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ASTRONOMY AND ASTROPHYSICS

Stellar evolution with rotation

II. A new approach for shear mixing

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Abstract. Recent observations show He- and N-enhancements in fast rotating O-type stars, while studies on shear mixing in rotating stars have shown that the μ-gradients generally inhibit mixing processes. However, these studies (including ours) ignored the other sources of turbulence, such as semiconvection and horizontal turbulence, which may be present in the medium and may modify the onset of shear mixing. Indeed, in massive stars most of the zone where μ-gradients would inhibit mixing according to the Richardson criterion is semiconvective, i.e. such a zone would experience some turbulence anyway.

This leads us to introduce the following working hypothesis: in a semiconvection region (or in any zone with other sources of turbulence) *some fraction of the local energy excess in the shear is degraded by turbulence to change the local entropy gradient*. Consistently with this hypothesis we derive the effects of the shear on the entropy gradient, then on the T- and μ-gradients, and express the fraction of the μ-gradient which can be diffused. From the basic equations describing the evolution of temperature perturbations we obtain the velocities of fluid elements under some specific conditions, and then we get the associated diffusion coefficient D. Interestingly enough, the values of D tend towards the diffusion coefficient for semiconvection, when the shears become negligible, and towards the coefficient by Zahn (1992; cf. also Maeder and Meynet 1996) when shears dominate.

We also examine the coupling of shear mixing and thermal transport; a third order equation expressing the combined effects is obtained. The solutions for shears in semiconvective and radiative zones are examined in detail. The main result of the above developments is the slight progressive erosion of the μ-barriers in stars, for cases where the usual form of the Richardson criterion would have imposed an unsuperable threshold.

In Appendices A and B we rediscuss the diffusion coefficient for semiconvection and find a more general expression, not limited to the adiabatic case.

Key words: stars: interiors – rotation – stars: evolution – diffusion

1. Introduction

The problem of rotational mixing is of great importance and actuality in stellar evolution. Several discrepancies between models and observations have been found, which all point in favour of more mixing in stellar models (cf. Maeder 1995a). As long as these discrepancies are not explained we cannot trust the various model outputs.

Some of the physical processes inducing rotational mixing have been studied for three quarters of a century. Recently the various processes have been reviewed by Zahn (1992, 1993, 1994) who shows that shear mixing should be the most efficient mechanism. He also established the equations for the transports of angular momentum and chemical species. In Paper I of this series (Meynet and Maeder 1996) we have solved in a new way the equations of stellar structure for the so-called "shellular rotation", including the effects of rotational mixing. The results were negative: no significant mixing as is required by the observations of massive stars (cf. Herrero et al. 1992; Venn 1993) occured!

The physical reason for this difficulty was clearly identified. It resides in *the threshold imposed by the Richardson criterion including μ-gradients which demands an excessively large shear $\Omega \frac{d\ell n\Omega}{d\ell nr}$ to overcome the μ-gradient ∇_μ generated by nuclear evolution* (Ω is the angular rotational velocity). Despite the fact that the threshold due to the Richardson criterion is somehow lowered by the inclusion of thermal effects (Maeder 1995b; Maeder and Meynet 1996), the negative conclusion remains; by a wide margin the models of Paper I showed no significant mixing. Let us also note that it was found by Chaboyer et al. (1995) that the inhibiting effects of μ-gradients should be reduced by a factor of 10 to explain the observed Li depletion on the main sequence.

To overcome the above discrepancy between models and observations we must certainly reconsider the threshold imposed by the Richardson criterion and the related hydrodynamical effects. In Sect. 2 we make some critical remarks about the current picture of shear mixing. In Sects. 3 to 5 we develop a new approach based on an energy criterion to obtain the diffusion coefficient. In Sect. 6 we introduce coupling with thermal effects and examine the various solutions (Sect. 7). In the Appendices, technical details are being discussed, in particular about semiconvection in relation with the work by Kato (1966), Langer et al. (1983) and Kippenhahn (1969, 1974).

2. Critical remarks about the current picture of shear mixing

There are three main arguments which suggest a revision of the usual treatment adopted in previous works (cf. Zahn 1992; Maeder and Meynet 1996; Meynet and Maeder 1997).

1. Firstly, as mentioned above, there are various observational evidences showing additional mixing in massive stars. In particular, the observations of O-stars clearly show He-enrichments for stars with a rotational velocity above 150 km/s (cf. Herrero et al. 1992). Recent works on B and A supergiants also show the presence of additional mixing (Venn 1993, 1995).

2. All studies on shear instabilities, including ours, consider the occurrence of shears in otherwise stable radiative layers. They assume that if the excess energy $\frac{1}{4}\rho(dU)^2$ in the shear is larger than the energy necessary to produce the ascending of an eddy in the medium with the considered T and μ gradients, mixing then occurs (U being the horizontal velocity, z the vertical depth in the star). This is the basic idea of the Richardson criterion. However, this approach completely ignores that other turbulent processes may already be present in the considered layers, in particular semiconvection and the horizontal turbulence suggested by Zahn (1992).

Semiconvection is a double diffusive instability which leads to a vibrational instability with growing amplitudes (Kato 1966; Langer et al. 1983; Kippenhahn and Weigert 1990). Recent numerical simulations confirm that semiconvection results in turbulent motions and mixing (cf. Merryfield 1995). Indeed, our current stellar models show that in massive stars most of the zone with a significant μ-gradient (and thus where mixing may have a real effect) is semiconvective and thus subject to some turbulence long before it is formally predicted by Richardson's criterion. Also, as suggested by Chaboyer and Zahn (1992), Zahn (1992), rotating stars are likely to have a highly anisotropic turbulence with a strong horizontal component.

The presence of other sources of turbulence may considerably modify the threshold and the efficiency of shear mixing. In particular, it is likely that *the excess of energy present in the shear may feed the already existing turbulent spectrum and thus contribute to mixing in stellar interiors as soon as some energy from the shear is available.* In that respect we recall that the Richardson criterion imposes some threshold, namely

$$\frac{1}{4}\left(\frac{dU}{dz}\right)^2 > \frac{g\varphi\nabla_\mu}{H_p}$$

for shear mixing in a radiative zone (cf. Maeder and Meynet 1996; symbols have the usual meaning as indicated below).

3. The hypothesis outlined above is worthy of particular interest, since the first numerical models of rotating stars (Paper I) show that we very often have the following intermediate situation with

$$R_i\,(\mu = 0) = \frac{g\delta(\nabla' - \nabla)}{H_p\left(dU/dz\right)^2} < 1/4 \tag{2.1}$$

and simultaneously

$$R_i(\mu \neq 0) = \frac{g\delta\left(\nabla' - \nabla + \frac{\varphi}{\delta}\nabla_\mu\right)}{H_p\left(dU/dz\right)^2} > \frac{1}{4} \tag{2.2}$$

R_i is the Richardson number, ∇' and ∇ are respectively the internal and external thermal gradient, $\nabla_\mu = (\partial\ell n\mu/\partial\ell nP)_{T,\mu}$, g the local gravity, H_p the pressure scale height, (dU/dz) expresses the shear of horizontal velocities U, $\delta = -(\partial\ell n\rho/\partial\ell nT)_{P,\,\mu}$, $\varphi = (\partial\ell n\rho/\partial\ell n\mu)_{P,T}$.

