Mem. S.A.It. Vol. 75, 660
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Memorie della

A convective model consistent with chemistry

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Abstract. We present a convective model that guarantees self-consistency for the chemistry and the energy budgets. We address its relevance to the thermally pulsing asymptotic giant branch phase by using models computed with a mixing length prescription for convection. We find that salt fingers occur at the base of the intershell convective region. We also find that differential reactivity may play a role in the intershell region as well as at the base of the convective envelope after H shell burning has ignited. However, fully self-consistent stellar evolution computations still need to be undertaken and we provide hints to overcome a few numerical problems generated by our convective model.

Key words. convection – AGB stars – thermal pulses – numerics

1. Motivation

The prelude to type Ia supernovae explosions is a convective phase during which electron captures and emissions take place and yield neutrino losses (Paczyński 1972). The net amount of energy released and the change in the electron fraction at the time of the explosion have always been uncertain owing to the lack of a convective model self-consistent within the energy and chemistry budgets (Bruenn 1973; Couch & Arnett 1975; Iben 1978, 1982; Barkat & Wheeler 1990; Mochkovitch 1996; Stein, Barkat & Wheeler 1999; Bisnovatyi-Kogan 2001). Former attempts (Eggleton 1983; Grossman et al. 1993; Canuto 1999) to describe the interplay between convection and chemistry have all left open the question of energy conservation.

Since this problem is solved in the radiative case we combine two radiative columns of fluid in order to get a self-consistent model of convection (Lesaffre, Podsiadlowski & Tout 2004). We plan to implement this convective model in a stellar evolution code to address the ignition conditions of type Ia supernovae. In the present work we assess whether this model may yield new results during the thermal pulses of asymptotic giant branch stars (the TP-AGB phase).

Section 2 presents the two-streams model compared with mixing-length theory (MLT) of Böhm-Vitense (1958). Section 3 examines the features that might be relevant during the TP-AGB phase. Section 4 considers a few numerical difficulties related to the implementation of this model. We summarise our results and conclude in Section 5.

2. The convective model - a two-streams model

To derive our convective model we considered two radiative columns of fluid side by

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side moving with different velocities which exchange mass, momentum and energy. We write down the equations of radiation hydrodynamics in each stream and we assume a model for the exchange terms.

The resulting formalism provides a framework for convective models that guarantees self-consistency for the chemistry and the energy budget in the flows, allows time-dependence, is non-local and accounts for the interaction of the convective motions with the global contraction or expansion of the star. In the one-stream limit the formalism reproduces several existing convective models and allows them to treat the chemistry in the flows. Details of the method can be found in Lesaffre, Podsiadlowski & Tout (2004).

2.1. Equations for the mean fluid

We present here one way of putting the equations for the evolution of the mean energy and chemical composition which emphasise their similarities[1] :

$$\frac{\mathrm{D}e}{\mathrm{D}t} + p\frac{\mathrm{D}}{\mathrm{D}t}(\frac{1}{\rho}) = \epsilon - \frac{\partial L_{\mathrm{rad}}}{\partial m} - \frac{\partial L_{\mathrm{conv}}}{\partial m} \quad (1)$$

and

$$\frac{\mathrm{D}\mathbf{N}}{\mathrm{D}t} = \mathbf{R} - \frac{\partial \mathbf{F}_{\mathrm{diff}}}{\partial m} - \frac{\partial \mathbf{F}_{\mathrm{conv}}}{\partial m}, \quad (2)$$

where e, p, ρ and $\mathbf{N}$ are respectively the specific energy, pressure, mass density and composition vector (number per unit mass). The net energy generation rate (nuclear burning and neutrino losses) is ϵ. The rate of change of $\mathbf{N}$ due to nuclear reactions is $\mathbf{R}$. The radiative and convective luminosities are L_{rad} and L_{conv}. The flows of particles due to atomic diffusion and convection are $\mathbf{F}_{\mathrm{diff}}$ and $\mathbf{F}_{\mathrm{conv}}$.

The two-streams model gives expressions for L_{conv} and $\mathbf{F}_{\mathrm{conv}}$ in terms of the convective velocity u (drift velocity between the two streams) and the enthalpy and composition differences between the two streams.

[1] in particular we put the work term to zero thereby assuming a fully dissipative process for the momentum exchange between the two streams.

2.2. The minimal extension to MLT

To obtain the convective speed in MLT we assume a stationary state in the sense that the buoyancy acceleration is exactly balanced by the dissipation of convective motions. We keep this approximation in all the following.

The buoyancy of a fluid element is proportional to its *density* excess compared with its surroundings. We further assume that this density difference is proportional only to the temperature difference. This yields the convective speed

$$u_{\mathrm{MLT}} = u_1 \sqrt{\delta(\nabla - \nabla_a)}, \quad (3)$$

where u_1 is a characteristic speed and $\delta = -(\frac{\partial \ln \rho}{\partial \ln T})_{\mathrm{p,N}}$ and ∇ and ∇_a have have their usual meaning.

