given by equation (6) in Paxton et al. (2013). Referring to Cantiello & Langer (2010) we see that

$$B = \left(\frac{\phi}{\delta}\right) \nabla_{\mu}$$

and hence

$$C_1 = \frac{3}{2} \alpha_{\text{th}}.$$  

We use the Ledoux criterion for convection, and $\alpha_{\text{MLT}} = 1.6$ in the Böhm-Vitense (1958) implementation of the mixing-length theory. MESA selects its time-step via a two-stage process (Paxton et al. 2011). A time-step is calculated using a scheme based on digital control theory, which is then subjected to a wide range of tests that reduce this time-step if certain properties are changing faster than specified. Such tests include limits similar to those discussed above for MONSTAR and STARS, including restrictions on changes in the solution mesh, composition, nuclear burning rates, etc.

3.4 STAREVOL-GENEVA-V2.3

Our final code is actually two variants of the STAREVOL code used extensively by Forestini, Siess, Charbonnel and collaborators. The first of these is the 2000 version of STAREVOL (Siess, Dufour & Forestini 2000) as used by Charbonnel & Zahn (2007) and Charbonnel & Lagarde (2010). We shall call this the STAREVOL-GENEVA-V2.3 code, or se-g-v2.3 for short. This code also uses the same opacity as the others above, $\alpha_{\text{MLT}} = 1.6$ and separate solution for the structure and the composition. The results we quote for this code are taken from Charbonnel & Lagarde (2010).
3.5 STAREVOL-V5.5

This code was largely rewritten during the development of the binary stellar evolution code BINSTAR (Siess et al. 2013). In this version the nuclear burning and diffusive transport of the chemicals are coupled and solved simultaneously, although it is of course possible to disable that option and solve separately for the nucleosynthesis and then the mixing. We will use this feature later in some of our tests. A major upgrade in the new version of this code is the differing of the equations, and the ability to simultaneously solve for the structure variables as well as the composition (including both nuclear burning and mixing), as is done in STARS. However, this fully coupled solution mode is slower and, as far as thermohaline mixing on the RGB is concerned, tests showed that it does not alter significantly the evolution of the surface abundances. Therefore we do not use this method in any of the tests described below. Rather, we solve for the structure and then the coupled mixing and burning (except in clearly identified tests where we uncouple the mixing and burning). We shall refer to this code as SE-V5.5.

In both STAREVOL versions, the same criteria are used to determine the evolution time-step $\delta t$. We employ the common sort of time-step constraints associated with changes in the structure variables. We check that at every grid point the physical variables do not change by more than a specified value between consecutive models. We further limit the time-step during the pre-main-sequence and RGB phases not to exceed a fraction of the Kelvin–Helmholtz time-scale $\tau_{KH}$. The expression we use is

$$ t_{KH} = \frac{g M^2}{R L} . \tag{10} $$

A more appropriate estimate would be to consider the envelope relaxation time-scale

$$ t_{KHenv} = \frac{g M_{env} M}{R_{env} L} . \tag{11} $$

but this does not make a significant difference. For low- and intermediate-mass stars climbing the RGB, the constraint on $\delta t$ is set ultimately by the requirement that the time-step does not exceed some specified fraction of the Kelvin–Helmholtz time-scale ($\tau_{KH}$). In SE-V5.5, this limit is set to $\delta t < 0.3 \tau_{KH}$.

3.6 The test case

Our test case will be a model of 1.25 M$_\odot$ with ‘solar’ composition, as defined in Asplund, Grevesse & Sauval (2005), meaning $X = 0.7383$, $Y = 0.2495$ and $Z = 0.0122$. In particular we take the initial mass fraction of $^3$He to be $8 \times 10^{-3}$ and the initial $^7$Li is given by $A(Li) = 3.25$ on the zero-age main sequence. This is the case presented in some detail in Charbonnel & Lagarde (2010) and thus it allows us to compare the results for that work, using SE-G-v2.3, with the other codes above, giving us a total of five essentially independent implementations of the thermohaline mixing algorithm to compare.

To introduce the important physics we show in Fig. 2 the internal structure of our test model not long after thermohaline mixing has started, when $L = 110 L_\odot$, just above the luminosity function (LF) bump in the HR diagram. Because we will be concerned with mixing time-scales we have used radius on the $x$-axis instead of mass. For our purposes in this paper it is far more intuitive to see the distances rather than masses. Note that in the deepest layers where the temperature is higher the shortest time-scale is that for Li destruction. Moving further out to cooler regions we see that there is a small region where Li production dominates, and further out again the mixing time-scales becomes the shortest. Hence the effect of thermohaline mixing is to feed material to the hot region where $^7$Li is rapidly destroyed. The destruction can be very quick, with time-scales as low as days, at the time shown in the figure. Hence the important determinant for the global evolution of the Li abundance is the time-scale of feeding Li-rich material from the envelope into the hot region where it is almost instantly destroyed. Conversely, if Li (or any other species) is significantly produced then the important time-scale is again that of the mixing which now drives the increase in the envelope abundance. Hence it is vital to resolve this mixing adequately.

4 THE START OF THERMOHALINE MIXING

We start by showing in Fig. 3 the results from all of our codes for the case $C_t = 1000$. It is pleasing to see that the plots all have a similar shape, showing the decrease in Li caused by FDU at log(L) $\simeq$ 0.7, reaching a similar value $A(Li) \simeq 1.5$ until the start of thermohaline mixing, which occurs at log(L) $\simeq$ 1.7–2.0 depending on the code.

![Figure 2. Internal structure in our test case soon after thermohaline mixing has begun, when $L = 110 L_\odot$, as calculated with SE-V5.5. The plots cover the region from the location of the minimum in $\mu$ near the left-hand edge where $D_{\text{thm}}$ goes to zero, and the bottom of the convective envelope, shown by cross-hatching near the right hand edge. The top panel shows the variation of $D_{\text{thm}}$, the middle panel shows abundances of key species (in mass fraction), and important time-scales are shown in the lower panel. Specifically, these are the Li production time-scale, i.e. the time-scale of the $^7$Be + e$^-$ reaction; the Li destruction time-scale, being the time-scale for $^7$Li + p; and the time-scale for mixing to transport material from the given position to the bottom of the convective envelope, defined by the sum of the local values ($\delta r)^2/D_{\text{thm}}$ across the region, where $\delta r$ is the width of the local mass shell.](http://mnras.oxfordjournals.org/Downloaded from | MNRAS 446, 2673–2688 (2015))
luminosity as Lagarde (2010) we define the local minimum and maximum in the bump in the LF seen in globular clusters. Following Charbonnel structure, and the radiated luminosity temporarily decreases before increase in hydrogen fuel causes a hydrostatic readjustment of the hydrogen burning shell approaches the step in composition caused

\[ L \]

that the deeper the maximum extent of FDU the lower is \( A(Li) \). This then results in a further decrease of Li, except in some codes where there is a small increase found near the end of the evolution, at the tip of the giant branch. Clearly the final \( A(Li) \) value after FDU is a topic of considerable importance; rather than discuss the details here we refer the reader to a recent paper on the subject by Angelou et al. (2014).