Relation 2.1 means that the excess energy in the shear would be able to overturn the stable thermal gradient, but relation 2.2 shows that when the μ-gradient is accounted for, the medium is stabilized. The term ∇_μ is often an order of magnitude larger than $(\nabla' - \nabla)$. The situation has some analogy with the classical problem set by the Schwarzschild and Ledoux criteria.

Indeed, there is much more than an analogy between semiconvection and criteria 2.1 and 2.2. If we write $(dU/dz) \longrightarrow 0$, we obtain

$$\left(\nabla' - \nabla\right) < 0 \tag{2.3}$$

and

$$\left(\nabla' - \nabla + \frac{\varphi}{\delta}\,\nabla_\mu\right) > 0 \tag{2.4}$$

that is to say precisely the Schwarzschild and Ledoux criteria. *Thus, the Richardson criterion in the form 2.1 and 2.2 contains the Schwarzschild and Ledoux criterion as a limit for* negligible shears $(dU/dz) \longrightarrow 0$. A zone where criterion 2.3 and 2.4 are simultaneously satisfied is called a semiconvective zone. Let us call a zone satisfying both 2.1 and 2.2 simultaneously *a "semiconvective shear zone"*.

In such a semiconvective shear zone, the shear does not contain enough energy to produce the complete overturn of the medium. However, even without a full overturn there can be some degree of partial mixing, i.e. some change of the entropy gradient, at the expense of the energy excess in the shear. It is precisely that degree of partial mixing we want to estimate in this work.

3. Partial mixing in a semiconvective shear zone. The diffused fraction f_μ

Let us consider a semiconvective shear zone. Even without a shear such a zone would experience some turbulence. The additional mechanical energy is likely to feed in some way the turbulent spectrum. A detailed analysis of these effects is likely to be a task of great complexity by analytical means and should be investigated by numerical hydrodynamical 3D-simulations. However, we need some tractable expression for the current 1D-calculations of stellar evolution, which still have a great interest

for rotating stars thanks to the existence of shellular rotation as shown by Zahn (1992). Thus, we shall try to make a global approach of that complex problem by considering the effects of the shear on the entropy gradient in a star. Let us then make the following working hypothesis: *in a semiconvective shear zone, a fraction α of the excess energy in the shear is used to change the entropy gradient, i.e. to extract entropy from the interior by smoothing the μ-gradient*. This hypothesis is likely to be a reasonable one. It might also apply to the radiative zone of rotating stars where efficient horizontal turbulence is present (shellular rotation). But as for any working hypothesis, we do not know whether it is correct, and what we want to do is to explore consistently its logical consequences to test its validity.
Let us consider the motion of a turbulent eddy in a medium and express the variation of its internal density ρ', as a function of internal pressure and entropy

$$\delta\rho' = \left(\frac{\partial\rho}{\partial P}\right)_S \delta\, P' + \left(\frac{\partial\rho}{\partial S}\right)_P \delta\, S' \tag{3.5}$$

where primes refer to internal quantities. For subsonic motions the gravity force acting on the turbulent element is

$$g\left(\delta\rho' - \delta\rho\right) = -\,g\left(\frac{\partial\rho}{\partial S}\right)_P \left(\delta S - \delta S'\right) \tag{3.6}$$

where non-primed quantities refer to the external medium. We also have

$$\left(\frac{\partial\rho}{\partial S}\right)_P = \frac{\left(\frac{\partial\rho}{\partial T}\right)_P}{\left(\frac{\partial S}{\partial T}\right)_P} = \frac{T}{C_P}\left(\frac{\partial\rho}{\partial T}\right)_P \tag{3.7}$$

where C_P is the specific heat at constant pressure.
For an upward displacement over a distance $-\delta z$ the work required to transport the matter is by unit of mass

$$\delta W = \frac{g}{\rho}\left(\frac{\partial\rho}{\partial S}\right)_P \left(\delta S - \delta S'\right)\delta z \tag{3.8}$$

There we assume that the average force is 1/2 of that given by 3.6 and that there are two blobs to be exchanged.
A shear flow contains an excess energy δK with respect to uniform motions

$$\delta K = \frac{1}{2}\left[U^2 + (U+\delta U)^2\right] - \frac{1}{2}\cdot 2\left(U + \frac{\delta U}{2}\right)^2 = \frac{\delta U^2}{4} \tag{3.9}$$

δK is independent of the sign of dU/dz. With expressions 3.8 and 3.9 our working hypothesis writes simply

$$\frac{dS - dS'}{dz} = \frac{\alpha\rho}{4\,g}\left(\frac{\partial S}{\partial\rho}\right)_P \left(\frac{dU}{dz}\right)^2 \tag{3.10}$$

where the fraction $\alpha \leq 1$. With 3.7, this becomes

$$\frac{dS - dS'}{dz} = \frac{-\alpha}{4\,g}\,\frac{C_P}{\delta}\left(\frac{dU}{dz}\right)^2 \tag{3.11}$$

$\delta = 1$ for a perfect gas and $\delta = (4-3\beta)/\beta$ for a mixture of perfect gas and radiation with $\beta = P_{gas}/P_{tot}$. Consistently with our working hypothesis, expression 3.11 gives the general relation between the shear and the change of the entropy gradient We see that the entropy gradient in the medium $dS/dr = -dS/dz$ will grow outwards for increasing shears; however, the detailed result depends on how dS' varies. For adiabatic motions we would have $dS' = 0$, but as shown below we must examine the content of dS' much more precisely.
The difference of the entropy gradients depends on the local physical variables. In terms of temperature T and mean molecular weight μ we can write

$$\frac{dS - dS'}{dz} = -\left(\frac{\partial S}{\partial\rho}\right)_P \rho\left[\delta\left(\frac{d\ell nT}{dz} - \frac{d\ell nT'}{dz}\right) + \varphi\left(\frac{d\ell n\mu'}{dz} - \frac{d\ell n\mu}{dz}\right)\right] \tag{3.12}$$

