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ON THE NUMERICAL TREATMENT AND DEPENDENCE OF THE THIRD DREDGE-UP PHENOMENON

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ABSTRACT

We present results of an investigation into the behavior of the base of the convective envelope of models of asymptotic giant branch stars during third dredge-up. We find that the extent, and even the presence, of third dredge-up depends critically on the treatment of convection within a stellar structure calculation.

Subject headings: convection — stars: AGB and post-AGB — stars: evolution — stars: interiors

1. INTRODUCTION

Determining the position of convective boundaries in stellar models is a long-standing problem. Formally, a boundary is defined (from the Schwarzschild criterion) to be located where the adiabatic and radiative temperature gradients, ∇_{ad} and ∇_{rad}, are equal. However, this merely tells us where the acceleration of the convective elements goes to zero. The region between this and where the velocity reaches zero is called the "overshoot" region. Much effort has been made to modify the commonly used mixing-length theory (MLT) of convection to extend beyond the formal boundary in order to calculate the extent of the overshoot region (e.g., Shaviv & Salpeter 1973; Maeder 1975 ; Bressan et al. 1981; Langer 1986). These techniques were shown by Renzini (1987) to produce nonphysical situations, and he concluded that only a new theory of convection could resolve the problem.

Although several new convective theories and modifications to the MLT have been proposed (Canuto & Mazzitelli 1991; Forestini et al. 1991; Gehmeyr & Winkler 1992; Lydon et al. 1992; Grossman et al. 1993; Singh et al. 1994, 1995), we use the standard MLT for our work. We shall look at phenomenological techniques to try to better approximate the true boundary. This is of paramount importance in models of thermally pulsing asymptotic giant branch (TP-AGB) stars during the third dredge-up phase. AGB stars consist of a degenerate carbon-oxygen core, surrounded by a helium-rich region, above which lies a hydrogen-rich convective envelope. Following thermal pulses of the helium-burning shell, the convective envelope moves inward in mass, penetrating the hydrogen-exhausted regions. This is known as third dredge-up. As convection moves inward, a chemical discontinuity develops at the boundary. The radiative temperature gradient is defined as

$$\nabla_{rad} = \frac{3}{16\pi acG}\frac{\kappa lp}{mT^4},$$

where κ, p, l, m, and T are opacity, pressure, luminosity, mass, and temperature, respectively. The chemical discontinuity associated with third dredge-up results in a discontinuity in κ, which likewise causes a discontinuity in ∇_{rad}. This last discontinuity then inhibits further growth in the convective envelope since large readjustments of temperature and other state variables must occur in order to raise ∇_{rad}/∇_{ad} in the radiative zone above unity. However, any mixing beyond the abundance discontinuity encourages further penetration since each mass element obtains ∇_{rad}/∇_{ad} well above unity when mixed, and thus the discontinuity is propagated.

That third dredge-up does occur is well supported by observations of carbon stars on the AGB. Codes that do not include some method of mixing beyond the Schwarzschild boundary (although this may depend on the mixing algorithm; see below) may not see third dredge-up and, hence, may not produce carbon star models. In addition, unless ∇_{rad}/∇_{ad} approaches unity at the convective boundary, we have the unstable situation of a finite acceleration at the base of the envelope. Clearly, the inclusion of some form of extra mixing is a physical necessity.

One method, employed by Boothroyd & Sackmann (1988), extends the convective zone until a point is reached where, even if mixed into the convective zone, it would remain radiative. A different method is used by Lattanzio (1986), who calculates the ratio of the temperature gradients, ∇_{rad}/∇_{ad}, and linearly extrapolates the ratio from the last two convective mesh points to the first radiative point. If the extrapolated value is greater than unity, then that point is included in the convective zone. If less than unity, the point remains radiative. This scheme allows, at most, one radiative point to be added to the convective zone per iteration, and it is the method used in this work.[1] It tries to ensure that the last convective point is close to neutral buoyancy (i.e., $\nabla_{rad}/\nabla_{ad} = 1$). This is distinct from that which is usually called "overshoot" in the literature, meaning the extension of the mixed region by finite velocity at the boundary (even though the acceleration is zero).