The next important difference is when the thermohaline mixing process starts to affect the surface composition. Obviously, this depends on the maximum depth of the convective envelope during FDU, but there is also another effect at play. For the surface Li abundance to show any change, we need the material at the bottom of the convective envelope to be transported to where it is hot enough for Li to be destroyed. The thermohaline mixing begins in the region where \( \mu \) has decreased. But this does not initially extend all the way to the bottom of the convective envelope. The region of the \( \mu \) inversion must develop, through mixing and burning, so that there is a negative \( \nabla \mu \) from the minimum in \( \mu \) to the bottom of the convective envelope. It is only then that the surface Li value will be seen to drop. The luminosity at which this happens is reported in Table 2 as \( L_{\text{lim}} \) (or \( L_c \) in the notation of Charbonnel & Lagarde 2010).

So just how long does it take for the thermohaline region to make contact with the convective envelope? Fig. 4 shows the results for two cases: SE-G-V2.3 (Charbonnel & Lagarde 2010) and MONSTAR. The time delay between the start of thermohaline mixing and the appearance of its effects at the surface is given in Table 2 as \( \Delta t_{\text{lim}} \). In SE-G-V2.3 the connection between the two mixing zones takes about 45 million years, whereas in MONSTAR it occurs in about 3 million years. The development of this region is crucially dependent on the propagation of the \( \mu \) inversion and requires an accurate determination of the mixing because it is the mixing which feeds the burning and produces the inversion. Fresh material rich in \(^4\)He must be brought down to the burning region, where it is transmuted into material with a lower \( \mu \) prior to being transported away from the burning region. If the time-step is too large then we do not follow this development accurately with the result that the thermohaline mixing takes longer to connect to the convective envelope and hence for the surface abundances to show the effect of the burning.

Table 1. First dredge-up parameters for our calculations. For each of the codes used (listed in the first column) we give the minimum and maximum luminosities at the bump, \( L_{b,\text{min}} \) and \( L_{b,\text{max}} \), respectively, as well as the deepest penetration of the convective envelope \( M_{\text{FDU}} \) during first dredge-up, and the luminosity \( L_{\text{FDU}} \) at that time. All values are in solar units.

| Code   | \( L_{b,\text{min}}/L_{\odot} \) | \( L_{b,\text{max}}/L_{\odot} \) | \( M_{\text{FDU}}/M_{\odot} \) | \( L_{\text{FDU}}/L_{\odot} \) |
|--------|---------------------------------|---------------------------------|-------------------------------|-------------------------------|
| MONSTAR| 47                              | 57                              | 0.272                         | 25                            |
| STARS  | 49                              | 52                              | 0.262                         | 27                            |
| MESA   | 40                              | 47                              | 0.257                         | 20                            |
| SE-G-V2.3| 37                             | 45                              | 0.256                         | –                             |
| SE-V5.5| 42                              | 50                              | 0.262                         | 20                            |

Note that the mixing is driven by a \( \mu \) inversion that is as small as one part in \( 10^6 \) or so initially. Indeed, as soon as any decrease in \( \mu \) is resolved, then the algorithm will start mixing. How this propagates will depend on how the \( \mu \) inversion is resolved and one can understand why small time-steps are needed. One can also imagine that in a real star, with magnetic fields, rotation, gravity waves, etc., such small variations may not be established as easily as in this idealization we are modelling (Maeder et al. 2013). We remind the reader that we are concerned here with an accurate calculation within the paradigm of the theory, rather than a test of the validity of the theory itself.

In any event we tried some tests with SE-V5.5. We took large time-steps, \( \delta t \), limited to be less than the total stellar Kelvin–Helmholtz time-scale, \( \tau_{\text{KH}} \), and small time-steps limited to \( 0.3\tau_{\text{KH}} \). The differences are seen in Fig. 5, with \( \Delta t_{\text{lim}} \approx 9.57 \) million years for the larger time-steps but reduced to only 2.19 million years when the smaller time-steps were used; we discuss the reasons for this below.

The next test was also performed with SE-V5.5. The Kelvin–Helmholtz time-scale for the model is 68 000 yr at this stage of the evolution. Hence we used fixed \( \delta t \) of 68 000 yr for the structure but took 10 nucleosynthesis sub-steps where we kept the structure constant but mixed and burnt the composition. We did not update \( D_{\text{lim}} \) or \( \nabla \mu \), just the composition. This produced a slower growth of the different codes at FDU is a topic of considerable importance; rather than discuss the details here we refer the reader to a recent paper on the RGB.

The time delay between the start of thermohaline mixing and the appearance of its effects at the surface is given in Table 2 as \( \Delta t_{\text{lim}} \). In SE-G-V2.3 the connection between the two mixing zones takes about 45 million years, whereas in MONSTAR it occurs in about 3 million years. The development of this region is crucially dependent on the propagation of the \( \mu \) inversion and requires an accurate determination of the mixing because it is the mixing which feeds the burning and produces the inversion. Fresh material rich in \(^4\)He must be brought down to the burning region, where it is transmuted into material with a lower \( \mu \) prior to being transported away from the burning region. If the time-step is too large then we do not follow this development accurately with the result that the thermohaline mixing takes longer to connect to the convective envelope and hence for the surface abundances to show the effect of the burning.

Note that the mixing is driven by a \( \mu \) inversion that is as small as one part in \( 10^6 \) or so initially. Indeed, as soon as any decrease in \( \mu \) is resolved, then the algorithm will start mixing. How this propagates will depend on how the \( \mu \) inversion is resolved and one can understand why small time-steps are needed. One can also imagine that in a real star, with magnetic fields, rotation, gravity waves, etc., such small variations may not be established as easily as in this idealization we are modelling (Maeder et al. 2013). We remind the reader that we are concerned here with an accurate calculation within the paradigm of the theory, rather than a test of the validity of the theory itself.

In any event we tried some tests with SE-V5.5. We took large time-steps, \( \delta t \), limited to be less than the total stellar Kelvin–Helmholtz time-scale, \( \tau_{\text{KH}} \), and small time-steps limited to \( 0.3\tau_{\text{KH}} \). The differences are seen in Fig. 5, with \( \Delta t_{\text{lim}} \approx 9.57 \) million years for the larger time-steps but reduced to only 2.19 million years when the smaller time-steps were used; we discuss the reasons for this below.

