

The effects of element diffusion on the pulsational properties of variable DA white dwarf stars

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ABSTRACT

We explore the effects of element diffusion due to gravitational settling and thermal and chemical diffusion on the pulsational properties of DA white dwarfs. To this end, we employ an updated evolutionary code coupled with a pulsational, finite difference code for computing the linear, non-radial g-modes in the adiabatic approximation. We follow the evolution of a $0.55\text{-}M_{\odot}$ white dwarf model in a self-consistent way with the evolution of chemical abundance distribution as given by time-dependent diffusion processes. Results are compared with the standard treatment of diffusive equilibrium in the trace element approximation. Appreciable differences are found between the two employed treatments. We conclude that time-dependent element diffusion plays an important role in determining the whole oscillation pattern and the temporal derivative of the periods in DAV white dwarfs.

In addition, we discuss the plausibility of the standard description employed in accounting for diffusion in most white dwarf asteroseismological studies.

Key words: stars: evolution – stars: interiors – stars: oscillations – white dwarfs.

1 INTRODUCTION

Asteroseismology is a method used to extract information about the internal structure and evolution of stars by means of the study of their oscillatory pattern. This technique, which is very sophisticated in the case of the Sun, has also undergone a strong development in other stars, in particular the pulsating white dwarfs (WDs; for reviews, see, e.g., Brown & Gilliland 1994; Gautschy & Saio 1995, 1996).

Pulsating WDs show multiperiodic luminosity variations in three ranges of effective temperatures (T_{eff}) corresponding to the currently named DOV, DBV and DAV (see e.g. the reviews by Winget 1988 and Kepler & Bradley 1995). Of interest for this work are the DAVs (hydrogen-dominated atmospheres), or ZZ Ceti, which pulsate in the instability strip corresponding to $12\,500 \approx T_{\text{eff}} \approx 10\,700$ K. The periodicities in the light curves of pulsating WDs are naturally explained in terms of non-radial g-modes of low harmonic degree ($\ell \leq 2$), driven by the ‘ κ mechanism’ working in a partial ionization region near the stellar surface (Dolez & Vauclair 1981; Winget et al. 1982). Other physically plausible

mechanism for overstability of g-modes in ZZ Ceti stars is the ‘convective driving mechanism’ (see Brickhill 1991 and Goldreich & Wu 1999 for details). The periods (P) are found within a range of $100 \leq P \leq 1200$ s and photometric amplitudes reach up to 0.30 mag.

Asteroseismology of WDs has recently reached important success, supplying independent constraints to several structural quantities. As a few examples we mention the cases of DOV PG 1159–035 (Winget et al. 1991), DBV GD 358 (Bradley & Winget 1994), and the DAVs G117-B15A and R548 (Bradley 1996, 1998).

The main observable feature in WD pulsations is the period pattern, which can be accurately measured. Another important quantity is the temporal derivative of the period (\dot{P}), which allows one to measure the cooling time-scale of WDs and to provide constraints on the chemical composition of the core. In this sense, the star DAV G117-B15A is particularly noteworthy. Its observed periods are 215.2, 271 and 304.4 s. For the 215.2 s mode it has been possible to find its temporal derivative to be $\dot{P} = (2.3 \pm 1.4) \times 10^{-15} \text{ s s}^{-1}$ (Kepler et al. 2000).

As mentioned, one of the main purposes of asteroseismology of WDs is to disentangle the observed periodic signals in terms of the internal structure and the evolution of such objects. In view of the detailed available observations, it is very important to study the pulsational properties of DAVs in the frame of evolutionary models as physically sound as possible. In this regard, most of existing calculations treat the chemical profile at the hydrogen–helium interface (the most relevant one in the context of ZZ Ceti pulsations) on the basis of the equilibrium diffusion in the trace

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element approximation, hereafter the EDTE approximation, (Tassoul, Fontaine & Winget 1990, hereafter TFW; Bradley, Winget & Wood 1992; Bradley 1996; also see the Appendix). In the treatment used by these authors, the chemical profile may change solely as a result of changes in the state of ionization in the plasma (see the Appendix). Thus, if the compositional transition region occurs at thermodynamical conditions at which the plasma is fully ionized, then such a treatment predicts fixed profiles. However, even in the case of thick hydrogen envelopes (when both hydrogen and helium are completely ionized deep in the star), element diffusion modifies the chemical abundance distribution within the star, and this is true even during evolutionary stages corresponding to the ZZ Ceti domain (see Iben & MacDonald 1985, particularly their fig. 4).

