Comments on the thermohaline instability in accreting white dwarfs

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1 Introduction

The thermohaline instability, sometimes also called saltfinger instability, is a well-known instability in oceanography. A warm layer of saltwater on top of a cold body of freshwater may be dynamically stable, if the density of the saltwater is smaller than that of the freshwater because of its higher temperature. However, if an element of the saltwater is perturbed into the freshwater, it may lose its heat faster than its salt, leading to an increase in density and an exponentially increasing perturbation. This thermohaline instability leads to a complete mixing of the two fluids. Because this instability depends on the timescales of two diffusion processes, it is also sometimes called double-diffusive instability.

In the case of stars, the role of the salt is played by the molecular weight. A layer with higher molecular weight on top of a layer with smaller weight may be dynamically stable, but subject to a similar double-diffusive instability. Classical papers in the astrophysical context are Ulrich (1972) and Kippenhahn et al. (1980, =KRT80).

2 The instability in the picture of KRT80

The instability starts from a boundary layer separating the two layers, with higher molecular weight μ on top. A front of a molecular weight gradient expands into the homogenous region below, with decreasing velocity (proportional to the decreasing gradient), leaving behind a (nearly) homogenous layer. This can be described as a global mixing process for the average concentration $\bar{c}$ of heavy elements in a spherical shell Δr

$$\frac{d\bar{c}}{dt} \propto \frac{d\Delta r}{dt} \propto w \propto \bar{c} \tag{1}$$

with expansion velocity w and a solution of the nature $\bar{c} \propto \exp(-t/\tau_{th})$. This behavior is partly analogous to a diffusion process, where an inhomogenous mixture asymptotically approaches a homogenous state in the available volume.

KRT80 consequently define a diffusion coefficient D_{th}, written here in slightly different notation used by more recent papers

$$D_{th} = C_{th} \frac{4acT^3}{3c_p\kappa\rho^2} \left[\frac{-\nabla\mu}{\nabla_{ad} - \nabla}\right] = C_{th}\,\alpha\,\frac{1}{R_0} \tag{2}$$

with

$$\nabla = \left.\frac{\partial \ln T}{\partial \ln p}\right|_{star} \qquad \nabla_{ad} = \left.\frac{\partial \ln T}{\partial \ln p}\right|_{ad} \qquad \nabla\mu = \left.\frac{\partial \ln \mu}{\partial \ln p}\right|_{star} \tag{3}$$

and the thermal diffusivity α

$$\alpha = \frac{4acT^3}{3c_P\kappa\rho^2} \tag{4}$$

and the abbreviation

$$\frac{1}{R_0} = \left[\frac{-\nabla\mu}{\nabla_{ad} - \nabla}\right]. \tag{5}$$

The other symbols T, p, ρ, c_p have their usual thermodynamic meaning; κ is the absorption coefficient (cm2/g). We note that the above formulation assumes an ideal gas with (at least locally) constant

ionization. The more general approach (also discussed in KRT80) involves additional factors which ensure that only the gradient due to changing composition enters in $\nabla \mu$. C_{th} is a constant, which has the value 12 in KRT80. However, values more than two orders of magnitude larger have also been used in the literature.

From this diffusion coefficient KRT80 derive the timescale

$$\tau_{th} \approx \frac{L^2}{D_{th}}, \tag{6}$$

which depends on the geometrical size L of the involved regions. In their derivations and in the specific examples KRT80 treat this as a global mixing process involving sizeable fractions of the star. They never define or use any diffusion velocities, which could be applied locally like a molecular diffusion velocity. One could, however, derive an estimate of an average velocity related to this expansion process as

$$v_{th} = \frac{L}{\tau_{th}} = \frac{D_{th}}{L}. \tag{7}$$

Comparing this with the calculation of a local diffusion velocity as in Deal et al. (2013, =DDVV13) and earlier papers of this group

$$v_{th} = D_{th} \frac{\partial \ln c}{\partial r} = -\frac{D_{th}}{H_p} \frac{\partial \ln c}{\partial \ln p} \tag{8}$$

we can conclude that these estimates agree for a typical length scale (size of "blobs", mean free path),

$$L = \frac{H_p}{\partial \ln c / \partial \ln p} \tag{9}$$

which in our numerical example below means a length scale of the pressure scale height or larger.