2. BEHAVIOR OF ∇_{rad}/∇_{ad} DURING THIRD DREDGE-UP

To study the evolution of AGB stars, we use a version of the Mount Stromlo Stellar Structure Program (Wood & Zarro 1981) with updated radiative opacities (Rogers & Iglesias 1992). Conductive opacities are calculated from a program supplied by McDonald (1992) that uses opacities from various sources (Hubbard & Lampe 1969; Iben 1975;

[1] Since this procedure is used at each iteration, it permits the growth of the convective zone to be determined by the demand for neutrality in a way that is almost (but not quite) independent of space and time discretization. An analysis of the dependence on mesh spacing and time stepping is not reported here.

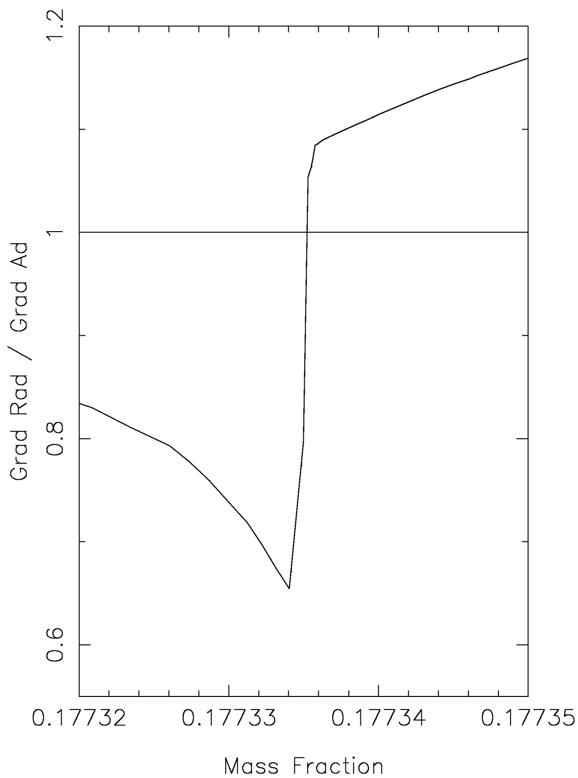

FIG. 1*a*