The next test was also performed with SE-V5.5. The Kelvin–Helmholtz time-scale for the model is 68 000 yr at this stage of the evolution. Hence we used fixed \( \delta t \) of 68 000 yr for the structure but took 10 nucleosynthesis sub-steps where we kept the structure constant but mixed and burnt the composition. We did not update \( D_{\text{lim}} \) or \( \nabla \mu \), just the composition. This produced a slower growth of the different codes at FDU is a topic of considerable importance; rather than discuss the details here we refer the reader to a recent paper on the RGB.
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Table 2. The start of thermohaline mixing. For each of the codes used (listed in the first column) we provide the value of \( C_t \) used, the luminosity \( L_{\text{thm}} \) (in solar units) when the surface composition shows the effects of thermohaline mixing (i.e. when the thermohaline region makes contact with the convective envelope), and the time \( \Delta t_{\text{thm}} \) elapsed between the beginning of thermohaline mixing and the appearance of its effects at the surface (in units of 10\(^6\) yr). The third column lists the particular case being examined: ‘norm’ refers to the typical values (for that code) for space and time resolutions; changes to the standard time-step criteria are given as factors of \( \delta t \) or restrictions in terms of the Kelvin–Helmholtz time-scale \( \tau_{\text{KH}} \); mesh-spacing criteria are detailed in the text or given as the total number of \( N \) of zones. The case \( M = 0 \) had mass-loss turned off, but updating \( \nu \) and \( D_{\text{thm}} \) after each iteration in the nucleosynthesis routine. In a run of 1.5 million years the thermohaline region had only reached about 1/3 of the way to the convective envelope. We conclude that there is no alternative but to take small time-steps during this part of the evolution as it determines when the surface abundance will begin to change. It is crucial that the value of \( D_{\text{thm}} \) be updated after even small changes in the composition – this drives the mixing and hence feeds back on itself. We are reasonably confident that the correct value for \( \Delta t_{\text{thm}} \) is within the 1D diffusive model of Kippenhahn et al. (1980) and Ulrich (1972) for this particular stellar model\] is about 1 million years. This is significantly different to the Charbonnel & Lagarde (2010) value of 45 million years, which presumably did not resolve this initial phase adequately. It is this delay that is responsible for the offset in the SE-G-V2.3 results for Li destruction, as shown in Fig. 3. This is also why the value of \( L_{\text{thm}} \) is much larger (at 94 \( L_\odot \)) than the other codes tested (at about 50–60\( L_\odot \)); see Table 2 for a list of the tests performed.

Finally, we should be able to estimate the time-scale for the growth of the thermohaline region from the structure. We have an estimate of the time-scale of a diffusion process to move matter over a distance \( \delta r \) as \( \tau \simeq (\delta r)^2 / D_{\text{thm}} \). Note that this is the time for material in the thermohaline region to move a distance \( \delta r \). One may initially think that this is not the rate at which the borders of the zone grow. For example, the convective turnover time in a convective envelope is in no way related to the time it takes for first dredge-up to reach its deepest extent. The material inside the convective envelope moves with one speed, quite independent of the rate at which the edge of the convective zone moves. In this case the inner edge of the convective envelope is determined by the stellar structure responding to the expansion of the star as it ascends the giant branch, and is quite independent of the concomitant changes in abundance. The speed with which the inner edge of the convective envelope moves inwards is typically \( v_{\text{DU}} \simeq 10^{-3} \text{ cm s}^{-1} \), quite different to the speed of matter in the convective envelope, which the mixing length theory gives as \( v_{\text{conv}} \simeq 10^2 \text{ cm s}^{-1} \). In the case of diffusion, however, the two speeds are the same. The edge of the mixed region moves precisely because it is diffusing into the homogeneous region. Thus the growth of the thermohaline mixing region can be estimated from \( D_{\text{thm}} \) in the region. When thermohaline mixing first appears, long before the region has made contact with the convective envelope, we have \( D_{\text{thm}} \simeq 10^{-10} \text{ cm}^2 \text{ s}^{-1} \). Later when the regions have nearly joined \( D_{\text{thm}} \) has grown to \( 10^{10} \text{ cm}^2 \text{ s}^{-1} \). Given that the mixing must cross a region of about 0.5\( R_\odot \) we estimate that at the start the initial time-scale for reaching the envelope is \( \tau \simeq (\delta r)^2 / D_{\text{thm}} \simeq 3–30 \text{ Myr} \). But the diffusion coefficient increases rapidly and by the time the regions have joined the time-scale is down to \( \tau \simeq 0.03 \text{ Myr} \). This can only give us a crude consistency check, but it supports the result of our calculations giving about 1 million years for the actual time.

We also performed some tests where we varied the spatial mesh, and these are reported in Table 2. We found that the mesh spacing was not nearly as critical as the time-step, a result which will reappear below.
Figure 4. The start of thermohaline mixing in SE-G-V2.3 (left panel) and MONSTAR (right panel), with $C_t = 1000$. Shaded regions show the locations in mass of convective mixing (dark shading) and thermohaline mixing (light shading) as a function of time since the zero-age main sequence. Also marked are the boundaries of the hydrogen-burning shell (green dashed line for SE-G-V2.3; blue shaded region for MONSTAR). Also shown are the luminosities when thermohaline mixing begins and when the mixed region connects to the envelope (these are effectively the same in MONSTAR).

Figure 5. The start of thermohaline mixing in SE-V5.5 with time-steps limited to $0.3\tau_{KH}$ (left panel) and $\tau_{KH}$ (right panel). Time is set to zero when thermohaline mixing first appears. The hydrogen burning shell is present between the two dashed lines and the location of its maximum energy output is shown by the dotted line. The blue shaded region shows the extent of thermohaline mixing, and the grey shaded region the convective envelope.

5 THE EVOLUTION OF THE SURFACE ABUNDANCE OF $^7$LI

We show the results for $C_t = 100$ in Fig. 6. Note that we do not have results for SE-G-V2.3 for this case. There is some scatter in the results, and by the time the models reach the tip of the giant branch there is 1 dex spread in the predicted final values for the Li content. This is clearly not acceptable, but as we will see, the situation gets worse as $C_t$ increases.

We have already shown in Fig. 3 the cases with $C_t = 1000$, including SE-G-V2.3 this time, from Charbonnel & Lagarde (2010). The early evolution is the same in all codes, but once the thermohaline mixing starts we get a very diverse spread of results. There is a spread of up to 2 dex in the Li abundance from different codes, and we even see an increase in the surface A(Li) near the tip of the giant branch in some cases, but not all. When we move to $C_t = 10000$ (Fig. 7) then all codes except SE-G-V2.3 show the increase of Li near the tip of the RGB, and a maximum spread in A(Li) between codes of over 3 dex. To try to determine the cause of this variation we have performed a number of tests with the different codes.