The whole discussion in this section implies that the thermohaline instability is a one-time event, which leads from an unstable stratification to a homogenous mixture with a calculable timescale. One example, where this scenario might be applicable, is the impact of 0.03 M_{jup} object on a star discussed in Théado & Vauclair (2012).

3 Application of the thermohaline instability in DDVV13

We see several possible problems in the way the instability is applied and treated in Deal et al. (2013), and partially also in some earlier papers of this group.

3.1 Local vs. global mixing

As discussed above the thermohaline instability leads to a global mixing with no well-defined local diffusion velocity. Adding v_{th} acting on the bulk material and the molecular diffusion velocity v_{12}, which is a relative velocity between a heavy atom and the main bulk material, different for each species can be regarded as a technical trick to facilitate computations. It is, however, really meaningful only in the two limiting cases, where either of the two processes is negligible. The analogy with convection, where this method of combining "convective mixing" and diffusion is also sometimes used, is misleading: the mixing coefficient in the dynamically unstable convection zone is always orders of magnitude larger than any molecular diffusion, and it is zero outside the cvz (+ overshooting region). A combination of the two mixing processes therefore has never any practical importance.

3.2 Definition of the thermohaline diffusion coefficient

Wide variations of the thermohaline diffusion coefficients (e.g. by varying the constant C_{th} or other means) have been used in the literature. DDVV13 state that their coefficient is calibrated with numerical simulations by Traxler et al. (2011). However, the coefficient determined in that paper is a purely empirical fit without physical basis. Moreover, the simulations are carried out for Prandtl and Lewis numbers of ≈ 0.1, whereas in the astrophysical context (see below) these numbers are $\approx 10^{-7} - 10^{-8}$, requiring an extrapolation of a numerical fit over seven orders of magnitude. Although Traxler et al.

(2011) use a scaling law for the transfer to astrophysical conditions, this relies on the validity of the asymptotic behavior suggested by their results (Wachlin et al. 2011).

The thermohaline instability applies only in a region where $\nabla < \nabla_{ad} + \nabla_\mu$ (with $\nabla_\mu < 0$). This is the limit of dynamical instability in case of a negative μ gradient (the Ledoux criterion for convection), which would lead to very rapid mixing. The expression in brackets in eq. 2 ($= 1/R_0$) goes to the limit 1, when approaching this critical gradient. In stark contrast to this behavior, DDVV13 replace $1/R_0$ by an expression, which has a singularity at the limit of the dynamically stable region. This virtually assures an instability at the boundary for arbitrary small μ gradients and cannot be physically sound. We therefore use the KRT80 formulation in our numerical estimates.

3.3 Thermohaline instability as a continuous process

DDVV13 – and earlier papers by the same group as well as other authors – make a bold step from a one-time instability to a process continuous in space and time by combining the thermohaline instability with accretion and molecular diffusion. In addition to the issues discussed above, this introduces new questions about timescales, which we discuss below in our numerical example.

Table 1: Properties of G29-38

stellar parameters	
effective temperature [K]	11820 ± 100
surface gravity log g [cm/s^2]	8.40 ± 0.10
data at the bottom of the convection zone	
fractional depth $\log(M_{cvz}/M)$	-13.96
pressure [dyn/cm^2]	$8.43\,10^8$
density [g/cm^3]	$6.93\,10^{-5}$
temperature [K]	77040
pressure scale height H_p [cm]	$5\,10^4$
average charge of hydrogen Z_1	0.99
average charge of calcium Z_2	3.24
current abundance of calcium c_{cvz}	$2.63\,10^{-7}$
molecular diffusion coefficient D_{12} [cm^2/s]	4.027
molecular diffusion velocity v_{12} [cm/s]	$6.11\,10^{-3}$
molecular diffusion timescale [s]	$9.07\,10^6$
thermal diffusivity α [cm^2/s]	$7\,10^7$
Lewis number D_{12}/α	$5.75\,10^{-8}$
inverse Lewis number	$1.74\,10^7$