It is the aim of this work to perform new pulsation calculations in DA WDs by relaxing both the trace element approximation and the diffusive equilibrium assumption. To this end, we carry out time-dependent diffusion calculations for a multicomponent plasma in a self-consistent way with stellar evolution. Detailed diffusion calculations consistent with stellar evolution have recently been performed by MacDonald, Hernanz & José (1998) to study the problem of carbon pollution in cool WDs, and by Althaus, Serenelli & Benvenuto (2001) to assess the role played by diffusion in the occurrence of hydrogen thermonuclear flashes in low-mass, helium-core WDs. In addition, Dehner & Kawaler (1995) have considered time-dependent diffusion in evolving, hot WDs in the interest of exploring the possibility of an evolutionary link between DO PG 1159 stars and the much cooler DB WDs. In the context of pulsations, the change in the chemical composition (particularly at the hydrogen–helium interface) induced by diffusion processes is expected to affect the shape of the Ledoux term B and hence the Brunt–Väisälä frequency (see Brassard et al. 1991 for a discussion of the calculation of the Brunt–Väisälä frequency in the context of WDs).

In order to gauge the actual importance of time-dependent diffusion in the computation of theoretical P and \dot{P} , we have to calculate the WD cooling using a full evolutionary code considering diffusion coupled to a pulsational code. To our knowledge, this is the first time that such a kind of calculation has been undertaken in the context of DA WDs. Note that in such a kind of treatment the internal chemical profile is the consequence of realistic evolutionary models. Here, we present calculations of linear, adiabatic, non-radial pulsations of DAV models with a mass of $0.55 M_{\odot}$ (which is representative of the mass of G117-B15A). In particular, we shall calculate two evolutionary sequences, one considering time-dependent element diffusion and the other in the frame of the standard EDTE approximation.

The remainder of this paper is organized as follows. In Section 2 we describe our evolutionary-pulsational computer code, paying special attention to the method for simulating the diffusion of elements in a time-dependent approach. Section 3 is devoted to presenting the calculations we performed. Finally, in Section 4 we discuss our results and make some concluding remarks.

2 OUR COMPUTER CODE

2.1 Evolutionary code and diffusion equations

The evolutionary code we employed is detailed in Althaus & Benvenuto (1997, 1998). This code is based on a very detailed and up-to-date physical description such as OPAL radiative (Iglesias & Rogers 1996) and molecular (Alexander & Ferguson 1994)

opacities. The equation of state is an updated version of that of Magni & Mazzitelli (1979). High-density conductive opacity and neutrino emission rates are taken from the works of Itoh and collaborators (see Althaus & Benvenuto 1997 for details). Also, a complete network of thermonuclear reaction rates corresponding to the proton-proton chain and the CNO bi-cycle is included. Nuclear reaction rates are from Caughlan & Fowler (1988) and electron screening is treated as in Wallace, Woosley & Weaver (1982).

Gravitational settling and chemical and thermal diffusion have been fully taken into account following the treatment for multicomponent gases presented by Burgers (1969). Thus, we avoid the trace element approximation usually invoked in most WD studies. Radiative levitation, which is important for determining photospheric composition of hot WDs (Fontaine & Michaud 1979), has been neglected.