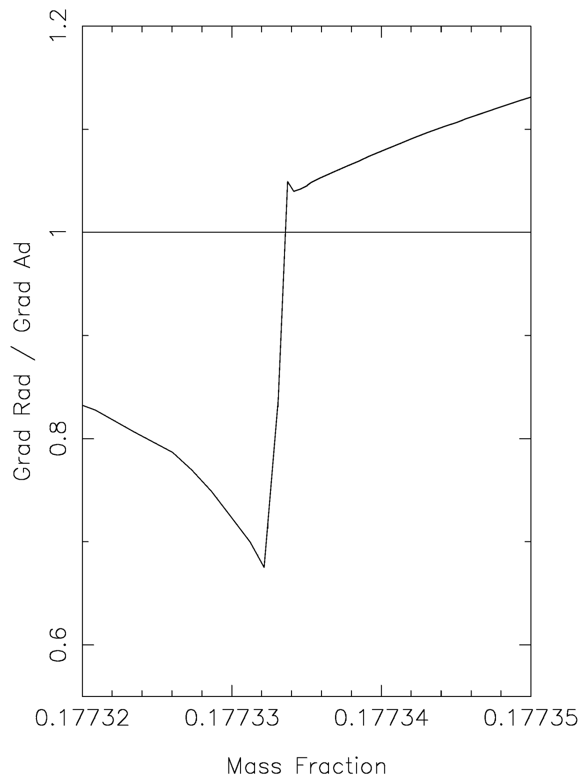

FIG. 1*b*

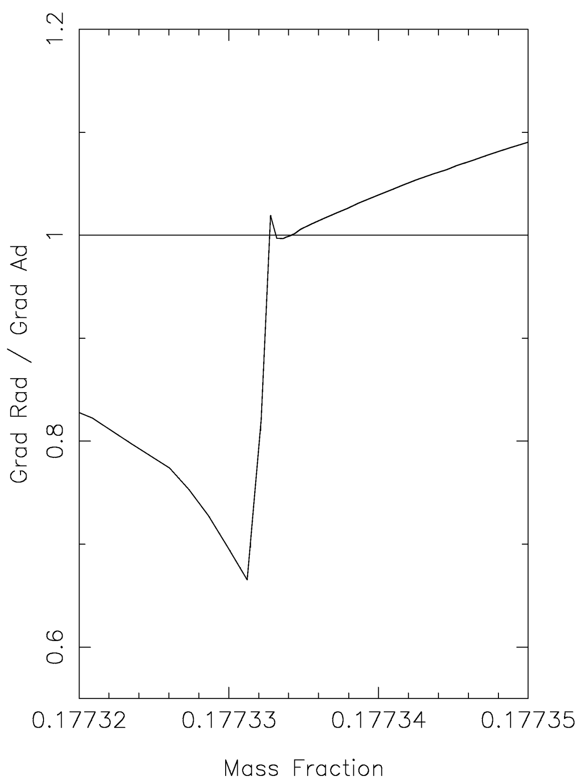

FIG. 1*c*

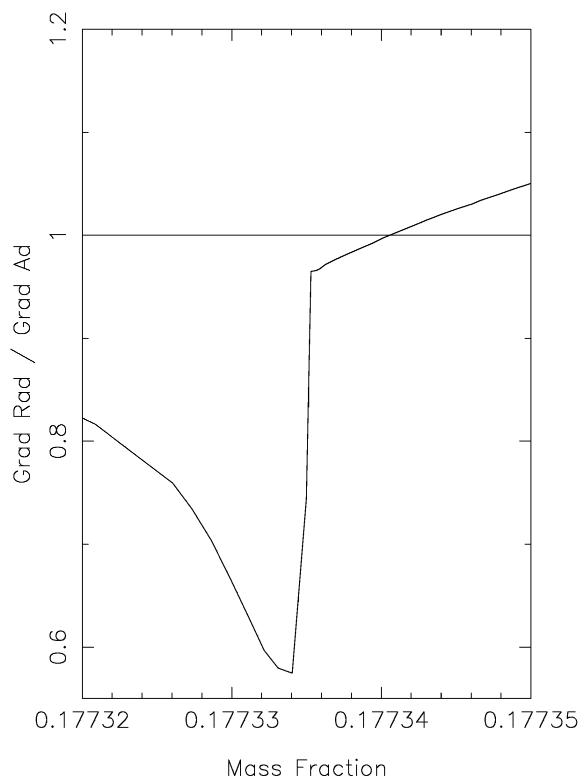

FIG. 1*d*

FIG. 1.—∇_{rad}/∇_{ad} vs. mass for a 5 $M_\odot$ model with $Z = 0.004$ during third dredge-up, showing the discontinuity at the base of the convective envelope. The line at $\nabla_{rad}/\nabla_{ad} = 1$ marks convective neutrality according to the Schwarzschild criterion. (*a*) Third iteration; (*b*) fifth iteration, in which a drop in ∇_{rad}/∇_{ad} just above the base of the envelope is clearly visible; (*c*) sixth iteration, the dip in ∇_{rad}/∇_{ad} has dropped below unity, producing a small radiative zone; (*d*) seventh iteration, in which the convective envelope has retreated; (*e*) eighth iteration; (*f*) ninth iteration.