5.1 Testing temporal resolution

We begin by testing the effect of the time-step, since we have seen how crucial this is in the early stages of the evolution. We chose the...
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Figure 6. Surface $A(Li)$ plotted as a function of the luminosity $L$ for our test case model with $C_t = 100$. The figure shows the evolution from the main sequence to the tip of the giant branch. The lines show various codes run with default resolution and time-stepping. The black dotted line is STARS, the red solid line MONSTAR, the blue long-dashed line SE-V5.5 and the purple short-dashed line MESA.

Figure 7. Surface $A(Li)$ plotted as a function of the luminosity $L$ for our test case model with $C_t = 1000$. The figure shows the evolution from the main sequence to the tip of the giant branch. The lines show various codes run with default resolution and time-stepping. The black dotted line is STARS, the green dot–dashed line SE-G-V2.3, the red solid line MONSTAR, the blue long-dashed line SE-V5.5 and the purple short-dashed line MESA.

Figure 8. The effects of varying the time-step on surface $A(Li)$ as a function of luminosity $L$ for our test case model with $C_t = 1000$. The figure shows the evolution from the main sequence to the tip of the giant branch. The green lines are STARS run with default time-step (dashes) and time-step reduced by a factor of 10 (dots). The red lines are MONSTAR with default time-step (dashes) and time-step increased by a factor of 10 (solid). Blue lines are SE-V5.5 with the default time-step (dashes), the time-step increased by a factor of 3 (solid line) and reduced by a factor of 10 (dotted line).

First consider the runs done with SE-V5.5. The ‘normal’ case and the case with time-steps reduced by a factor of 3 seem to give essentially the same results. Contrarily, if the time-step is increased by a factor of 3 then the results start to differ, with less Li being destroyed due to the code not being able to follow accurately the flow of material into the top of the hydrogen burning shell where Li is efficiently destroyed.

Now consider the MONSTAR runs. Here the standard case seems to agree well with the converged cases found with the SE-V5.5 code. However if the time-step is increased by a factor of 10 then the code is able to match the Li destruction initially, but it starts to depart from the (presumably) correct solution and indeed begins to produce Li as the model nears the tip of the RGB. Note that Li production is seen in the normal case also, for this code, but the production is not as significant with the smaller time-step. Upon closer examination there is also a hint of an increase in Li in the well-resolved calculations by the SE-V5.5 code. We address the cause of this rise in Li in Section 7.

Two tests were run with the STARS code also, as shown in Fig. 8. This code does not destroy as much Li as MONSTAR and SE-V5.5, and it has not yet converged on our inferred solution. We note that it does show the same trends as the other codes, in that increasing the time-step stops the calculation from adequately following the flow of material from the convective envelope into the hot burning region resulting in a lower Li depletion, as will be explained in Section 5.3.

As stated earlier, STARS normally uses the composition at the previous time-step to calculate $\mu$. This is not ideal for the present case where there is strongly coupled feedback between the mixing and the composition. To test this we ran cases where $\mu$ was calculated using the current composition. These are reported in Table 2 with

case with $C_t = 1000$, which is the preferred value for explaining various observations, as discussed above. Tests were run with three codes, using the ‘normal’ time-step constraints, which we refer to as ‘$\delta t$’, and then with increased or decreased time-steps given as multiples of this standard $\delta t$. The results are shown in Fig. 8.
We performed tests on the spatial resolution using STARS and SE-V5.5.

### 5.2 Testing spatial resolution

δ reduced to ensure convergence, and the results are very similar to

\[ M_{\text{NRAS}} = 446, \text{respect}, \text{although again the STARS code seems to be less efficient in} \]

resolution shows that less Li is burned. Both codes agree in this

region, being 60, 100 and 170, respectively. Again, increasing the

are defined in terms of the number of zones in the thermohaline

Similar results were found for the SE-V5.5 code in the three cases

the time resolution, and the reason for this will be discussed below.

Figure 9. The effects of varying the spatial resolution on surface A(Li) as a

function of luminosity L for our test case model with \( C_1 = 1000 \). The figure

shows the evolution from the main sequence to the tip of the giant branch.
The green lines are STARS runs with low resolution (499 mesh points, solid

line) and medium resolution (1999 mesh points, dotted line). Blue lines are

SE-V5.5 with the default resolution (100 zones in the thermohaline region,
dashed line), low resolution (60 zones in the thermohaline region, solid

and high resolution (170 zones in the thermohaline region, dotted line).

the notation ‘μ’ and either the normal time-step criteria, δt, or 1/10

of those criteria, δt = 0.1. In practice, the time-steps had to be greatly

reduced to ensure convergence, and the results are very similar to

the standard case with δt = 0.1.

### 5.3 Understanding the resolution tests

Consider solving the diffusion equation for a quantity \( u \)

\[
\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}
\]  

over a region with \( N \) zones of constant width \( \delta x \) and with constant
time-step \( \delta t \) and constant diffusion coefficient \( D \). We can write this

as a fully implicit scheme as

\[
\frac{u^{n+1}_j - u^n_j}{\delta t} = D \left( \frac{u^{n+1}_{j+1} - 2u^{n+1}_j + u^{n+1}_{j-1}}{(\delta x)^2} \right)
\]  

(13)

where superscripts refer to the time-step and subscripts refer to the

spatial zone. We assume the boundary conditions \( u_0 = \text{constant} \)

and \( u_N = \text{constant} \). Hence can write this as the matrix equation

\[
u^n = M u^{n+1}
\]  

(14)

where

\[
u^n = (u^n_0, u^n_1, \ldots, u^n_N)^T
\]  

(15)

and

\[
M = \begin{pmatrix}
1 & 0 & 0 & 0 & \cdots & 0 \\
-\alpha & 1 + 2\alpha & -\alpha & 0 & \cdots & 0 \\
0 & -\alpha & 1 + 2\alpha & -\alpha & \cdots & 0 \\
0 & 0 & -\alpha & 1 + 2\alpha & -\alpha & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 1
\end{pmatrix}
\]  

(16)

Here the parameter \( \alpha \) is simply

\[
\alpha = D \delta t / (\delta x)^2.
\]  

(17)

This is a tri-diagonal system which can be solved easily by the

Thomas Algorithm, for example. It is always stable because the
diagonal elements are always larger than the sum of the magnitudes of
the sub- and super-diagonal elements, i.e.

\[
|1 + 2\alpha| > |\alpha| + |\alpha|
\]  

(18)

for all \( \alpha > 0 \), which is the case here.

The salient feature here is that, for this case with constant space and
time-steps, the solution is determined entirely by \( \alpha \), which
enables us to relate the chosen spatial and temporal mesh to the

solution. For example, halving the time-step \( \delta t \) reduces \( \alpha \) by a

factor of 2. This is the same as using the original time-step but
with \( D \) reduced by a factor of 2. Hence we expect the solution with

eriner time-steps to be similar to solving the original equation with a

smaller \( D \). Similarly, if we halve the spatial mesh \( \delta x \) then \( \alpha \) increases
by a factor of 4, so that is equivalent to using the initial \( \delta x \) but

an increase in \( D \) by a factor of 4.