But the density is also sensitive to the composition, especially in degenerate matter. The corresponding convective velocity involves the Ledoux criterion rather than the Schwarzschild criterion. So

$$u = u_1 \sqrt{\delta(\nabla - \nabla_a) - \phi\nabla_\mu}, \quad (4)$$

where $\phi = (\frac{\partial \ln \rho}{\partial \ln \mu})_{\mathrm{p,T}}$ and ∇_μ is the molecular weight (μ) gradient. This introduces a dependence of the convective speed on chemical gradients.

The convective luminosity is then expressed in terms of the enthalpy excess. MLT assumes that it is proportional to the temperature excess via the specific heat c_{p} which yields the convective luminosity

$$L_{\mathrm{MLT}} = 4\pi r^2 \rho u_{\mathrm{MLT}} c_{\mathrm{p}} \Delta T, \quad (5)$$

where ΔT is the temperature excess and r is the distance to the centre of the star.

However, the enthalpy h also has a dependence on composition. This yields the more general expression

$$L_{\mathrm{conv}} = 4\pi r^2 \rho u (c_{\mathrm{p}} \Delta T + \boldsymbol{\mu}'.\Delta\mathbf{N}), \quad (6)$$

where $\boldsymbol{\mu}' = T(\frac{\partial h}{\partial \mathbf{N}})_{\mathrm{T,p}}$ and $\Delta\mathbf{N}$ is the vector of composition excesses. This yields also a dependence of the convective luminosity on chemical variables.

In either case the chemical flow is expressed as

$$\mathbf{F}_{\rm diff} = 4\pi r^2 \rho u \Delta \mathbf{N}, \quad (7)$$

where λ is the mixing length. The convective mixing is hence a diffusion process.

Equations (1), (2), (4), (6) and (7) provide the smallest extension of MLT which is consistent with the energy and chemistry budgets. We later refer to this model as MLTc.

2.3. Differential reactivity

In the one-stream limit of our convective model the time evolution of the chemical excesses obeys

$$\frac{\lambda}{u}\frac{\mathrm{D}\Delta\mathbf{N}}{\mathrm{D}t} = -\lambda\frac{\partial \mathbf{N}}{\partial r} - 2\Delta\mathbf{N} + \frac{\lambda}{u}\Delta\mathbf{R}. \quad (8)$$

The last term illustrates the differential reactivity of the fluid elements in the ascending and descending streams. This term is present in all former attempts to include chemical effects in a convective model. Note that if this term is significant it is likely to selectively modify the chemical mixing according to different species. For example, only strongly reacting species will be affected.

3. Relevance to the TP-AGB phase

We consider the 5 $M_\odot$ models of Z=0.02 from Stancliffe et al. (2004) at various phases of the 14$^{\rm th}$ thermal pulse. For each of these models, we extract every other point of the grid in order to get more accurate chemical gradients. We then compute a few variables of MLTc on these models to assess the relevance of different physical effects.

3.1. Schwarzschild versus Ledoux

We compared the Schwarzschild criterion to the Ledoux criterion. A significant difference was observed only at the He burning shell during the thermal pulse. Salt fingers are expected as is shown on Figure 1.

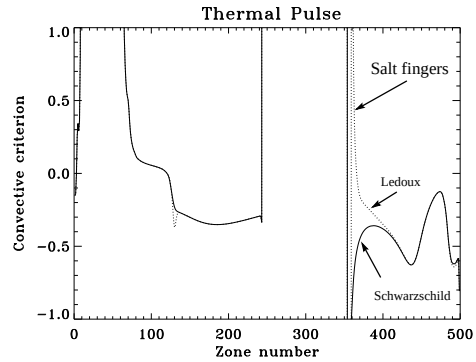

Fig. 1. Schwarzschild ($\nabla - \nabla_a$) and Ledoux ($\nabla - \nabla_a - (\phi/\delta)\nabla_\mu$) criteria for convection are compared for a model near the peak of the 14$^{\rm th}$ thermal pulse of a 5 $M_\odot$ model.

3.2. Differential reactivity

In order to assess the role of the differential reactivity we compared the thermal diffusion time scale over a pressure scale height, the local convective turn-over time scale and the chemical time scale, maximum of $|\frac{\partial R_j/N_j}{\partial \ln T}|$ for j species with mass fraction geater than 10%. Figures 2 and 3 show these time scales for the TP and the second half of the third dredge up (TDUP) phase (after H shell burning has reignited).

The thermal time scale is taken as a good estimate for the typical time scale for the evolution. Since the convective turn-over time scale is always much shorter it is fair to take a stationary model for convection.