4 A numerical example

In the following, we adopt the scenario and the equations used in DDVV13, but replace the singularity in the diffusion coefficient with the, in our view, physically more meaningful definition of KRT80. We then have

$$D_{th} = C_{th}\,\alpha\left[\frac{-\nabla_\mu}{\nabla_{ad}-\nabla}\right] = C_{th}\,\alpha\,\frac{1}{R_0} \tag{10}$$

with $C_{th} = 12$. For a trace element with concentration $c \ll 1$, ideal gas equation of state and constant ionization it can be shown that

$$\frac{d\ln\mu}{d\ln p} = \left[\frac{A_2}{A_1} - \frac{Z_2+1}{Z_1+1}\right]\frac{dc}{d\ln p} \tag{11}$$

with A, Z the atomic masses and charges of element 1 and 2. The thermohaline diffusion coefficient then is

$$D_{th} = \frac{C_{th}\,\alpha}{\nabla_{ad}-\nabla}\left[\frac{A_2}{A_1} - \frac{Z_2+1}{Z_1+1}\right]\frac{dc}{d\ln p} \tag{12}$$

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and the diffusion velocity

$$v_{th} = D_{th} \frac{d\ln c}{dr} = \frac{D_{th}}{H_p} \frac{d\ln c}{d\ln p} = \frac{C_{th}\,\alpha}{H_p} \frac{1}{\nabla_{ad} - \nabla} \left[\frac{A_2}{A_1} - \frac{Z_2 + 1}{Z_1 + 1} \right] c \left(\frac{d\ln c}{d\ln p} \right)^2 . \tag{13}$$

Another quantity of interest is the timescale for the growth of the instability in the linear approximation (KRT80)

$$\tau_{growth} = \frac{L^2}{\alpha} \frac{\nabla_{ad} + \nabla_\mu - \nabla}{\nabla_\mu} \tag{14}$$

The molecular diffusion coefficient D_{12} and the velocity v_{12} are calculated as in Koester (2009).

The numerical example we use is the variable DA G29-38, with the parameters recently determined by Xu et al. (2013). The heavy element considered is Ca. Table 1 collects relevant data for the star as well as at the bottom of the convection zone (cvz). Our scenario is the following: the star starts with a homogenous pure hydrogen envelope. When accretion of calcium (taken as representative heavy element, because it is most often observed) from circumstellar matter starts, the abundance in the cvz (assumed to be homogeneous because of extremely rapid mixing) builds up until a steady state between accretion and diffusion below the cvz is reached. We assume that the current abundance of c_{cvz} is a steady state, since it has not changed since the detection of Ca in 1997.

With a vanishing μ gradient, eq. 2 predicts $D_{th} = 0$ everywhere, except direct at the border of the stability region, where it is undefined. This is an artifact of assuming an infinitely sharp transition, which does not exist in nature. We assume that convective overshoot, molecular diffusion, and possibly other processes (in this particular case e.g. the pulsations) lead to a transition region of width $\beta\,H_p$, where the concentration changes from c_{cvz} to zero. We evaluate the conditions for thermohaline instability in the middle of this transition region. We thus have

$$\frac{dc}{d\ln p} \longrightarrow \frac{c_{cvz}}{\beta} \tag{15}$$

For $\beta \approx 1$ (see eq. 9 above) and the low observed Ca abundances in white dwarfs, the μ gradient ∇_μ is thus extremely small and Schwarzschild and Ledoux limits practically agree. The difference $\nabla_{ad} - \nabla$ increases rapidly across the boundary to ≈ 0.2 in a small fraction of H_p and stays near or above this value throughout the hydrogen envelope. We use this value as representative for the transition region. Inserting the numbers from the model we find

$$v_{th} = 6.237\,10^6\, \frac{c_{cvz}}{\beta^2} \tag{16}$$

Whereas the molecular diffusion velocity is independent of c, since the concentration gradient term is always negligible compared to the gravitational settling terms, the "thermohaline diffusion velocity" approaches zero for the small abundances at the beginning of an accretion event. Even for an abundance of $c = 10^{-10}$ and $\beta \approx 1$, v_{th} is smaller than v_{12} by a factor of 9.