The quantity $\varphi = 1$ for a mixture of perfect gas and radiation. For a turbulent eddy which would preserve its identity, the internal change of the μ-gradient is

$$\frac{d\ell n\mu'}{dz} = 0$$

If one makes the usual assumption that the turbulent eddy at its starting level has the average local composition, the μ-excess after a small trip Δr is

$$D\mu = \frac{\mu}{H_p}\,\nabla_\mu\,\Delta r \tag{3.13}$$

Such a fluid element in a shear flow can only rise if the Richardson criterion is satisfied. However, in a mildly turbulent medium, the composition is not likely to be homogeneous and a fluid element at the considered starting level r_0 may have a μ-deficiency (or excess) $\Delta\mu_0 = (\mu - \mu')_0$. After an upwards displacement by Δr, such elements, if they keep their integrity during the displacement, will in general have an excess

$$D\mu^* = D\mu - \Delta\mu_0 \tag{3.14}$$

For $\Delta\mu_0 > 0$, one has $D\mu^* < D\mu$ and we may consider the ratio $f_\mu = D\mu^*/D\mu$, which we call *the transported or diffused fraction*. If $f_\mu = 1$, the cell just transports the composition of its original level, if $f_\mu = 0$, nothing is transported. In order to lift a turbulent element with $f_\mu < 1$, Richardsons's criterion needs not to be satisfied, since less energy is required to drive the motion. For such an element the change of entropy can be written

$$\frac{dS - dS'}{dz} = -\left(\frac{\partial S}{\partial\rho}\right)_P \frac{\rho\delta}{H_p}\left[\left(\nabla - \nabla'\right) - \frac{\varphi}{\delta} f_\mu \nabla_\mu\right] \tag{3.15}$$

Thus, from 3.11 and 3.16, we get an estimate of the fraction f_μ which can be transported by a given shear flow

$$f_\mu = \frac{\alpha}{4}\,\frac{H_p}{g\varphi\nabla_\mu}\left(\frac{dU}{dz}\right)^2 - \frac{\delta}{\varphi}\,\frac{(\nabla' - \nabla)}{\nabla_\mu} \tag{3.16}$$

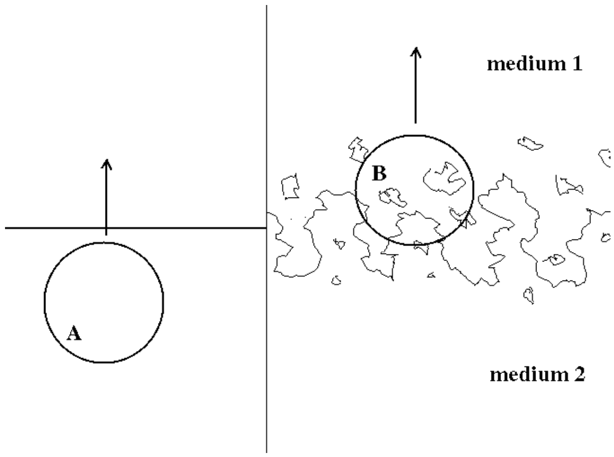

Fig. 1. Schematic representation of mixing criteria through a chemical discontinuity. Left) The criterion for eddy A to move from medium 2 to medium 1 ($\mu_2 > \mu_1$) is the Richardson criterion. Right) In a turbulent medium there is enough energy in the shear to move upwards a turbulent eddy containing a mass fraction f_μ of the lower medium.

Fig. 1 illustrates in a simplified way the meaning of f_μ. If there is some turbulence at the interface between two media of different mean compositions, the excess energy of the shear may be high enough to move upwards a bubble B containing a fraction f_μ of the lower medium. To move A upwards in medium 1, the Richardson criterion should first be satisfied.

The first term in the right part of 3.16 corresponds to the mixing of elements induced by the shear. We notice that the diffused fraction grows with $(dU/dz)^2$. The second term corresponds to the effects of the thermal gradient. It is positive in a semiconvective zone, since the unstable thermal gradient also contributes to mixing. In a radiative zone this term is negative, since in order to transport matter one has to overcome the stable thermal gradient. It is to be noticed that we consider the difference of thermal gradients $(\nabla' - \nabla)$ in 3.16 rather than $(\nabla_{ad} - \nabla)$, since the transport of matter is not necessarily adiabatic. Even more, we will see that non adiabatic effects generally play a major role.

4. The thermal adjustment velocity

Let us now consider what happens to a fluid element which has an excess $D\mu$ of mean molecular weight with respect to its surroundings. Mechanical and thermal equilibrium are impossible for this fluid element. Even if at some location in the medium the blob happens to reach temporarily mechanical equilibrium, the thermal instabilities would destroy the equilibrium since the fluid element will radiate energy into its surroundings and will progressively start sinking like salt fingers. Kippenhahn (1969, 1974) and Kippenhahn and Weigert (1990) have estimated the sinking velocity v_μ for a simple physical situation consisting of two homogeneous media of compositions μ_1 and $\mu_2 (\mu_1 < \mu_2)$. An eddy of composition μ_2 (lower medium) transported into the upper medium will sink with a stationary velocity

$$v_\mu = \frac{-H_p}{(\nabla_{ad} - \nabla)\tau_{adj}} \frac{\varphi}{\delta} \frac{D\mu}{\mu} \tag{4.17}$$

τ_{adj} is the adjustment time; for a sphere with diameter d one has

$$\tau_{adj} = \frac{\kappa\rho^2 C_p d^2}{16\, acT^3} \tag{4.18}$$

One can also write

$$\tau_{adj} = \frac{d^2}{12\, K} \quad \text{with} \quad K = \frac{4acT^3}{3\kappa\rho^2 C_p} \tag{4.19}$$

where K is the thermal diffusivity. The velocity v_μ is an important characteristic of the stellar medium (cf. Kippenhahn 1974). It is indeed the minimum sinking velocity of a fluid element with an excess $D\mu$. Let us call v_μ the Kippenhahn velocity.

The physical conditions used in deriving expression 4.17 are, however, oversimplified. We must consider a more realistic situation with a medium having a continuous μ-gradient ∇_μ in which we study the motion of a cell having a μ-excess $D\mu$. The following equation applies quite generally (cf. Kippenhahn 1969).

$$\frac{\partial}{\partial t}\left(\frac{DT}{T}\right) = \frac{v_\mu}{H_p}(\nabla - \nabla_{ad}) - \frac{DT}{T\tau_{adj}} \tag{4.20}$$

Indeed, this equation is equivalent to that obtained by Kato (1966; Eq. 7) from the first order perturbations of the equation of energy transfer, if we identify the perturbation T_1 by Kato with the quantity DT in 4.20. Also, the radiative losses are expressed with $K\nabla^2 T_1$ by Kato (1966), while they are expressed with DT/τ_{adj} by Kippenhahn and Weigert (1990). See also Appendix A below on the application of the expressions by Kato and by Kippenhahn and Weigert to semiconvection. In a homogeneous medium Kippenhahn assumes

$$\frac{\partial}{\partial t}\left(\frac{DT}{T}\right) = 0 \tag{4.21}$$

since for a succession of equilibrium stages one has $DT/T = \frac{\varphi}{\delta}\left(D\mu/\mu\right)$ and $D\mu/\mu$ is constant due to homogeneity. In this way, the expression (4.17) for the velocity was derived.