Thus increasing the resolution in space and in time has opposite
effects on the solution, which is consistent with the tests performed in

the previous section. Of course, these changes are only indicative; for

instance, when halving the time-step we should actually compare the

solution after two time-steps with the original solution with the

single time-step. Similarly when we double the number of mass

shells we should compare every second mesh-point in the new

solution with the original solution. Nevertheless, the discussion here

gives some explanation for why the solution behaves differently for

changes in \( \delta x \) and \( \delta t \).

### 6 Determining appropriate resolutions for an accurate solution

#### 6.1 Time-steps

Understanding the dependence of the solutions on the time and

mesh spacing is important but it does not guide us in finding an
appropriate discretization for our calculations. We now address this question, through an examination of Fig. 2. The lowest panel in the figure shows the important time-scales. For the majority of the evolution the Li is destroyed through mixing to the hot region at the bottom of the thermohaline zone. Hence it is crucial to determine the rate at which this mixing occurs. In the region where destruction dominates, this nuclear burning is very fast. The efficiency of the destruction thus depends on how rapidly it can be fed by the mixing. Likewise, in the case where production dominates, which we discuss below, the rate of increase is determined by the rate at which the created Li can be injected into the envelope.

Thus, the region where the Li production and destruction time-scales are equal is going to be crucial in determining the evolution of the surface Li content. Let us call this the equilibrium point. We must adequately resolve the region between this point and the convective envelope if we are to follow the Li transport accurately. If the time-step is too long, or the spatial mesh too large, we connect the two regions at a different rate to what they would achieve in reality. We will define the time-scale for mixing from this point to the bottom of the convective envelope as \( \tau_0 \), and we suggest this is used as a typical time-step for the calculation.

To calculate this \( \tau_0 \) we note that \( D \simeq v_l l_i \) where \( v \) is the local mixing velocity and \( l \) is the mean free path, or mixing length, of the moving parcel of gas. Hence at mass shell \( i \) we have

\[
v_i = \frac{D_i}{l_i}.
\]

Let \( \delta r_i \) be the radial width of each mass shell. Then the mixing time-scale from shell \( i \) to the convective envelope is

\[
\tau_0 = \sum_i \frac{\delta r_i}{v_i} = \sum_i \frac{\delta r_i l_i}{D_i}
\]

where the sum extends from the current mesh point to the bottom of the convective envelope. If we write \( l_i = a_i \delta r_i \) for some real numbers \( a_i \) then we get

\[
\tau_0 = \sum_i \frac{a_i (\delta r_i)^2}{D_i} \propto \sum_i (\delta r_i)^2.
\]

Hence we will define our preferred time-step \( \delta t_0 \) by

\[
\delta t_0 = \tau_0 = \sum_i \frac{(\delta r_i)^2}{D_i}
\]

with the knowledge that we have ignored some constants, but maintained the essence of the physics.

We return to our standard case with \( C_t = 1000 \) and run tests with \texttt{SE-V5.5} using a time-step that is limited by \( f \times \delta t_0 \) with \( f = 0.1, 1.0, 3.0 \) and 10.0. Clearly \( f \) is related to the \( a_i \) above, and we consider that it must be determined empirically. The results of these tests are shown in Fig. 10. We see that we appear to have converged on a solution for all except the case with \( f = 10 \). This confirms our claim that the important time is of order \( \tau_0 \) and as long as the step stays near this value, the solution should be reliable. Note that for these tests we disabled the other time-step criteria; this means that for the \( f = 10 \) case for example, we continued to use \( \delta t = 10 \tau_0 \) even though we would normally be using a smaller \( \delta t \) as determined by another condition (e.g. \( \delta t < 0.3 \tau_{\text{K LX}} \), as is normally used in \texttt{SE-V5.5}). Hence if a normal time-step condition produces a \( \delta t \) that is below the critical value, then naturally the solution is reached. But to be sure of this, we suggest adding a condition that \( \delta t \) not exceed say \( 3 \tau_0 \). This should ensure an acceptable solution.

We note that the \texttt{SE-V5.5} code solves simultaneously for the burning and mixing, whereas not all codes do this; e.g. \texttt{MONSTAR} and \texttt{SE-G-V2.3} do not. Hence we perform tests also with \texttt{MONSTAR} to check if this affects the preferred choice of \( \delta t \). We anticipate slightly the next section, and perform these tests with our preferred mesh spacing \( \delta h_0 \); although as we will show below, this is not crucial. Fig. 11 shows results for \( C_t = 1000 \) (left) and 10 000 (right) for various \( f \) as multiples of \( \delta t_0 \). Although the early changes in Li content are not dependent on the time-step, a converged solution at later times requires a step no larger than about \( \delta t_0 / 8 \). This is about an order of magnitude smaller than required by \texttt{SE-V5.5} and reflects the advantage of a simultaneous solution for the burning and mixing.

To confirm this we repeated the calculations with \texttt{SE-V5.5} with the mixing and burning algorithms decoupled, as is done in many codes, including \texttt{MONSTAR} and \texttt{SE-G-V2.3}. The results are shown in Fig. 12, for tests with time-steps of \( f \times \delta t_0 \). Clearly to converge on the solution in this case requires a value of \( f \lesssim 0.1 \), in agreement with the results from \texttt{MONSTAR}. We conclude that our critical time-step is verified, but whether one should use a limit of a few \( \delta t_0 \) or a few \( \delta t_0 / 10 \) depends on the solution scheme for the chemical composition that is used in the code in question.

Note also that it is imperative to apply this condition from the start of the thermohaline mixing; i.e. from the time when a \( \mu \) minimum first emerges. If the time-step is too large initially then we follow a solution that is not appropriate. Using a smaller time-step later just ensures that we accurately follow an incorrect solution branch. There is no short cut -- a small \( \delta t \) must be used from the start of the thermohaline mixing period.