A similar conclusion can be reached from the excitation timescale in the linear approximation of the instability. For the same conditions as above we obtain

$$\tau_{growth} = 1.95\,10^9\,\mathrm{s} \tag{17}$$

more than a factor of 100 larger than the molecular diffusion timescale. Finally the simple but most important question is if a thermohaline instability could be excited. The condition is that R_0 should be smaller than the inverse Lewis number $1/Le$, since otherwise particles of the perturbation element could be exchanged with the surroundings more rapidly than heat. In the situation discussed above we find

$$R_0 = 2\,10^9 \gg 1/Le = 1.74\,10^7 . \tag{18}$$

The conclusion does not depend on the choice of the thickness of the transition region (β). As long as it is finite there will always be a regime in the beginning of the accretion process where the timescale for molecular diffusion is much shorter than for the build-up of a significant μ discontinuity.

We thus conclude that in the beginning of the accretion episode (molecular) diffusion equilibrium near the convective boundary is always reached before the thermohaline instability becomes significant. As a next step we have therefore assumed that

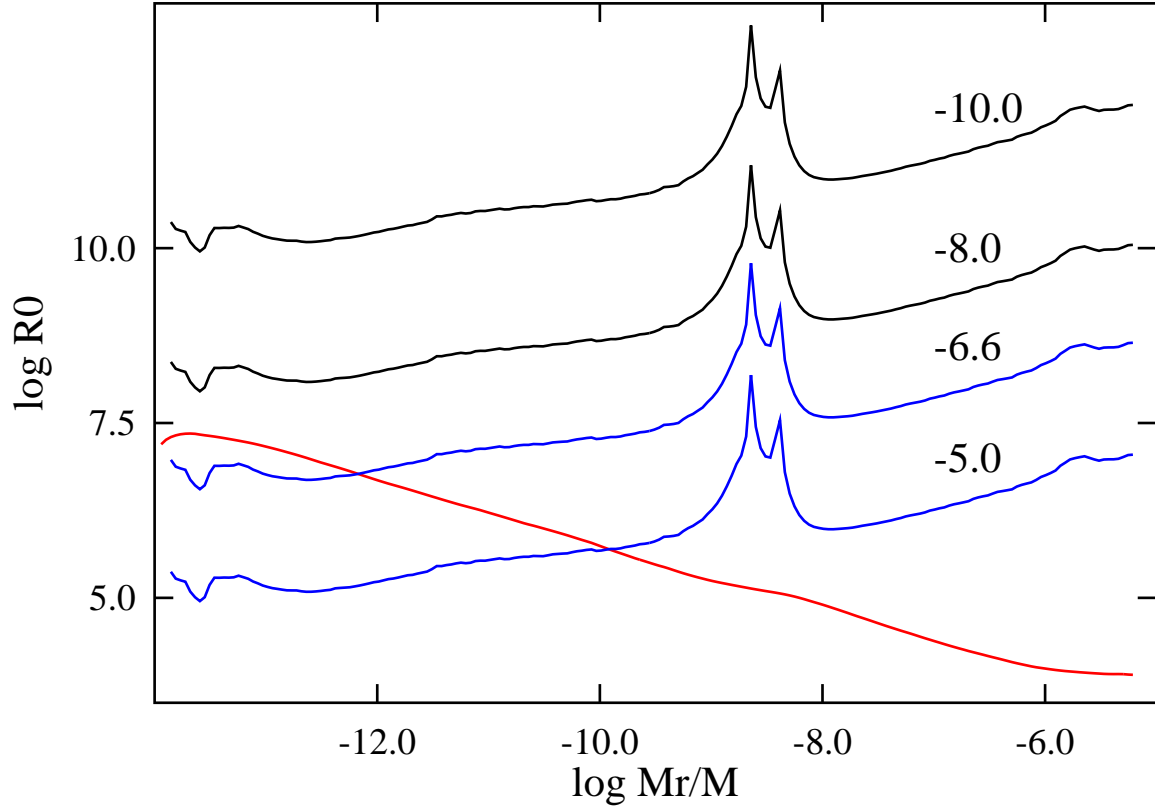$$\rho\,c\,v_{12} = \mathrm{const} \tag{19}$$