As a result of gravity, partial pressure, thermal gradients and induced electric fields (we neglect stellar rotation and magnetic fields), the diffusion velocities in a multicomponent plasma satisfy the set of $N - 1$ independent linear equations (Burgers 1969)

$$\frac{dp_i}{dr} - \frac{\rho_i}{\rho} \frac{d\rho}{dr} - n_i Z_i e E = \sum_{j \neq i}^N K_{ij} (w_j - w_i) + \sum_{j \neq i}^N K_{ij} z_{ij} \frac{m_j r_i - m_i r_j}{m_i + m_j}, \quad (1)$$

and heat flow equation (N equations)

$$\begin{aligned} \frac{5}{2} n_i k_B \nabla T = & - \frac{5}{2} \sum_{j \neq i}^N K_{ij} z_{ij} \frac{m_j}{m_i + m_j} (w_j - w_i) - \frac{2}{5} K_{ii} z_{ii}'' r_i \\ & - \sum_{j \neq i}^N \frac{K_{ij}}{(m_i + m_j)^2} \left(3m_i^2 + m_j^2 z_{ij} + 0.8m_i m_j z_{ij}'' \right) r_i \\ & + \sum_{j \neq i}^N \frac{K_{ij} m_i m_j}{(m_i + m_j)^2} \left(3 + z_{ij} - 0.8z_{ij}'' \right) r_j. \end{aligned} \quad (2)$$

In these equations, p_i , ρ_i , n_i , Z_i and m_i means, respectively, the partial pressure, mass density, number density, mean charge and mass for species i (N means the number of ionic species plus electron). The quantities T and k_B are the temperature and Boltzmann constant. The unknown variables are the diffusion velocities with respect to the centre of mass, w_i , and the residual heat flows r_i (for ions and electrons). In addition the electric field E has to be determined. The resistance coefficients (K_{ij} , z_{ij} , z_{ij}'' and z_{ij}''') are from Paquette et al (1986).

The set of equations is completed by using the conditions for no net mass flow with respect to the centre of mass

$$\sum_i A_i n_i w_i = 0, \quad (3)$$

and no electrical current

$$\sum_i Z_i n_i w_i = 0. \quad (4)$$

In terms of the gradient in the number density we can transform equation (1) to

$$\begin{aligned} \frac{1}{n_i} \left[\sum_{j \neq i}^N K_{ij} (w_i - w_j) + \sum_{j \neq i}^N K_{ij} z_{ij} \frac{m_i r_j - m_j r_i}{m_i + m_j} \right] - Z_i e E \\ = \alpha_i - k_B T \frac{d \ln n_i}{dr}, \end{aligned} \quad (5)$$

where

$$\alpha_i = -A_i m_H g - k_B T \frac{d \ln T}{dr}, \quad (6)$$

where A_i , m_H and g are the atomic mass number, hydrogen atom mass and gravity, respectively. Let us write the unknowns w_i , r_i and E in terms of the gradient of ion densities in the form

$$w_i = w_i^{gt} - \sum_{ions(j)} \sigma_{ij} \frac{d \ln n_j}{dr}, \quad (7)$$

where w_i^{gt} means the velocity component due to gravitational settling and thermal diffusion. With equations (2) and (5) together with (3) and (4) we can easily find the components w_i^{gt} and σ_{ij} by matrix inversions (LU decomposition). The evolution of the abundance distribution throughout the star is found by solving the continuity equation. In particular, we follow the evolution of the isotopes ^1H , ^4He , ^{12}C , ^{14}N and ^{16}O . To calculate the dependence of the structure of our WD models on the evolving abundances self-consistently, the diffusion equations have been coupled to the evolutionary code.

2.2 The pulsational code

In order to compute the g-modes of the WD models, we have coupled our evolutionary code to our new, finite difference, pulsational code described in Córscico & Benvenuto (2002), which solves the equations for linear, adiabatic, non-radial pulsations (Unno et al. 1989).

We describe now how these codes work together. To begin with, an interval in P and T_{eff} (T_{eff} -strip) is chosen. The evolutionary code computes the model cooling until the hot edge of the T_{eff} -strip is reached. Then, the program calls the pulsation routine to begin the scan for modes. When a mode is found, the code generates an approximate solution which is iteratively improved to convergence and stored. This procedure is repeated until the period interval is covered. Then the evolutionary code generates the next stellar model and calls pulsation routines again. The previously stored modes are now taken as initial approximation to the modes of the new stellar model and iterated to convergence. Such a procedure is automatically repeated for all evolutionary models inside the T_{eff} -strip. The computational strategy described above has been successfully applied in fitting the observed periods of G117-B15A to impose constraints on the mass of axions (Córscico et al. 2001a) and in computing the period structure of low-mass, helium WDs (Córscico & Benvenuto 2002).