Let us now consider a medium with a non-zero μ-gradient ∇_μ; the differences for radiatively stable and semiconvective layers will be specified later. Let us also consider as initial conditions the case of a fluid element temporarily in equilibrium at some level with an excess $D\mu$ and a corresponding excess DT. In a medium with $\nabla_\mu \neq 0$, $D\mu$ varies with location (cf. 3.13) and there is no stationary Kippenhahn's velocity resulting from the coupled equations

$$\frac{\partial v}{\partial t} = g\left(\delta\frac{DT}{T} - \varphi\frac{D\mu}{\mu}\right) \tag{4.22}$$

with 4.20 and 3.13. This system of equations has been studied for a long time (cf. Kato 1966) and we do not come back to this treatment.

There is, however, an essential remark to be made in this context. In fact, the only cases relevant for mild mixing in stellar evolution are those with a small Peclet number

$$Pe = \frac{\tau_{adj}}{\tau_{dyn}} \ll 1 \tag{4.23}$$

where τ_{adj} is given by 4.19 and τ_{dyn} is the dynamical timescale of mixing motions. Indeed, if $Pe \gtrsim 1$, mixing would occur on timescales shorter than the Kelvin-Helmoltz timescale and the stars would be fully mixed very quickly! $Pe \ll 1$ implies that

$$\left|\frac{1}{v}\frac{\partial v}{\partial t}\right| \ll \left|\frac{1}{(\frac{DT}{T})}\frac{\partial}{\partial t}\left(\frac{DT}{T}\right)\right| \tag{4.24}$$

and thus the cell rapidly adjusts its temperature to the surroundings and is almost in thermal equilibrium with it. As a consequence of the cooling, the cell goes down. From 4.22 and 4.24 we can make the following approximation:

$$\frac{\partial}{\partial t}\left(\frac{DT}{T}\right) \simeq \frac{\partial}{\partial t}\left(\frac{\varphi}{\delta}\frac{D\mu}{\mu}\right) = \frac{\partial}{\partial t}\left(\frac{\varphi}{\delta}\frac{\nabla_\mu}{H_p}\Delta r\right) = \frac{\varphi}{\delta}\frac{\nabla_\mu}{H_p}v_\mu \tag{4.25}$$

and thus 4.20 leads to

$$v_\mu = -\frac{H_p}{\left(\frac{\varphi}{\delta}\nabla_\mu + \nabla_{ad} - \nabla\right)}\frac{\varphi}{\delta}\frac{D\mu}{\mu}\frac{1}{\tau_{adj}} \tag{4.26}$$

This is a generalisation of Kippenhahn's sinking velocity, however we must stress that it is only valid for $Pe \ll 1$. Interestingly enough, this expression of v_μ applies whatever $\frac{D\mu}{\mu}$ may be, provided the cell keeps its identity during the trip Δr, because then the second equality in 4.25 is valid. In particular, we may consider a fluid element with a specific excess $D\mu^*$, and we verify that, according to 3.14, one well has

$$\frac{\partial}{\partial t}\left(D\mu^*/\mu\right) = \frac{\partial}{\partial t}\left(D\mu/\mu\right) \tag{4.27}$$

We may now consider the sinking motion of a fluid element which has been lifted upwards with a μ-excess $D\mu^*$ as a result of the excess energy available in the shears.

5. The diffusion coefficient for shear mixing

From the previous expressions, the sinking velocity of a fluid element having an excess $D\mu^*$ is, by using the expressions 3.16 for f_μ and 4.19 for τ_{adj}

$$v_\mu = \frac{-3\alpha K\left(\frac{dU}{dz}\right)^2 H_p\Delta r}{\delta\left(\frac{\varphi}{\delta}\nabla_\mu + \nabla_{ad} - \nabla\right)d^2 g} + \frac{12K\left(\nabla' - \nabla\right)\Delta r}{\left(\frac{\varphi}{\delta}\nabla_\mu + \nabla_{ad} - \nabla\right)d^2} \tag{5.28}$$

The corresponding diffusion coefficient of a fluid element is defined by

$$D = \frac{1}{3}\left|v_\mu\right|\Delta r \tag{5.29}$$

where we consider that the ratio $\Delta r^2/d^2$ of the characteristic scales is of the order of unity. We thus obtain

$$D = \frac{K}{\left(\frac{\varphi}{\delta}\nabla_\mu + \nabla_{ad} - \nabla\right)}\left[\frac{\alpha H_p}{g\delta}\left(\frac{dU}{dz}\right)^2 - 4\left(\nabla' - \nabla\right)\right] \tag{5.30}$$

The internal gradient ∇' is related to the adiabatic gradient ∇_{ad} by the following expression (cf. Maeder 1995b), in which Γ can be expressed in terms of the Peclet number $Pe = v\ell/K$ by $Pe = 6\Gamma$. (We recall that the Peclet number is the ratio of the cooling to the dynamical timescale for a turbulent eddy).

$$\nabla' - \nabla = \frac{\Gamma}{\Gamma + 1}\left(\nabla_{ad} - \nabla\right) \tag{5.31}$$

and thus

$$D = \frac{K}{N^2_{ad}(\mu)}\left[\alpha\left(\frac{dU}{dz}\right)^2 - \frac{4\Gamma}{\Gamma+1}N^2_{ad}\left(\mu = 0\right)\right] \tag{5.32}$$

with the Brunt-Väisälä frequency

$$N^2_{ad}\left(\mu\right) = \frac{g\delta}{H_p}\left[\frac{\varphi}{\delta}\nabla_\mu + \nabla_{ad} - \nabla\right] \tag{5.33}$$

First discussion about D

At this stage several important remarks can be made on the diffusion coefficient in the form (5.30) or (5.32).

1. We firstly notice that the leading term in D is $K(dU/dz)^2/N^2_{ad}(\mu)$ which is similar to what was found in previous works on shear mixing (cf. Zahn 1992; Maeder & Meynet 1996).

2. In a semiconvective zone, the thermal term $-4(\nabla' - \nabla)$ is positive and thus it adds its effect to that of the shear, both contributing to chemical transport. Oppositely, in a radiative zone, the term $-4(\nabla' - \nabla)$ is negative and thus, in order to produce mixing, the shear has to overcome the thermal stable gradient. We shall see below (cf. §6) that the coupling with thermal transport may somehow smooth this term.

3. In the limiting case $(\frac{dU}{dz}) \longrightarrow 0$ in a semiconvective zone, we are left with

$$D = \frac{4K\left(\nabla - \nabla'\right)}{\left(\frac{\varphi}{\delta}\nabla_\mu + \nabla_{ad} - \nabla\right)} \tag{5.34}$$

It is most remarkable that this value of D is the same as the diffusion coefficient D obtained for semiconvective mixing! In the Appendices A and B we derive, in two different ways, the diffusion coefficient D (cf. also Langer et al. 1983) and we find a result identical to expression 5.34, apart from a minor difference in the numerical factor in front of the expression. (In Appendix B we obtain $\frac{\pi^2}{2} = 4.93$ instead of 4 in 5.34, this minor difference resulting from slightly different geometrical approaches.)