\[\text{Figure 10. Tests for the time-step criteria on the evolution of lithium abundance during the giant branch. } A(\text{Li}) \text{ is plotted as a function of luminosity } L. \text{ The mixing parameter } C_t = 1000. \text{ Different lines show different multiples } f \text{ of the preferred time-step } \delta t_0 \text{ as defined in equation (22). The solid red line shows } f = 0.1, \text{ the dashed blue line (under the solid red line) } f = 1, \text{ the green dotted line } f = 3 \text{ and the purple dot–dashed line } f = 10.\]

\[\text{Figure 11 shows results for } C_t = 1000 \text{ (left) and } 10 000 \text{ (right) for various } f \text{ as multiples of } \delta t_0 \text{. Although the early changes in Li content are not dependent on the time-step, a converged solution at later times requires a step no larger than about } \delta t_0 / 8 \text{. This is about an order of magnitude smaller than required by } \texttt{SE-V5.5} \text{ and reflects the advantage of a simultaneous solution for the burning and mixing.}\]

\[\text{To confirm this we repeated the calculations with } \texttt{SE-V5.5} \text{ with the mixing and burning algorithms decoupled, as is done in many codes, including } \texttt{MONSTAR} \text{ and } \texttt{SE-G-V2.3}. \text{ The results are shown in Fig. 12, for tests with time-steps of } f \times \delta t_0 \text{. Clearly to converge on the solution in this case requires a value of } f \lesssim 0.1, \text{ in agreement with the results from } \texttt{MONSTAR}. \text{ We conclude that our critical time-step is verified, but whether one should use a limit of a few } \delta t_0 \text{ or a few } \delta t_0 / 10 \text{ depends on the solution scheme for the chemical composition that is used in the code in question.}\]

\[\text{Note also that it is imperative to apply this condition from the start of the thermohaline mixing; i.e. from the time when a } \mu \text{ minimum first emerges. If the time-step is too large initially then we follow a solution that is not appropriate. Using a smaller time-step later just ensures that we accurately follow an incorrect solution branch. There is no short cut -- a small } \delta t \text{ must be used from the start of the thermohaline mixing period.}\]
Figure 11. Tests of the effect of the time-step at fine mesh spacing, performed with the MONSTAR code. The lithium abundance $A(Li)$ is plotted as a function of luminosity $L$. The left panel shows $C_t = 1000$, the right panel $C_t = 10000$. Each calculation used a maximum mesh spacing of $\delta m_0$. The lines show calculations with time-steps of $\delta t_0/8$ (solid thin line), $\delta t_0/4$ (dashed thin line), $\delta t_0/2$ (dotted thin line), $\delta t_0$ (dash–dotted thick line), and $2\delta t_0$ (long-dashed thick line).

Figure 12. Results from SE-V5.5 with the calculations of mixing and burning of composition decoupled. The blue dot–dashed line is for $f = 0.1$, the green dashed line is for $f = 1$ and the red dotted line is for $f = 3$. The black curve shows the solution obtained with a simultaneous solution for mixing and burning and a time-step of $\delta t_0$ (i.e. $f = 1$). All calculations use $C_t = 1000$.

6.2 Mesh spacing

We also performed tests on the mesh spacing used in the calculations. Because the thermohaline mixing is being driven by variations in $\mu$, which are in turn driven by the burning of $^3$He, we concentrate on fully resolving variations in the $^3$He content. Based on experience with such problems, we defined a preferred maximum mass spacing $\delta m_0$ so that the maximum change in the mass fraction of $^3$He between mesh points is no more than 1 per cent of the maximum value of the $^3$He abundance throughout the star. We performed the tests with MONSTAR and the standard model, with $C_t = 1000$ and the very sensitive case of $C_t = 10000$. The results are shown in Fig. 13, where we have used our preferred time-step of $\delta t_0/8$. These plots clearly show that if the time-step is short enough, then the mesh spacing is not critical, although it is more important in the $C_t = 10000$ case, as may be expected. But even here, we have to use $100\delta m_0$ to produce a significant degradation of the results.

6.3 Combining space and time resolution

The choices of space and time resolution are in fact related. For a sufficiently poor resolution in one variable it is unlikely that the correct solution will be recovered for any choice of the other variable. Here we test the interdependence of the spatial and temporal resolution criteria. Again, tests were performed with the MONSTAR code and for the two cases $C_t = 1000$ and $C_t = 10000$. For each we have varied the time-step significantly for two choices of the mesh spacing: $\delta m_0$ and $100\delta m_0$. Let us first examine the case for $C_t = 1000$ in the left panel of Fig. 11. Clearly the solution converges as the time-step is lowered, and with a maximum $\delta t = \delta t_0/8$ we believe we have essentially found the solution. With larger time-steps we obtain values that are quite different to the true solution, although the variations are not large until we begin producing Li towards the tip of the RGB (see Section 7 for a discussion of this phenomenon). For the case with $C_t = 10000$ in the right panel of Fig. 11 the runs with larger $\delta t$ are clearly wrong, with large discontinuities produced in the surface Li abundance. As the time-step is decreased, however, we again appear to converge on a solution.

We now wish to determine how sensitive is this result to the mesh spacing. Hence we repeat the two tests above, but using a maximum mesh spacing of $100\delta m_0$, as shown in Fig. 14. First we look at the left panel, for $C_t = 1000$. Again, as we decrease the time-steps the solution converges. What is interesting, however, is the red line, which is the converged solution using a mesh spacing that is 100 times smaller. This solution with $\delta m_0 = 100\delta m_0$, i.e. the thin red line and the thin black line are essentially the same. This tells us that it is the time-step that is by far the most important parameter in finding the solution to this problem. Provided the time-step is small enough, the mesh spacing is not critical, to within relatively large
Figure 13. Tests of the effect of the mesh spacing performed with the MONSTAR code. The lithium abundance $A(\text{Li})$ is plotted as a function of luminosity $L$. The left panel shows $C_t = 1000$, the right panel $C_t = 10000$. Each calculation used a maximum time-step of $\delta t_0/8$. The lines show calculations with mesh spacing of $\delta m_0/2$ (solid black line), $\delta m_0$ (dashed red line), $2 \delta m_0$ (dotted blue line) and $100 \delta m_0$ (dash–dotted brown line).

Figure 14. Tests of the effect of the time-step at coarse mesh spacing, performed with the MONSTAR code. The lithium abundance $A(\text{Li})$ is plotted as a function of luminosity $L$. The left panel shows $C_t = 1000$, the right panel $C_t = 10000$. Each calculation used a maximum mesh spacing of $100 \delta m_0$. The lines show calculations with time-steps of $\delta t_0/8$ (solid thin line), $\delta t_0/4$ (dashed thin line), $\delta t_0/2$ (dotted thin line), $\delta t_0$ (dash–dotted thick line), and $2 \delta t_0$ (long-dashed thick line).

factors. The same thing is seen in the right panel, for $C_t = 10000$. Here, with the larger time-steps there are discontinuities and large changes in the solution. Decreasing the time-steps removes the erratic behaviour and produces a smooth solution. Here again the red curve is the solution using 100 times smaller mesh spacing. In this more sensitive case there is still a difference between the solutions for the smallest time-step, so we conclude that in the extreme cases the mesh spacing is indeed important, although the crucial thing to be concerned with is the time-step chosen. The mesh spacing is important but not as critical, except in the most strongly mixed cases.