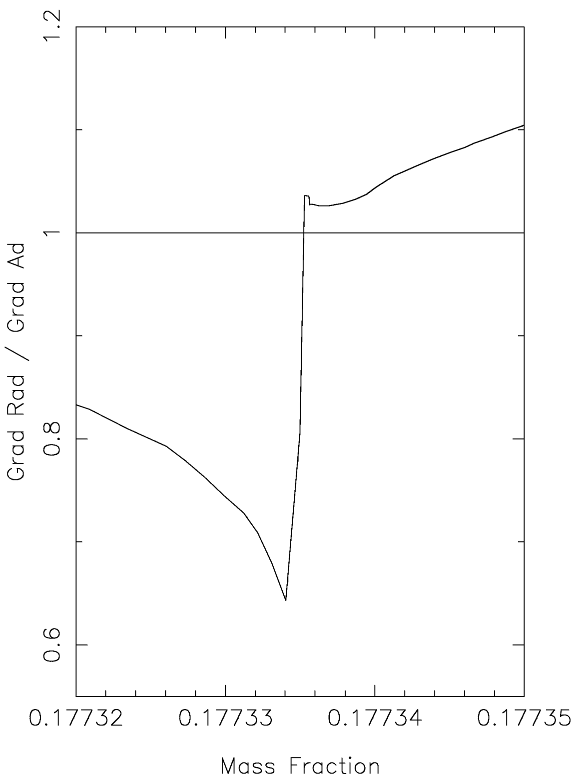

FIG. 1*e*

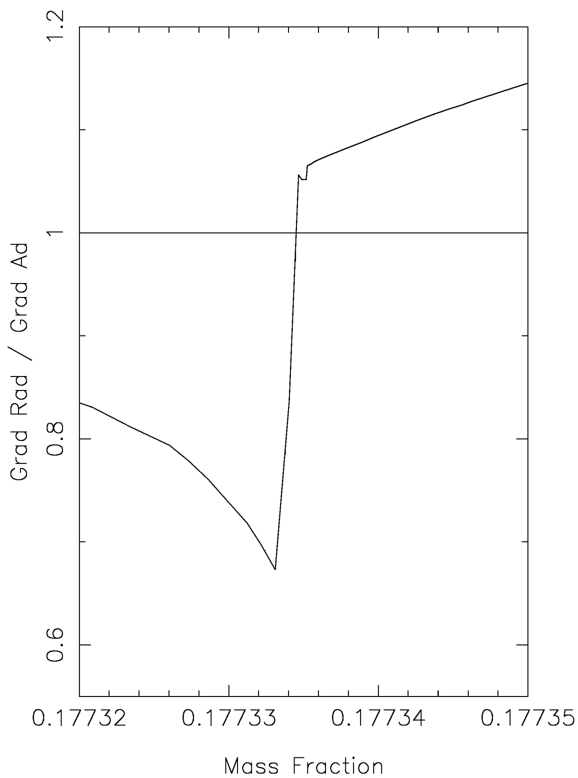

FIG. 1*f*

FIG. 1.—*Continued*

Itoh et al. 1983, 1984; Mitake et al. 1984; Raikh & Yakovlev 1982). The change in entropy of the convective envelope during third dredge-up is treated using Wood's (1981) method. The code begins with a model, uses the rate of composition change to step forward in time and make an initial estimate of a new model, and then iterates on the state variables until the equations of stellar structure are satisfied. The model is then deemed to have converged, and a new model is calculated. Convective boundaries are recalculated for each iteration according to the current conditions, and abundances are recalculated from the previous converged model to fit the new convective zones. Thus, the code does not retain memory of the abundances from the previous iteration (nor should it, since iterations are not time steps); this is an important point in the discussion below. Extension of convection beyond the Schwarzschild boundary is allowed, using the method described above.

In the past, it was not always possible to converge a model if the convective boundaries were allowed to change with each iteration. To overcome this problem, we find it necessary to (*a*) set a maximum value on the number of iterations allowed before changing the time step (we choose 60 as the maximum) and (*b*) allow the convective boundaries to change for the first 40 of these iterations only (Lattanzio 1986). The boundaries are then held at whatever position they occupied on the 40th iteration. In general, a model would converge within the first 10 iterations. Note that convergence difficulties are often found in stellar evolution calculations, especially for AGB models. They are usually not reported in publications until they become so severe as to prohibit further evolution (e.g., Boothroyd & Sackmann 1992).

A question naturally arises: why is it so difficult to converge the models during third dredge-up? We look closely at the behavior of ∇_{rad}/∇_{ad} with each iteration of a stellar model undergoing convergence difficulties during third dredge-up, and we find that the convective envelope initially moves steadily inward as expected (Fig. 1*a*). However, ∇_{rad}/∇_{ad} begins to decrease just above the base of the envelope (Fig. 1*b*) and eventually drops below unity, so that the convective envelope splits into two zones (Fig. 1*c*). During the following iterations, the envelope retreats (Figs 1*d* and 1*e*) until it has returned to (nearly) the conditions of the earlier iterations (Fig. 1*f*).