This noticeable correspondence is easily understandable, since Kippenhahn's velocity v_μ expresses the motion due to radiative losses (proportional to $(\nabla - \nabla')$), for a cell having some μ-excess in a medium with variable μ. The semiconvective velocity also results from radiative losses depending on $(\nabla - \nabla')$ for a cell oscillating in a medium of variable μ. In both cases it is the same physical process (i.e. the heat loss) which is responsible for the motion, although in Appendices A and B one considers an oscillating fluid element, while expression 5.34 was derived for just a sinking element. Thus we understand why the results are similar, apart from a small difference in the numerical factors.

4. Let us consider a radiative zone, i.e. a zone with $\nabla' > \nabla$ and let us examine the diffusion coefficient in the form 5.30. The second term on the right, i.e. $-4(\nabla' - \nabla)/(\frac{\varphi}{\delta}\nabla_\mu + \nabla_{ad} - \nabla)$, is negative. Thus, if D is to be positive and thus mixing to occur we must have for $\alpha = 1$

$$\frac{1}{4}\left(\frac{dU}{dz}\right)^2 > \frac{g\delta}{H_p}\left(\nabla' - \nabla\right) \tag{5.35}$$

This is merely the Richardson criterion, without taking the μ-gradient into account. Thus we see that mixing starts as soon as the shear energy is sufficient to overcome the stable T-gradient. It is then not necessary to have

$$\frac{1}{4}\left(\frac{dU}{dz}\right)^2 > \frac{g\varphi}{H_p}\nabla_\mu \tag{5.36}$$

as assumed in previous works. Thus, our working hypothesis that part or all of the shear energy is used to modify the entropy gradient implies more specifically that the shear mixing will start modifying the μ-gradient as soon as thermal stability can be overpassed, as expressed by 5.35.

We may remark that the previous treatments (cf. Zahn 1992; Maeder and Meynet 1992) and the one presented here both imply the validity of the Richardson criterion. However, while previous treatments included the term containing ∇_μ in the Richardson criterion, the present developments are different.

5. We may also shortly consider the limiting case $\Gamma = 0$, which is the limit for $K \longrightarrow \infty$, i.e. very large radiation losses. This leads from (5.31) to $\nabla' = \nabla$, i.e. a situation where the internal and external gradients are the same. The diffusion coefficient D becomes

$$D = \frac{\alpha K}{N^2_{ad}(\mu)}\left(\frac{dU}{dz}\right)^2 \tag{5.37}$$

which for an homogeneous medium is similar to the expression by Zahn (1992). We see the great importance of the value of Γ, which may considerably change the diffusion process (see Sect. 6 and Appendices A and B).

6. Coupling the shear mixing and thermal transport

The expression of the diffusion coefficient in the form (5.30) or (5.32) is incomplete because it contains Γ and ∇ which are unspecified and which in turn depend on the diffusion coefficient. Indeed, we have the following system of three coupled equations with three unknown quantities D, Γ and ∇:

$$D = \frac{\alpha K\left(\frac{dU}{dz}\right)^2 H_p}{g\delta\left(\frac{\varphi}{\delta}\nabla_\mu + \nabla_{ad} - \nabla\right)} - \frac{4\Gamma}{\Gamma+1}\,\frac{K\left(\nabla_{ad} - \nabla\right)}{\left(\frac{\varphi}{\delta}\nabla_\mu + \nabla_{ad} - \nabla\right)} \tag{5.32}$$

$$D = 2K\Gamma \tag{6.38}$$

$$\nabla = \frac{\nabla_{rad} + \left(\frac{6\Gamma^2}{1+\Gamma}\right)\nabla_{ad}}{1 + \left(\frac{6\Gamma^2}{1+\Gamma}\right)} \tag{6.39}$$

Expression (6.38) results from the definitions of D and Γ, while (6.39) results from the effects of the shear mixing on the thermal transport. Relation 6.39 was derived by expressing that the total heat transport is the sum of the radiative transfer and of the heat released by the turbulent fluid elements due to shear instabilities (cf. Maeder 1995b). It was indeed implicitely assumed that the energy necessary for the mixing is provided by the rotational energy. Of course, the shear energy will then decrease and this is consistently expressed by the equation for the transport of angular momentum (Zahn 1992). This procedure is perfectly correct in radiative shear zones. In semiconvective shear zones, however, some of the energy necessary to transport the elements could be taken at the expense of the total luminosity. Thus, in semiconvective shear zones the coupling expressed by (6.39) formally applies if the semiconvective energy is small with respect to rotational energy. For current models of rotating stars (cf. Paper I, Meynet and Maeder 1997), this condition is satisfied by several orders of magnitude. We may also note that the change of luminosity due to the transport is generally ignored in semiconvective zones (cf. Langer et al. 1985 and private communication).

The efficiency factor in (6.38) is the same as that in (5.32) and (6.39), because we consider that the velocities and sizes of the turbulent eddies, which contribute mostly to the matter transport, are the same which also contribute mostly to the thermal transport. This is quite consistent with the above assumption that the motions with velocity v_μ are determined by the thermal losses of turbulent eddies.

The interactions expressed by this system of three Eqs. (5.32, 6.38, 6.39) are rather complex. Let us take an example. A low value of Γ will of course heavily reduce the diffusion coefficient given by (6.38), but simultaneously a low Γ will also reduce the factor $\frac{\Gamma}{\Gamma+1}$ in (5.32), and thus for example in a radiative zone it will decrease the negative effect of the stable thermal gradient, thus favouring a larger D. Also, at the same time a low Γ would make $\nabla \longrightarrow \nabla_{rad}$, thus increasing the difference $(\nabla ad - \nabla)$ in expression (5.32) and favouring a smaller D. Thus the coupling of shear and thermal effects leads to several interesting interactions.

Let us now solve the above system of equations. We can eliminate D between (5.32) and (6.38) and ∇ by expression (6.39). Let us simplify the writing by calling

$$\nabla_u = \alpha \frac{H_p}{g\delta} \left(\frac{dU}{dz}\right)^2 \tag{6.40}$$

$$\nabla_m = \frac{\varphi}{\delta} \nabla_\mu \tag{6.41}$$

Thus we get

$$2\Gamma \left(\nabla_{ad} + \nabla_m \left(1 + \frac{6\Gamma^2}{1+\Gamma}\right) - \nabla_{rad}\right) = \nabla_u \left(1 + \frac{6\Gamma^2}{1+\Gamma}\right) - \frac{4\Gamma}{\Gamma+1} (\nabla_{ad} - \nabla_{rad}) \tag{6.42}$$

$$2\Gamma \left[(\nabla_{ad} - \nabla_{rad})(1+\Gamma) + 6\Gamma^2\nabla_m + \nabla_m (1+\Gamma)\right] = \nabla_u(1+\Gamma) + \nabla_u 6\Gamma^2 - 4\Gamma(\nabla_{ad} - \nabla_{rad}) \tag{6.43}$$

and finally

$$12\nabla_m\Gamma^3 + [2(\nabla_{ad} + \nabla_m - \nabla_{rad}) - 6\nabla_u]\Gamma^2 + [2(\nabla_{ad} + \nabla_m - \nabla_{rad}) + 4(\nabla_{ad} - \nabla_{rad}) - \nabla_u]\Gamma - \nabla_u = 0 \tag{6.44}$$