Finally, to check that our preferred mesh and time-spacing works, we show in Fig. 15 the results for $C_t = 1000$ and $C_t = 10000$ using both MONSTAR and SE-V5.5. Both codes use $\delta m = \delta m_0$, while SE-V5.5 uses $\delta t = \delta t_0$ and MONSTAR uses $\delta t = \delta t_0/8$, as determined earlier. We see that they do in fact agree sufficiently, and thus verify that the critical solution mesh proposed in this paper is suitable for calculations of the behaviour of Li during the RGB phase, in different evolution codes.

We have not tested our proposed solution mesh in the STARS code. This code uses an elegant implicit method to solve for its preferred solution mesh. This does not lend itself to the sort of tests and controls we derived here, so we do not try to apply them to this code. Nor have we implemented our preferred mesh in MESA. We have instead shown that our suggested solution mesh works well in two totally independent codes. We advise anyone who is interested in calculating thermohaline mixing of Li to perform tests of the code being used, guided by our preferred $\delta t_0$ and $\delta m_0$. 

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Figure 15. Calculations with our preferred time and mesh spacing. The lithium abundance A(Li) is plotted as a function of luminosity $L$. The left panel shows $C_t = 1000$, the right panel $C_t = 10000$. Solid black lines are results from MONSTAR; dashed green lines result from SE-V5.5.

7 THE PRODUCTION OF LITHIUM

We have seen that the models show a tendency to produce Li as they get near to the tip of the giant branch. This tendency is stronger as $C_t$ increases, being essentially absent when $C_t = 100$ but almost universal when $C_t = 10000$ (the only exception being for the SE-G-V2.3 code). Our aim in this section is to understand why this happens. That deep-mixing can produce Li is not a new result, having been discussed extensively by Sackmann & Boothroyd (1996). The question is how and why do our models change from efficient destruction of Li early on the RGB to efficient production later on the RGB. We defer to a companion paper (Church et al, in preparation) the question about whether real stars behave this way; our emphasis here is on the accurate solution of the numerical problem rather than a test of its applicability.

Here we look at the case with $C_t = 10000$ since this is where the Li production appears most easily. We show the results from SE-V5.5 in Fig. 16 and identify three phases of the evolution. In Phase 1 we see a decrease in the envelope Li content, which reaches a minimum at Phase 2, and then during Phase 3 the Li increases again.

The left, middle and right panels in Fig. 17 correspond to the three models denoted by asterisks in Fig. 16. The upper panels show three time-scales:

(i) $\tau_{\text{prod}}$ (blue line) which is the time-scale for the production of $^7\text{Li}$, which is also the time-scale for the destruction of $^7\text{Be}$ (since the rate of proton capture on $^7\text{Be}$ is negligible);
(ii) $\tau_{\text{dest}}$ (red line) which is the time-scale for the destruction of $^7\text{Li}$;
(iii) $\tau_{\text{mix}}$ (black line) which is the time-scale for the matter to diffuse from the given position to the bottom of the convective envelope;

and the lower panels show the abundance profiles of $^7\text{Li}$, $^7\text{Be}$ and $^3\text{He}$.

In the bottom left panel, we show the situation typical of phase 1. The Li content in the convective envelope (shown hashed) is higher than in the interior and Li will diffuse inward. Just below the envelope we see a region where the production of Li is much faster than the destruction time-scale. However this production is negligible compared to the amount of Li transported from the envelope reservoir. The production and mixing contribute mostly to filling in the little dip in Li seen at $r \approx 0.15 R_\odot$. A little further interior we see that Li destruction is the dominant process, and indeed it is the transport of Li from the surface into this region that leads to a reduction in its surface abundance. Note that there is a region of enhanced $^7\text{Be}$ which is produced by $\alpha$ captures on $^3\text{He}$. The destruction of $^7\text{Be}$ is only efficient at the very bottom of the thermonuclear region ($r \lesssim 0.06 R_\odot$) where we see a decrease in the $^3\text{He}$ $^7\text{Be}$ abundance profiles. As the other panels show, overall the $^7\text{Be}$ content increases during the rise up the RGB.

In the middle panel the Li profile has flattened, and hence the diffusion inward must cease. We have reached a local extremum (minimum) in the surface Li abundance. From the upper middle

Figure 16. The three phases of different Li behaviour highlighted in different colours. The asterisks indicate the specific models plotted in Figs 17 and 18.
Thermohaline mixing in red giants

Figure 17. Structure in the three models specified in Fig. 16. Model 1 (left) is during the phase of evolution where thermohaline mixing reduces the surface lithium abundance. Model 2 (middle) is where the surface lithium abundance is roughly constant. Model 3 (right) is from near the tip of the giant branch where the surface lithium abundance is increasing. The top panels show the important time-scales and the density. The dashed blue lines show the time-scale for the production of $^7$Li; the dotted red lines show the time-scale for its destruction. The solid black line shows the time-scale to mix from a given point to the base of the convective envelope. The magenta line shows the run of density in units of $g \text{ cm}^{-3}$. The bottom panels show composition for selected species. The solid black line is for $^7$Li, the red dotted line is for $^7$Be and the green dashed line is for $^3$He.

In summary, the main change in the structure as the star ascends the RGB is that the diffusion becomes much quicker, allowing the $^7$Be to escape from where it is produced. This is the classical Cameron–Fowler mechanism in operation.

It remains for us to understand why the mixing time-scale decreases as the model ascends the RGB. The mixing time-scale is just the time taken to diffuse from a given radius to the bottom of the envelope. This is the sum of the terms $(\delta r)^2/D_{\text{thm}}$ for each shell across the region, emphasizing again the reason why we have plotted our graphs against radius instead of mass. The spatial extent of this region stays essentially the same, as shown in Fig. 17. (Importantly, the mass in this region decreases from $9.38 \times 10^{-3} \, M_{\odot}$ through $3.45 \times 10^{-3} \, M_{\odot}$ to $1.93 \times 10^{-3} \, M_{\odot}$ for the three models shown in Fig. 17.) Hence we expect that $D_{\text{thm}}$ increases as the star ascends the RGB, and this is indeed what we find, as shown in Fig. 18.

The expression for $D_{\text{thm}}$ is given in equation (1). We have investigated each term in this expression for $D_{\text{thm}}$ to determine which is responsible for the increase. The dominant term is easily the thermal diffusivity $K$, and within $K$ the largest change is due to the decrease in density as the star expands along the RGB, as shown in the top panels of Fig. 17. This can be understood as altering the fundamental physical structure of the region. As the thermal diffusivity increases then the heat can be transported very easily, making the material with a lower $\mu$ even more buoyant, and increasing the diffusive motions.
In fact, any changes that result in an expansion in this region would act to favour Li production. Since the strength of the hydrogen burning shell scales directly with the initial CNO abundance, we would expect that Li production would be more favoured in higher metallicity stars.