Figure 1: Variation of $\log(R_0)$ through the hydrogen envelope below the convection zone for different concentrations c (black, from top to bottom $\log(c_{cvz}) = -10.0, -8.0, -6.6, -5.0$) and comparison with the inverse Lewis number (red). The bumps near $\log M_r/M = -8.5$ (and similar in Fig. 2) are caused by a nearly constant c and near zero gradient in that region. The concentration $\log(c_{cvz}) = -6.6$ corresponds to the currently observed abundance in G29-38, -5.0 is the total heavy element abundance, one of the highest currently known in any DA
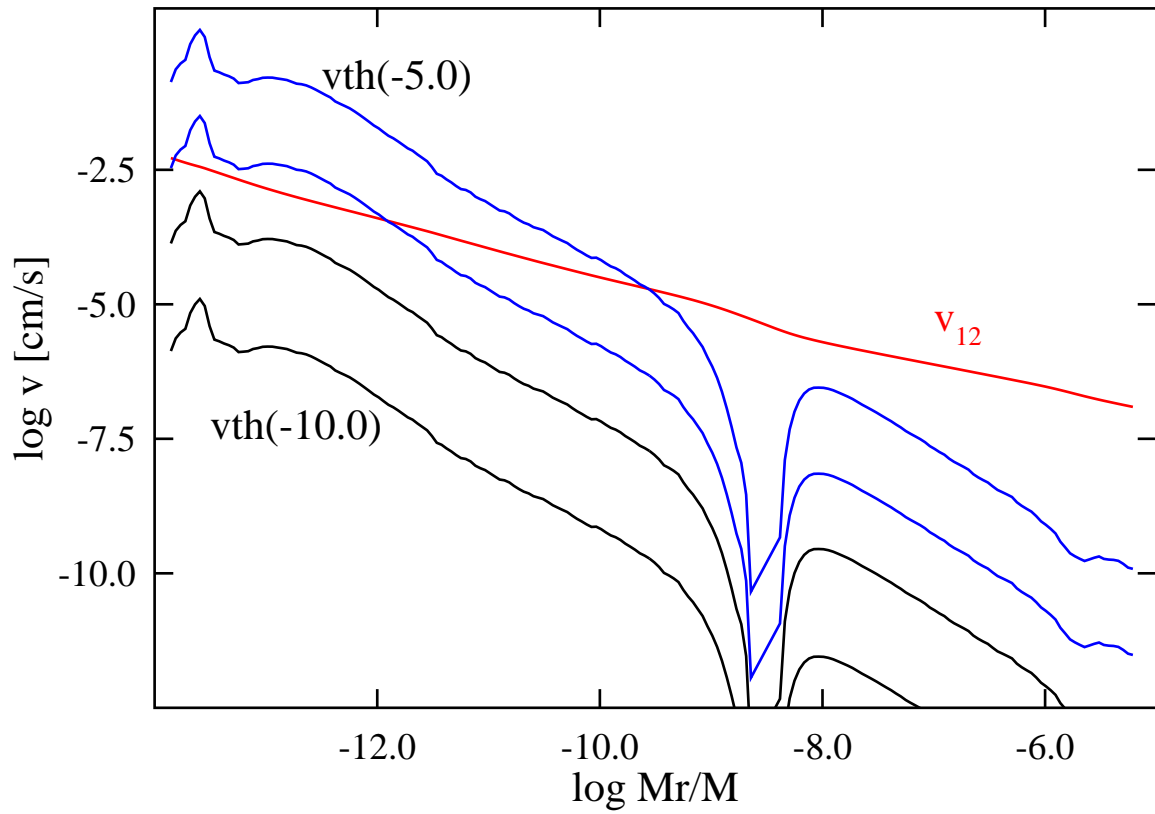
Figure 2: Variation of (logarithmic) diffusion velocities through the hydrogen envelope. Red: molecular diffusion; black: thermohaline diffusion for $\log(c_{cvz}) = -5.0, -6.6, -8.0, -10.0$ from top to bottom.
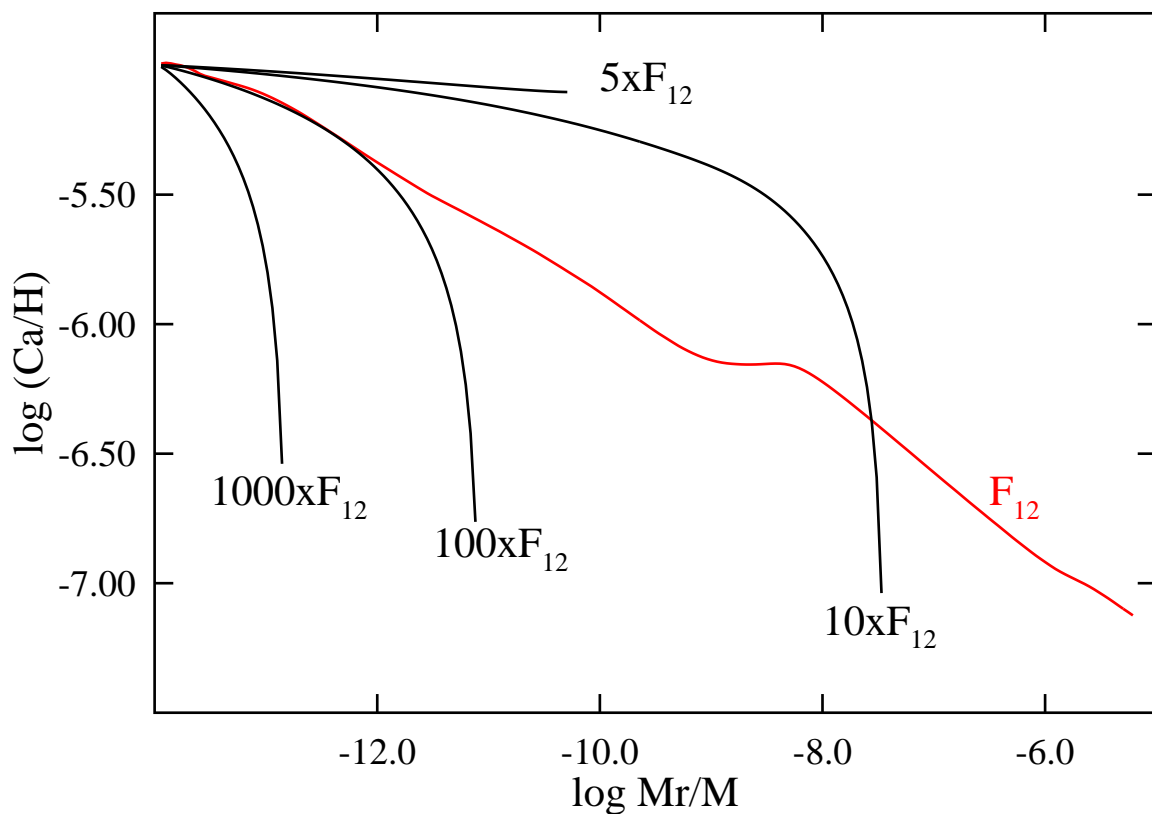
Figure 3: Steady state abundance stratification for molecular diffusion flux F_{12} alone (red), and for accretion fluxes 5 - 1000 times higher, at the same cvz abundance of -5.0. No steady state solution with thermohaline mixing exists throughout the hydrogen zone.
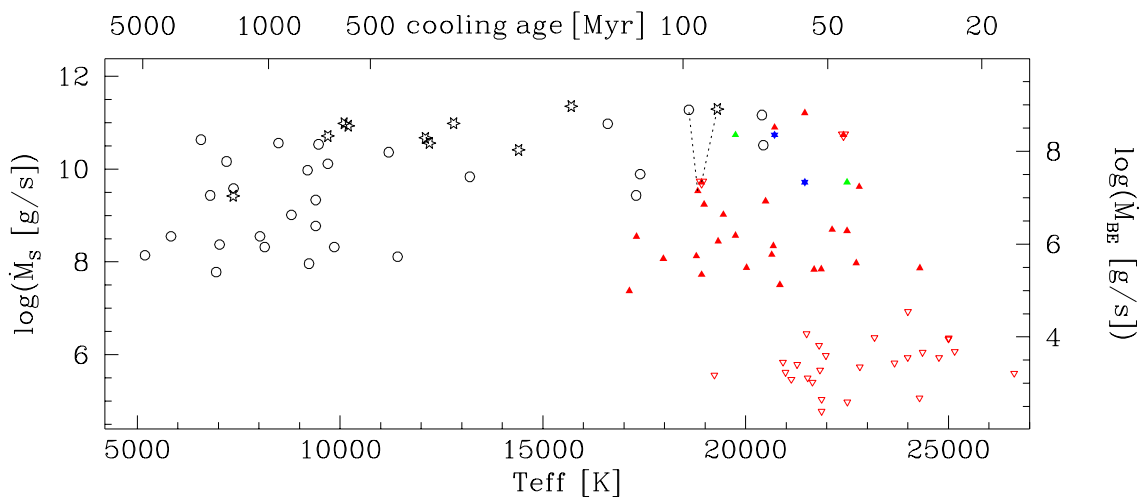