This is an equation of degree 3 in Γ. All coefficients are determined at any level in the star and it is easy to solve it numerically with appropriate routines from the NAG library. We have analysed expression (6.44) in detail and rather than discuss it with the Cardan formulae, we prefer to treat it as follows, because of its special form (see below). Let us define two parameters

$$p_u = \frac{\nabla_u}{\nabla_{ad} - \nabla_{rad}} \tag{6.45}$$

$$p_\mu = \frac{\nabla_m}{\nabla_{ad} - \nabla_{rad}} \tag{6.46}$$

Dividing expression (6.44) by $(\nabla_{ad} - \nabla_{rad})$, we can write it the following way:

$$12p_\mu\Gamma^3 + \left[2 + 2p_\mu - 6p_u\right]\Gamma^2 + \left[6 + 2p_\mu - p_u\right]\Gamma - p_u = 0 \tag{6.47}$$

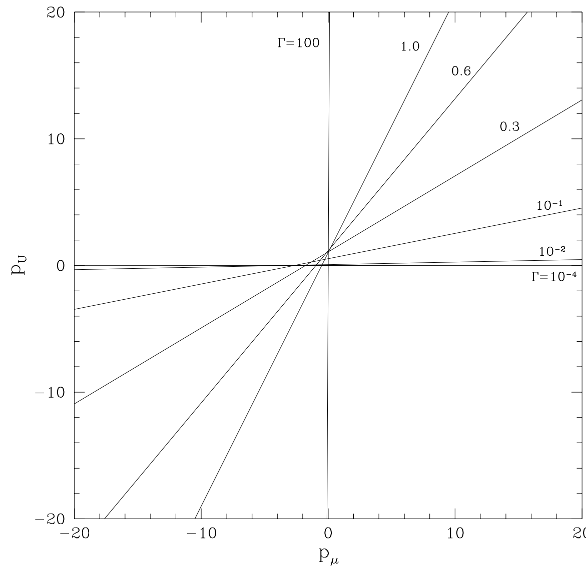

Fig. 2. The values of Γ as a function of p_u (shear parameter) and p_μ (chemical parameter). The straight lines are given by Eq. (6.49). The upper right corner concerns the radiative zone and the lower left corner the semiconvective zone.

We notice that Γ is a function of only two parameters p_u and p_μ. We also notice that since both ∇_u and ∇_m are positive, p_u and p_μ are always of the same sign, positive in a radiative zone and negative in a semiconvective zone. The general solution is of the form $\Gamma = \Gamma(p_u, p_\mu)$. Interestingly enough, since p_u and p_μ only appear linearly in the cubic (6.47), this means that for a given Γ we have a linear relation between p_u and p_μ. Relation (6.47) can therefore be written

$$p_\mu \left[12\Gamma^3 + 2\Gamma^2 + 2\Gamma\right] - p_u \left[6\Gamma^2 + \Gamma + 1\right] + 2\Gamma^2 + 6\Gamma = 0 \tag{6.48}$$

and thus

$$p_u = 2\Gamma p_\mu + \frac{2\Gamma^2 + 6\Gamma}{6\Gamma^2 + \Gamma + 1} \tag{6.49}$$

This is the equation of a straight in the plane p_u vs. p_μ; the slope and the ordinate at the origin are functions of Γ. Here we are only interested in real and positive roots for Γ, in view of its physical meaning.

Choosing a set of arbitrary real and positive Γ-values, we can easily represent graphically the relations between p_u and p_μ as a function of Γ. This way we obtain the iso-Γ lines in Fig. 2. For given p_u and p_μ values we can thus easily read the corresponding Γ-value. The application of the numerical solution from the NAG Library is in full agreement with the solutions of Fig. 2. We firstly notice that the real and positive Γ-values mainly (but not only, strictly speaking; see below) correspond to p_u and p_μ values in the upper right and lower left corners of Fig. 2. This is very much expected since the physically meaningful solutions

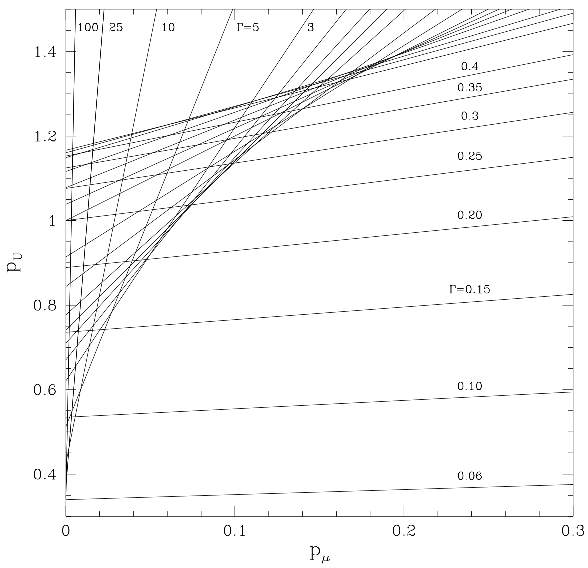

Fig. 3. Details of the region of Fig. 2 where multiple solutions of the cubic can occur. The value of Γ is indicated. Above $\Gamma = 0.4$ we have 0.5, 0.55, 0.6, 0.7, 0.8, 0.9, 1.0, 1.25, 1.5, 1.8, 2.0, 2.2 and 2.5.

for p_u and p_μ must be of the same signs. We also see that the solutions are in general unique, i.e. for given values of p_u and p_μ there is only one corresponding Γ value, except in a small region near the origin; this point will be discussed in Fig. 3 below.

7. Discussion of the solutions in radiative shear and semiconvective zones

Let us firstly turn to solutions in the upper right corner, which correspond to shears in a radiative zone with $\nabla_{ad} > \nabla_{rad}$. As shown by Fig. 2, in most of this quadrant, for any couple $(p_u,\, p_\mu)$ there is one unique real positive root Γ to Eq. (6.47). However, in a limited region near the origin multiple roots may occur. This situation results from the fact that the ordinate $p_u(0)$ at origin in the equation of the straight line (6.49) grows firstly with Γ, reaches a maximum $p_u(0)_{\rm max}$ for some finite value of Γ and then $p_u(0)$ goes down again for larger Γ values.
Indeed, the ordinate at origin

$$p_u(0) = \frac{2\Gamma^2 + 6\Gamma}{6\Gamma^2 + \Gamma + 1} \tag{7.50}$$

has a maximum for $\Gamma \simeq 0.483$ at $p_u(0)_{\rm max} = 1.167$. Then, for growing Γ values, the function $p_u(0)$ goes down, down to $p_u(0) = 1/3$ for $\Gamma \longrightarrow \infty$. Fig. 3 shows the details of the region where multiple solutions occur. It is a relatively small domain of the plane $(p_u,\, p_\mu)$ limited, as far as the upper right quadrant is concerned, by the vertical axis and two caustics. Along the vertical axis, the domain of multiple solution extends down to