But the chemical time scale is sometimes shorter than the convective turn-over time scale. This indicates situations where the differential reactivity term is no longer negligible. We point out two situations where this term should be taken into account. They are

- at the base of the convective envelope during TP and in the second half of TDUP and
- in he intershell convective zone during TP.

The first case is interesting because it might give rise to selective mixing in the region where the ^{13}C pocket is thought to be formed even though the process happens only after H-

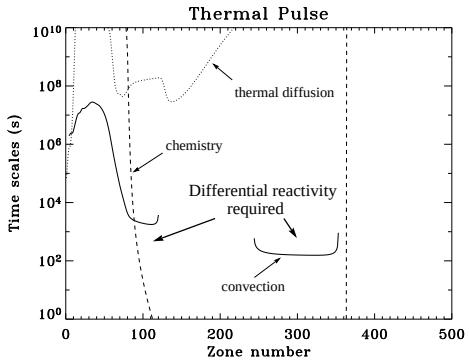

Fig. 2. Three characteristic time scales for thermal diffusion, convection and chemistry are compared for the same model as Figure 1.

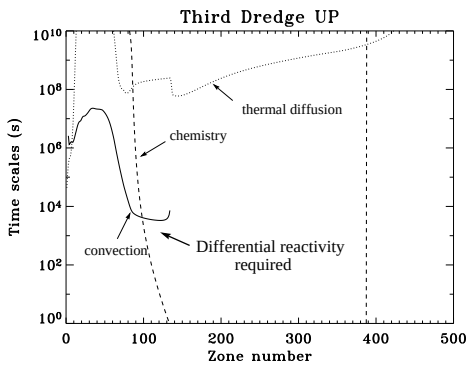

Fig. 3. Three characteristic time scales for thermal diffusion, convection and chemistry are compared for a model near the end of the TDUP phase after the 14th pulse.

shell burning has reignited. However numerical calculations need to be undertaken with a refined stellar evolution code to validate the extent of this effect.

4. Numerical difficulties

MLTc is formally very close to MLT but in practice it generates plenty of numerical difficulties...

4.1. Energy equation

When writing down the energy equation (1) we have the choice of using $\mathrm{d}e + p\mathrm{d}(1/\rho)$ or $\mathrm{d}s + \boldsymbol{\mu}.\mathrm{d}\mathbf{N}$ where s is the specific entropy and $\boldsymbol{\mu}$ is the vector of chemical potentials. Even though it is easier to implement, the former choice is often numerically ill-determined because the sum of two terms nearly cancels. The entropy form of the equation is hence a wiser choice.

4.2. Chemical gradients

The chemical profile can be very flat in well mixed convective regions. In this case it is a bad idea to compute the gradients by a difference scheme which introduces huge roundoff errors. In the case of MLTc these errors are propagated to the convective velocity. Hence a mixing and a numerical instability is triggered. We suggest the use of $\mathbf{F} = \mathbf{F}_{\mathrm{diff}} + \mathbf{F}_{\mathrm{conv}}$ as an additional variable in exactly the same way as $L = L_{\mathrm{rad}} + L_{\mathrm{conv}}$ is used in addition to T in standard stellar evolution codes. This allows us to compute accurately the mixing even in well mixed regions. It is crucial for degenerate matter where even small gradients affect the convective velocity.

4.3. Resolution at convective boundaries

To get smooth variations of the total flow $\mathbf{F}$ the condition

$$\Delta r \ll \sqrt{D\Delta t}, \tag{9}$$

where Δr is the grid spacing, Δt is the time step and D is the atomic diffusion coefficient, needs to be satisfied near the convective boundary. This implies a lower bound for the time step.

4.4. Back reaction

The back reaction of the chemical gradients on the convective velocity, and hence the chemical mixing, gives birth to a pathological case where Newton-Raphson is not able to converge. We are currently trying to fix this by using the chemical gradients at the previous time

step in the expression for the convective speed even though it damages the self-consistency of the solution.

5. Summary and conclusion

Using a two-streams configuration we have produced a convective model self-consistent within the energy and chemistry budget. We note that MLT is formally close to consistency with chemistry because only the chemical dependence of the convective velocity and luminosity need be introduced to get MLTc.

In the TP-AGB phase we expect a significant change to the convective velocity only during TPs at the He burning shell where salt fingers are expected. Differential reactivity is likely to play a role in the intershell convective region and at the base of the convective envelope and during TPs and the second half of TDUP. The latter case is exciting because it corresponds to where we think the ^{13}C pocket is formed.

However, we need to overcome quite a few numerical difficulties before we are able to implement MLTc in a stellar evolution code and assess the true impact of this model on various types of stars.

Acknowledgements. This work was funded through a European Research & Training Network on Type Ia Supernovae (HPRN-CT-20002-00303).

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