This behavior may be understood in terms of the method used for calculating abundances. Abundances are always calculated from the previous model, and no memory is preserved of the abundance profile of the previous iteration. Once the convective envelope splits, the second zone (located just below the convective envelope) reverts to its original premixed abundances (i.e., helium rich and not hydrogen rich) and is now radiatively stable. Similarly, as the envelope retreats, the matter previously engulfed by the envelope also reverts to its premixed abundances. The model now returns to its original conditions and abundances, and the entire process begins again (Fig. 2). We recognize this behavior to be reminiscent of semiconvection of the convective core during core helium burning (Castellani et al. 1971). Once caught in this cycle, the code will not converge unless the convective boundaries are fixed in some way.

To overcome this problem, which we refer to as "envelope breathing," we decided to mix down to the "split" on subsequent iterations, regardless of how the tem-

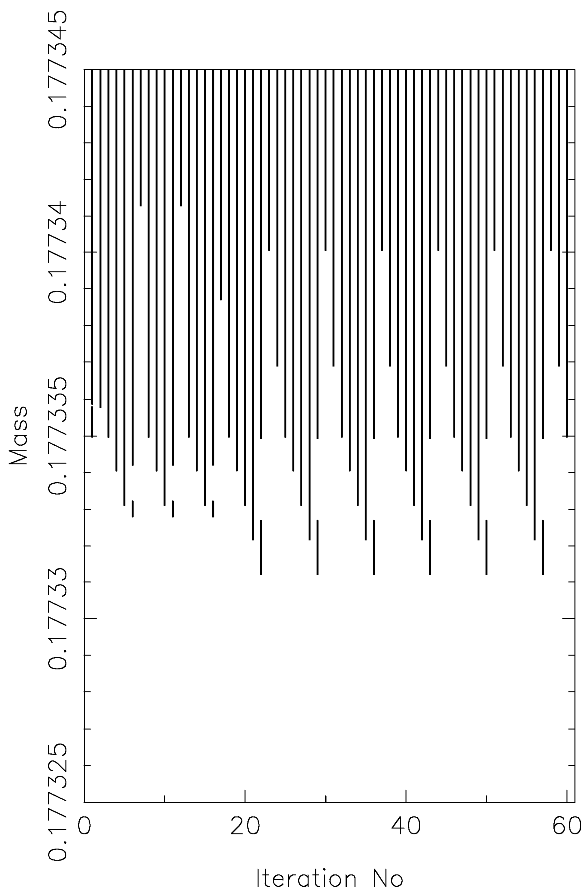

FIG. 2.—Diagram showing convection at the base of the envelope as a function of iteration number, for the model in Fig. 1. The progression and retreat of the envelope are clearly seen, together with the splitting of the envelope. Two separate cycles are evident: the first occurring within the first 15 iterations, repeating every six iterations, and the second occurring for later iterations, repeating every eight iterations. The difference lies in a new convergence criterion being introduced after the 15th iteration, to try and help convergence. This further demonstrates the sensitivity of calculations to numerical technique.