$$\frac{2\Gamma^2 + 6\Gamma}{6\Gamma^2 + \Gamma + 1} = \frac{1}{3} \tag{7.51}$$

i.e. down to $\Gamma = 1/17 = 0.059$. This means that for lower Γ values there is no multiple solution and, as mentioned above, most real cases correspond to very small Γ, much smaller than 1/17. However, in the domain of multiple solution, some ambiguity could possibly arise in some cases. We consider that the physically meaningful solutions should be those with

$$\left(\frac{\partial\Gamma}{\partial p_u}\right)_{p_m} > 0 \tag{7.52}$$

i.e. those solutions implying a growing coefficient D for a growing shear. This means that in the domain of intersections the solution with $\Gamma > 0.483$ should be disregarded. Such solutions would correspond to extreme diffusion coefficients for low shears and they are very likely unphysical. On the contrary, for $\Gamma < 0.483$ the behaviour of the solutions are quite regular and continuous both inside and outside the domain of multiple solutions, as shown by Figs. 2 and 3.
For weak shears in radiative and semiconvective zones (i.e. for small p_u and Γ values, cf. Fig. 2) we can take the following simple approximation for the cubic (6.47).

$$\left(6 + 2p_\mu - p_u\right)\Gamma - p_u \simeq 0 \tag{7.53}$$

and thus

$$\Gamma \simeq \frac{p_u}{6 + 2p_\mu - p_u} \simeq \frac{1}{2}\,\frac{p_u}{3 + p_\mu} \tag{7.54}$$

for $\Gamma << 1$. We can now write the diffusion coefficient D as follows

$$D = K\,\frac{\frac{\alpha H_p}{g\delta}\left(\frac{dU}{dz}\right)^2}{3\left(\nabla_{ad} - \nabla_{rad} + \frac{\varphi}{\delta}\nabla_\mu\right) - \frac{\varphi}{\delta}\nabla_\mu} \tag{7.55}$$

In models of rotating stars, Γ covers a broad range of values and it is preferable to solve the general Eq. (6.47). For larger values of p_u there is a rapid growth of Γ as illustrated by Fig. 2.
We notice that the cubic (6.47) also has some solutions in the upper left corner, i.e. in a region where p_u and p_μ have a different sign. These solutions may apply to cases where we have an inverse μ gradient and where a Rayleigh-Taylor instability may occur, with a shear superimposed.
The solutions for shears in a semiconvective zone are located in the lower left quadrant of Fig. 2, since we have $\nabla_{rad} - \nabla_{ad} > 0$, both p_u and p_μ being negative. Moreover, for semiconvection we also have

$$\nabla_{ad} - \nabla_{rad} + \frac{\varphi}{\delta}\nabla_\mu > 0$$

$$\text{i.e.} \qquad 1 + p_\mu < 0$$

$$\text{or} \qquad p_\mu < -1 \tag{7.56}$$

Thus, in the lower left quadrant only the part to the left of $p_\mu = -1$ corresponds to semiconvection (the part between $p_\mu = -1$ and 0 would correspond to convection in presence of a μ gradient). The solutions for mixing in semiconvective shear zones are also provided by Eq. (6.47). The diffusion coefficient in a semiconvective zone in the absence of shears is rediscussed in Appendices A and B below, which show large differences with respect to current expressions by Langer et al. (1983).

8. Conclusions

The main idea of this work is to consider that diffusion in semiconvective shear zones results from the motions of fluid elements which possess an excess of μ as large as permitted by the excess energy in the shears.

Since the necessary energy comes from the shear, the shear has to be decreased accordingly. This feedback is expressed by the equation governing the conservation of angular momentum. However, the shear at some location in lagrangian coordinates is continually resplenished in energy by the regular growth of the central concentration due to stellar evolution. All these various effects have to be combined in a consistent way. This will be done in future models. For now, it is very gratifying that the first calculations with the coefficient D obtained in this work show some He- and N-enrichments in fast rotating massive O-stars, as suggested by observations.

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Appendix A: on the coefficient for semiconvective diffusion by Langer et al.

The derivation of a diffusion coefficient D for semiconvection by Langer et al. (1983) was a major step forward in the treatment of semiconvective regions (cf. also Langer 1991, 1992; Langer et al. 1985). There are, however, several further clarifications needed.

A.1. Missing factor

The derivation by Langer et al. was based on the dispersion relation by Kato (1966; cf. also Shibahashi and Osaki 1966) for the first order perturbations of the basic equations of conservation. The perturbations are of the form

$$\delta f \sim e^{\mathrm{ikx} + \mathrm{st}} \tag{A1}$$

Langer et al. express the coefficient D as

$$D = \frac{1}{3}\, v_{eff}\, \ell_{mix} \tag{A2}$$

with $v_{eff} = \ell_{mix} \cdot s_r$, where s_r is the real part of s, the angular frequency in Eq. A1. Langer et al. obtain

$$D = \frac{\alpha s_r}{3k^2} = \frac{\alpha K}{6} \left(\frac{\nabla - \nabla_{ad}}{\nabla_{ad} - \nabla + \frac{\varphi}{\delta}\nabla_\mu} \right) \tag{A3}$$

where α is a numerical factor $\alpha \leq 1$. Indeed, we should rather have

$$v_{eff} = \frac{\ell_{mix} \cdot s_r}{2\pi} \quad \text{and} \quad \ell_{mix} = \frac{2\pi}{k} \tag{A4}$$

in view of the definitions in (A1). Thus we would obtain

$$D = \alpha \frac{2\pi s_r}{3k^2} = \frac{\alpha \cdot 2\pi K}{6} \, \frac{(\nabla - \nabla_{ad})}{(\nabla_{ad} - \nabla + \frac{\varphi}{\delta}\nabla_\mu)} \tag{A5}$$

which differs from expression (A3) by a factor of 2π.

A.2. Problem concerning the order of magnitude

Various studies (Langer 1991; Langer et al. 1989) have shown that according to observations it is necessary to reduce the diffusion coefficient D (Eq. A3) by using a factor $\alpha = 0.01 - 0.04$. If we take into account the factor 2π seen above, this means that the true value given by the theory should be reduced by a factor of $\sim$ 150 to 620. Two or three orders of magnitude are too much to be an acceptable minor adjustment. This means that the derivation of D for semiconvection needs to be fundamentally revised. In particular, we show below that the coefficient D by Langer et al. (1983) is only an upper bound in the limit of adiabaticity.

A.3. Limiting cases for $\tau_{dyn}/\tau_h \longrightarrow 0$ or ∞

We recall that the solution by Langer et al. is not the general solution of the Kato dispersion relation, but only the solution for the limiting case where the ratio τ_{dyn}/τ_h of the dynamical to cooling times is negligible, which means a case very close to adiabaticity. As shown below, the assumption $(\tau_{dyn}/\tau_h) \longrightarrow 0$ leads to a large overestimate of the diffusion coefficient if the motion is not adiabatic.