Figure 4: Total accretion fluxes for DAZ white dwarfs derived using the standard assumption of molecular diffusion. Note the constant range over a very large range of stellar parameters and observed Ca or Si abundances from 10^{-12} to $10^{-4.5}$. The open triangles in the lower right show Si supported by radiative levitation.

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and calculated the thermohaline velocities and timescales for the resulting c stratification. Figure 1 shows the results for the comparison of R_0 with the inverse Lewis number. For steady state abundances slightly smaller than the currently observed value for G29-38 – which is one of the largest observed Ca abundances – thermohaline diffusion does not occur anywhere in the hydrogen envelope. If we accept the use of the local combination of molecular and thermohaline diffusion we would conclude, that for the highest abundances a small effect just below the convection zone and affecting a fraction of $10^{-4.5}$ of the total hydrogen mass is possible. Since a thermohaline mixing velocity adds to the molecular diffusion velocity, the time needed to reach a stationary state at the bottom of the cvz for a given accretion flow is shorter than with molecular diffusion alone, and the equilibrium abundance in the cvz will be smaller.

5   No steady state solution possible with thermohaline mixing

A steady state solution (mass flux F of trace element constant over all layers and equal to the external accretion flux) is governed by the equation

$$\rho c \frac{A_2}{A_1} v = \rho \frac{A_2}{A_1} \left[\frac{C_{th}\,\alpha}{H_p} \frac{1}{\nabla_{ad} - \nabla} \left[\frac{A_2}{A_1} - \frac{Z_2 + 1}{Z_1 + 1} \right] \left(\frac{dc}{d\ln p} \right)^2 - \frac{D_{12}}{H_p} \left(\frac{dc}{d\ln p} \right) + v_{12}\, c \right] = F \qquad (20)$$

where the first term in the brackets is the thermohaline velocity, the second the molecular diffusion velocity from the concentration gradient (always negligible here), and the third the gravitational settling. This equation can be integrated using the abundance ($c(cvz)$) in the convection zone as starting value and the mass flux F as free parameter. $F = \rho v_{12} c A_2/A_1 = F_{12}$ with the quantities evaluated at the bottom of the cvz corresponds to the standard equilibrium solution, where the transport is by molecular diffusion alone (red curve in Fig. 3). We have also used larger values for the flux as claimed to be necessary by DDVV13. As one can already see from eq. 20, for $F \gg F_{12}$ the concentration gradient will get more negative for ever larger fluxes, inevitably leading to $c = 0$. For smaller F a few times F_{12} the solution for the gradient always becomes complex. **There exists no real stationary solution for $F > F_{12}$.** We conjecture that the consequence is that the abundance in the cvz will continue to rise until molecular diffusion can carry the whole flux and "standard" equilibrium is achieved. This can only be demonstrated by real numerical integrations like DDVV13, but continued to the final steady state.