8 SUMMARY AND CONCLUSIONS

Lithium continues to cause problems for many branches of astrophysics. At the very least we need to understand how it behaves in stars. We have seen in this paper that even within the constraints of a well-defined mathematical model for diffusive mixing we find dramatically different behaviours due to the high sensitivity of Li to physical conditions in the star. We find that although the dominant effect of thermonuclear mixing is to decrease the stellar surface content of Li on the RGB, the Cameron– Fowler mechanism can operate near the tip of the RGB for sufficiently high values of the parameter $C_i$ that appears in the 1D diffusion theory for thermonuclear mixing. Further, unless sufficient care is taken in the integration of the diffusion equation and the structure equations, one can easily find envelope lithium abundances that differ from a resolved solution by orders of magnitude. We present criteria to be used for determining the time-steps and spatial resolution needed for an accurate solution of the Li content during thermonuclear mixing. These criteria can be summarized as:

(i) the time-step $\delta t$ should satisfy

$$\delta t \lesssim f \times \sum_i (\delta r_i)^2/D_i$$

(23)

where the sum is taken from the point where the Li production and destruction time-scales are equal, to the bottom of the convective envelope; $f \approx 2$ is suitable for an implicit and simultaneous solution of burning and mixing, but if these processes are calculated separately then $f \lesssim 0.2$ is required;

(ii) the spatial mesh spacing $\delta m$ should be no larger than will permit a change in the $^3$He abundance of a few per cent of the maximum $^3$He value in the model.

Of these, the time-step criterion is the most important, in that if the behaviour is resolved in time then the spatial mesh is not crucial, except for higher values of $C_i$. We show that by using these criteria we find the results produced by the two totally independent codes are in agreement. It would be prudent for any interested in this problem to perform similar tests with the code they will be using, guided by our recommended mesh spacings.

Finally, we note that any mechanism that will determine the composition of fragile elements like Li is likely to be very sensitive to numerical details of the kind discussed here. Hence an analysis similar to that performed here would be wise when investigating any other proposed mechanism, especially one that has feedback between the composition profile and the details of the mixing.

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REFERENCES

Abia C., Isern J., 1996, ApJ, 460, 443
Angelou G. C., Church R. P., Stancliffe R. J., Lattanzio J. C., Smith G. H., 2011, ApJ, 728, 79
Angelou G., Stancliffe R. J., Church R. P., Lattanzio J. C., Smith G. H., 2012, ApJ, 749, 128
Angelou G., D’Orazi V., Constantino T. N., Church R. P., Stancliffe R. J., Lattanzio J. C., 2014, ApJ, submitted
Anthony-Twarog B. J., Deliyannis C. P., Twarog B. A., Crozall K. V., Cummings J. D., 2009, AJ, 138, 1171
Asplund M., Grevesse N., Sauval A. J., 2005, in Barnes T. G., III Bash F. N., eds, ASP Conf. Ser. Vol. 336, Cosmic Abundances as Records of Stellar Evolution and Nucleosynthesis. Astron. Soc. Pac., San Francisco, p. 25
Balachandran S., 1995, ApJ, 446, 203
Böhm-Vitense E., 1958, Z. Astrophys., 46, 108
Brown J. M., Garaud P., Stellmach S., 2013, ApJ, 768, 34
Cameron A. G. W., Fowler W. A., 1971, ApJ, 164, 111
Cantiello M., Langer N., 2010, A&A, 521, 9
Charbonnel C., 1995, ApJ, 453, L41
Charbonnel C., Lagarde N., 2010, A&A, 522, 10
Charbonnel C., Zahn J.-P., 2007, A&A, 467, 15
Cuby R. H., Fields B. D., Olive K. A., 2008, J. Cosmol. Astropart. Phys., 11, 12
D’Orazi V., Marino A. F., 2010, ApJ, 716, L166
Denissenkov P. A., 2010, ApJ, 723, 563
Denissenkov P. A., Merryfield W. J., 2011, ApJ, 727, L8
Eggleton P. P., 1971, MNRAS, 151, 351
Eggleton P. P., 1972, MNRAS, 156, 361
Eggleton P. P., Dearborn D. S., Lattanzio J. C., 2006, Science, 314, 1580
Eggleton P. P., Dearborn D. S., Lattanzio J. C., 2008, ApJ, 677, 581
Iglesias C., Rogers F., 1996, ApJ, 464, 943
Kippenhahn R., Ruzenplatt G., Thomas H. C., 1980, A&A, 91, 175
Lagarde N., Romano D., Charbonnel C., Tosi M., Chiappini C., Matteucci F., 2012, A&A, 542, A62
Maeder. A., Meynet G., Lagarde N., Charbonnel C., 2013, A&A, 553, 1
Mazzitelli I., D’Antona F. D., Ventura P., 1999, A&A, 348, 846
Medrano G., Garaud P., Stellmach S., 2014, ApJ, 792, L30
Meléndez J. et al., 2010, ApJS, 328, 193
Palmerini S., Cristallo S., Busso M., Abia C., Uettenhaler S., Gianfulla L., Majorca E., 2011, ApJ, 741, 26
Paxton W., Bildsten L., Dotter A., Herwig F., Lesaffre P., Timmes F. X., 2011, ApJS, 192, 3
Paxton W. et al., 2013, ApJS, 208, 4
Pinsonneault M., 1997, ARAA, 35, 557
Pols O. R., Tout C. A., Eggleton P. P., Han Z., 1995, MNRAS, 274, 964
Sackmann I.-J., Boothroyd A. I., 1992, ApJ, 392, L71
Sackmann I.-J., Boothroyd A. I., 1996, ApJ, 510, 217
Siess L., Dufour E., Forestini M., 2000, A&A, 358, 593
Siess L., Izzard R. G., Davis P. J., Deschamps R., 2013, A&A, 550, 100
Smith V. V., Lambert D. L., 1989a, ApJ, 345, L75
Smith V. V., Lambert D. L., 1989b, ApJ, 361, L69
Spite F., Spite M., 1982, A&A, 115, 357
Stancliffe R. J., 2006, MNRAS, 370, 1817
Stancliffe R. J., 2010, MNRAS, 403, 505
Stancliffe R. J., Eldridge J. J., 2009, MNRAS, 396, 1699
Stancliffe R. J., Lugaro M. A., Ugalde C., Tout C. A., Görres J., Wiescher M., 2005, MNRAS, 360, 375
Stancliffe R. J., Church R. P., Angelou G. C., Lattanzio J. C., 2009, MNRAS, 396, 2313
Traxler A., Garaud P., Stellmach S., 2011, ApJ, 728, L29
Ulrich R. K., 1972, ApJ, 172, 165
Wood P. R., Zarro D., 1981, ApJ, 247, 247

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