Indeed, other solutions of the dispersion equation by Kato can be searched, for example for $(\tau_h/\tau_{dyn}) \longrightarrow 0$, which corresponds to very large heat losses. In this case it is easily deduced that the solution of the dispersion relation by Kato (1966) should be

$$s = \frac{-1}{\tau_h} + \frac{1}{\tau_h} \frac{k_H^2}{k^2} \frac{4 - 3\beta}{\beta} \left[\nabla_{ad} - \nabla\right] \frac{\tau_h}{\tau_{dyn}} \tag{A6}$$

a solution which is completely different from that by Langer et al. Solution (A6) means that the various perturbations are exponentially decreasing at a fast rate since $1/\tau_h$ is very large. The motion velocity, which is a first order term, decreases at the same rate, and the diffusion coefficient is thus quite small.

We see that the results for D are highly depending on the degree of adiabaticity assumed. In that respect the adiabatic solution by Langer et al. is only an upper bound for semiconvection (which is essentially a non-adiabatic process).

A.4. A solution without the assumption of adiabaticity

The equation expressing the change of the temperature excess of a fluid element as a result of its motions and heat losses was derived by Kippenhahn (1969, 1974). A similar equation was derived by Kato (1966; Eq. 7).

$$\frac{\partial}{\partial t} \left(\frac{DT}{T} \right) = \frac{v_\mu}{H_p} \left(\nabla - \nabla_{ad}\right) - \frac{DT}{\tau_{adj} T} \tag{A7}$$

We do not assume adiabaticity, but on the contrary we assume that the motions are only due to heat losses. As shown by Kippenhahn, we may consider that the motion occurs through a succession of equilibrium states, and we obtain for $Pe \ll 1$

$$v_\mu = \frac{-H_p}{\left(\frac{\varphi}{\delta}\nabla_\mu - \nabla + \nabla_{ad}\right) \tau_{adj}} \quad \frac{DT}{T} \tag{A8}$$

The temperature difference between the moving eddy and the medium can be written quite generally for non adiabatic motions

$$\frac{DT}{T} = -\left(\nabla' - \nabla\right)\, \frac{\Delta r}{H_p} \tag{A9}$$

The diffusion coefficient $D = \frac{1}{3}|v_\mu|\Delta r$ becomes, with the above expressions and the assumption $\Delta r^2/d^2 = 1$

$$D = \frac{-4K\,\left(\nabla' - \nabla\right)}{\left(\frac{\varphi}{\delta}\nabla_\mu - \nabla + \nabla_{ad}\right)} \tag{A10}$$

Using (5.31), we finally get

$$D = \frac{4\Gamma}{\Gamma + 1}\quad \frac{-K\,(\nabla_{ad} - \nabla)}{\left(\frac{\varphi}{\delta}\nabla_\mu - \nabla + \nabla_{ad}\right)} \tag{A11}$$

This is just the second term in expressions 5.30 and 5.32.
In the limit of adiabaticity $\Gamma \longrightarrow \infty$, and D becomes

$$D = \frac{-4K\,(\nabla_{ad} - \nabla)}{\left(\frac{\varphi}{\delta}\nabla_\mu - \nabla + \nabla_{ad}\right)} \tag{A12}$$

a coefficient D which has the same functional dependences as that by Langer et al. (1983). Expression A11 is the same as that derived in Appendix B below. In the limit of extreme heat losses, one has $\Gamma \longrightarrow 0$ and D becomes zero. Expression A11 for the semiconvection diffusion coefficient is not restricted to the limiting case of adiabaticity as that by Langer. It is much more general, the term $\frac{\Gamma}{\Gamma+1}$ allows us to introduce the degree of adiabaticity in the solutions. Depending on the value of $\frac{\Gamma}{\Gamma+1}$, the coefficient A11 may differ by orders of magnitude from that obtained in the adiabatic limit, which may explain the numerical problems mentioned above.

Appendix B: derivation of the diffusion coefficient in the mixing-length framework

Here we make another derivation of the coefficient D for a semiconvective region. It is based on the mixing-length approach, which in this case has a certain advantage over the perturbation method. The method of perturbations, despite its intrinsic value, leads to equations which have tractable analytical solutions only in limiting cases, which are orders of magnitude away from observations as seen above.
In a semiconvective region one has

$$\nabla' < \nabla < \nabla' + \frac{\varphi}{\delta}\nabla_\mu \tag{B1}$$

where quantities with a prime refer to values interior to turbulent eddies. The energy lost by an eddy of size ℓ and surface A during a time Δt is

$$\Delta U = \frac{-4acT^3}{3\kappa\rho}\;\frac{\Delta t/2}{\ell/2}\;A\Delta t \tag{B2}$$

For subsonic motions with no changes of μ the corresponding density excess due to heat losses is

$$\Delta\rho = \frac{4acT^3\delta}{3\kappa\rho C_p}\;\frac{\Delta t/2}{T\,(\ell/2)}\;\frac{A}{V}\;\Delta t \tag{B3}$$

For a sphere the ratio A/V of surface to volume is $A/V = 6/\ell$. Expressing $\Delta T = T(\nabla - \nabla')\ell/H_p$, we get

$$\frac{\Delta\rho}{\rho} = \frac{6\delta K(\nabla - \nabla')\Delta t}{H_p\ell} \tag{B4}$$

where K is the thermal diffusivity. The excess of velocity gained after a time Δt is thus

$$\Delta v = \frac{6g\delta K(\nabla - \nabla')\Delta t^2}{H_P\ell} \tag{B5}$$

where average values over the time interval Δt are taken. What is to be taken for Δt? If we consider oscillatory motions around an equilibrium position, it seems reasonable to consider the motion at maximum deviation from the equilibrium position, i.e. after a quarter of the basic oscillatory period $2\pi/N$, where N is the Brunt-Väisälä frequency. Thus, one has $\Delta t^2 = \frac{\pi^2}{4}N^{-2}$, and Δv becomes

$$\Delta v = \frac{3\pi^2}{2}\;\frac{K(\nabla - \nabla')}{(\nabla_{ad} - \nabla + \frac{\varphi}{\delta}\nabla_\mu)\ell} \tag{B6}$$

The resulting diffusion coefficient

$$D = \frac{\pi^2}{2}\;\frac{K(\nabla - \nabla')}{(\nabla_{ad} - \nabla + \frac{\varphi}{\delta}\nabla_\mu)} \tag{B7}$$

and with expression (5.31) from Sect. 4

$$D = \frac{\pi^2}{2}\;\frac{\Gamma}{\Gamma + 1}\;\frac{(\nabla - \nabla_{ad})}{(\nabla_{ad} - \nabla + \frac{\varphi}{\delta}\nabla_\mu)} \tag{B8}$$

Apart from a minor difference in the numerical coefficient due to the fact that we consider here an oscillatory motion, this equation is the same as that found in Appendix A.4.

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