6   Astrophysical support

Since there are many open question about the application of the thermohaline instability in the astrophysical context, several authors have tried to find support through the explanation of astrophysical phenomena like the stellar abundance pattern on the giant branches. This has met with only limited success (Cantiello & Langer 2010; Wachlin et al. 2011; Théado & Vauclair 2012), and often an increase of the mixing efficiency by large factors, or invoking additional mixing processes, is required to get agreement with observations.

DDVV13 emphasize prominently in abstract and conclusions that their calculations can explain the differences in the maximum accretion rates derived for DA and DB white dwarfs. There is, however, another plausible explanation. In the models for helium-rich DB stars, the bottom of the convection zone reaches mass densities between 1 and 1000 g/cm^3. This range includes the regime of pressure ionization in helium. In the equation of state we use (Saumon et al. 1995) this regime is not treated explicitly but bridged by a smooth interpolation. The quantity most important for the convection zone calculation is the adiabatic gradient, since the structure is almost exactly adiabatic throughout the zone. Numerical experiments show that because of the cumulative effect of the inward integration a very small change in the adiabatic gradient can change the mass in the cvz by one or two orders of magnitude. As is demonstrated by Fig. 23 in Saumon et al. (1995) the adiabatic gradient is significantly different between various EOS calculations. It can also show irregular behavior, which is probably not realistic but caused by the numerical calculation of the necessary second derivatives, if the EOS is determined by a Free Energy minimization method. As a consequence, absolute values of diffusion timescales and diffusion fluxes in cool DBs depend on the details of the EOS and may be quite uncertain. Fortunately, the relative

values for different elements, which are important for the determination of the chemical composition of the accreted material, are much less affected.

On the other hand, the large study of metal pollution in DA white dwarfs of Koester et al. (2014) provides an argument that the current use of molecular diffusion only for the derivation of accretion fluxes is correct. Fig. 4 demonstrates, that the range of derived accretion rates remains the same between $10^{5.5}$ to $10^{8.5}$ g/s over the whole observed range from T_{eff} 5000 to 25000 K. This range spans cooling times from 20 Myr to 2 Gyr, diffusion timescales from days to 100000 yr, from purely radiative envelopes to very deep convection zones, and observed Ca abundances for 10^{-12} to 10^{-6}. It is highly unlikely that such a consistent result would be achieved with the inclusion of a thermohaline mixing description as in DDVV13.

7   Conclusions

We do not doubt that the thermohaline instability may play an important role in astrophysics. Possible examples are the cases discussed in KRT80 with differences of the molecular weight of the order of 1, or catastrophic events like the sudden infall of a $0.03\,M_{jup}$ object on a star (Théado & Vauclair 2012). However, the validity of extending the instability to a continuous process, the mixing with molecular diffusion, and the extrapolation of mixing efficiencies over 7 orders of magnitude in Lewis numbers, is not obvious.

Concerning the accretion on white dwarfs, with a gradual build-up of heavy element abundances and μ differences of 10^{-6} or smaller, the situation is quite different. We respect the important work of DDVV13 (and earlier papers), which has brought back this almost forgotten effect and demonstrated the need of further discussions and study. We do not claim that we know the final answer to this problem. The aim of this study is to present an alternative view of this scenario; further studies, calculations, and discussions will be necessary to come to a conclusion. With our current state of knowledge and the estimates presented above, we think that thermohaline convection does not play an important role in accreting white dwarfs. Although we do not know the details of the DDVV13 calculations, it is plausible, that the different conclusions originate from their use of infinitely sharp transitions between regions with different molecular weights, and, most importantly, from their use of a singular (infinitely large) diffusion coefficient at the border of the dynamically stable region. This guaranties an instability for any finite μ difference, but is not physically realistic.

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