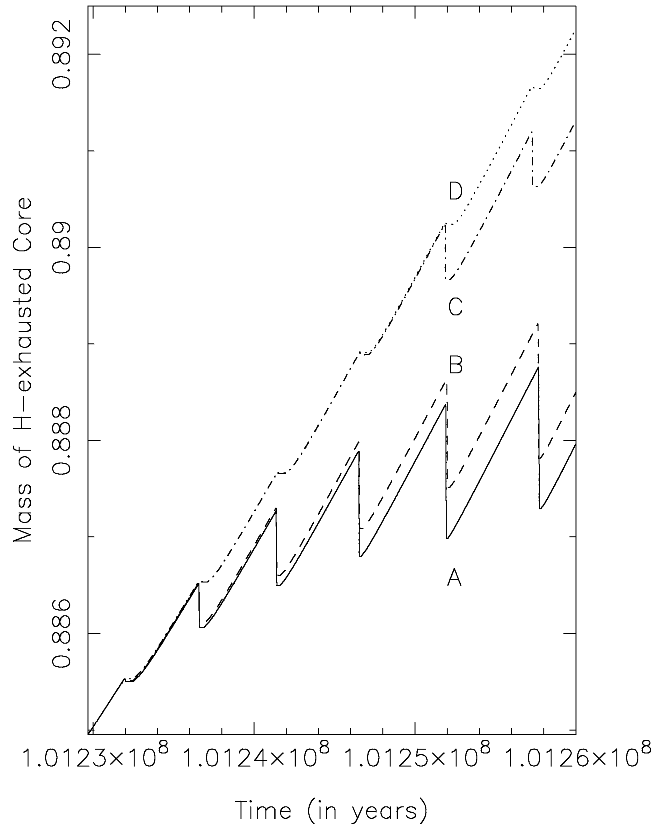

FIG. 3.—Mass of the H-exhausted core vs. time for four 5 $M_\odot$ models with $Z = 0.004$. The first six thermal pulses are shown. Case A (*solid line*) included the method of extending the envelope to the "split." Case B (*dashed line*) did not. Case C (*dot-dashed line*) did not allow the convective neutrality algorithm to include additional mesh points into the envelope. In case D (*dotted line*), mixing was performed after each model had converged, so that, at most, one mesh point per model would be added to the convective envelope by the convective neutrality algorithm. This was the only case that did not experience third dredge-up.

perature gradients alter afterward. We allow convection to extend even further downward, if required by the temperature gradients, but abundances are always mixed to the point of splitting even if convection formally retreats. Thus, we implicitly treat the iterative process as time dependent, which is now reasonable since the convective mixing is the only source of change in the stellar structure equations after a few iterations.

Figure 3 shows the mass of the H-exhausted core versus time for the first six thermal pulses of four 5 $M_\odot$ models with $Z = 0.004$. These models have exactly the same starting model and conditions, but case A (*solid line*) includes the method of dealing with "envelope breathing" as outlined above and case B (*dashed line*) does not. Both models allow the convective boundaries to change during the first 40 iterations since this is still necessary on occasion for convergence, even in case A. Both cases experience dredge-up during the second pulse, but it is larger in case A and grows more quickly during subsequent dredge-up events. By holding the convective boundaries at the 40th iteration, the choice of location of the base of the envelope in the converged model is not well determined and would lie somewhere between the minimum and the maximum extent. Naturally, we would expect to see less dredge-up in this instance, case B, than in case A.

3. THE NUMERICAL DEPENDENCY OF DREDGE-UP

By treating convective overshoot phenomenologically rather than physically, we need to understand how the depth of dredge-up is affected by numerical treatment, and which treatment yields results that are physically reasonable and accurate. The latter is probably best tested by comparison of models with stellar observations and is beyond the scope of this paper.

We already see that a simple method of dealing with "envelope breathing" allows the convective envelope to penetrate further inward than would otherwise be calculated. We investigate two further cases, also shown in Figure 3. Cases C (*dot-dash line*) and D (*dotted line*) do not include the method for handling "envelope breathing." Case C does not attempt to force convective neutrality at a convective boundary, according to Lattanzio's method as discussed above, but simply uses the Schwarzschild criterion. Case D does attempt to force neutrality but calculates abundances at a different stage to that usually used. Instead of determining abundances after each iteration, the abundance profiles are held as they were in the last model (changes due to nuclear burning are allowed) until the current model has converged. Abundances are then mixed for the converged model. This method is used in some stellar codes.

The differences between cases A and B have already been discussed. We first obtain dredge-up for case C during the fifth pulse (cf. the second pulse for cases A and B). In subsequent pulses, the extent of dredge-up grows, but more slowly. In case D, we see negligible dredge-up (or none at all), despite the inclusion of the convective neutrality algorithm. When mixing is not calculated concurrently, the boundaries can change little from model to model, and the convective neutrality algorithm allows at most one mesh point to be mixed into the convective envelope per model. This is clearly inadequate in case D.

4. DISCUSSION

The motivation for calculating the extent of dredge-up has been to obtain more accurate estimates of those elements whose surface abundances (e.g., carbon) are affected by this phenomenon. We note that simple, and reasonable, differences in computational details between codes could explain the differences in third dredge-up reported in the literature by various authors. Furthermore, from Figure 3, it is clear that dredge-up affects the structure and strength of thermal pulses (Sackmann 1977; Paczyński 1977). Those models that experience deep dredge-up have longer interpulse periods and smaller core masses than those that do not. Much of the evolution of stars during the TP-AGB phase is thought to be controlled by the size of the H-exhausted core, and a fuller understanding of the effects of deep dredge-up is needed. This will be addressed in a later paper.

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