We have tested our pulsational code with two carbon-oxygen DA WD models of $0.5 M_{\odot}$ and $0.85 M_{\odot}$, the structure of which was computed with the WDEC evolutionary code. The vibrational properties of such models were previously analysed by Bradley (1996). In the interests of a detailed comparison, we have considered a large amount of modes and we found that the differences between the two sets of modes remain below ≈ 0.1 per cent.

3 COMPUTATIONS

We have evolved a $0.55 M_{\odot}$ WD model with an internal carbon-oxygen chemical profile corresponding to that calculated by Salaris et al. (1997). Such a model has hydrogen and helium mass fractions of $M_{\text{H}}/M_* = 10^{-4}$ and $M_{\text{He}}/M_* = 10^{-2}$, respectively. These values are in good agreement with evolutionary predictions and

are also very similar to those found by Bradley (1998) for the case of G117-B15A. The internal chemical profile of our model is shown in Fig. 1. It is important to mention that at the bottom of the hydrogen envelope of our model, hydrogen and helium are fully ionized and this is so throughout the entire evolutionary stages we study in the present paper. Thus, the chemical abundance profile predicted by the trace element approach remains fixed during evolution. In computing radiative opacities, we have assumed $Z = 0$. We have treated convective transport in the frame of the ML3 version of the mixing length theory. The ML3 prescription, characterized by a high convective efficiency, assumes the mixing length to be two times the local pressure scaleheight (see Tassoul et al. 1990).

A realistic starting model for our evolutionary sequences was obtained by artificially brightening an initial WD configuration (see Benvenuto & Althaus 1998) up to $\log L/L_{\odot} = 2$. Such a procedure is known to produce an initial sequence of some unphysical models, but then relaxes to the correct cooling sequence (see Althaus & Benvenuto 2000 for further discussion) far before reaching the DAV instability strip. From then on element diffusion is incorporated. When the model reaches $T_{\text{eff}} = 14\,000$ K we start pulsational calculations. Specifically, we have calculated dipolar ($\ell = 1$) modes (which are usually encountered in ZZ Ceti light curves) with radial orders $k = 1, \dots, 21$, which cover a period interval of $100 \leq P \leq 1000$ s. Calculations are stopped at $T_{\text{eff}} = 10\,000$ K, thus, the T_{eff} -strip amply embraces the observed DAV instability strip. For the modes we have found to fulfil such conditions, we have computed periods and eigenfunctions. For computing the Brunt-Väisälä frequency, we have employed the appropriate prescription for degenerate models, given in Brassard et al. (1991). After period assessment we compute \dot{P} by numerical differentiation.

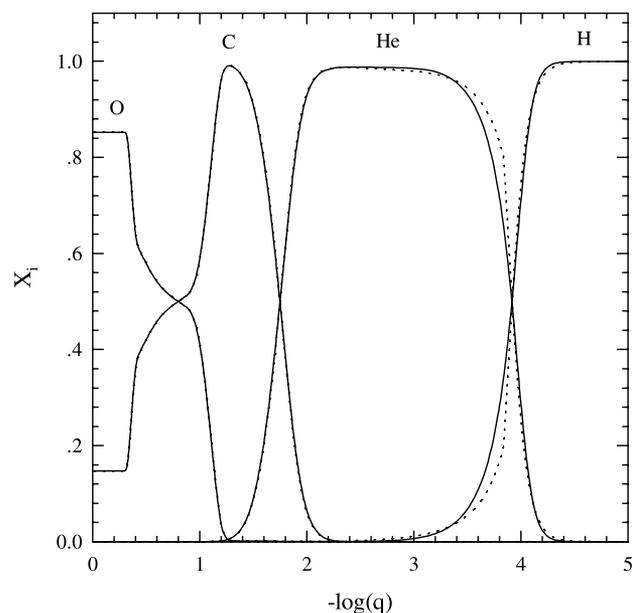


Figure 1. The internal chemical profiles of the $0.55 M_{\odot}$ carbon-oxygen WD model for hydrogen, helium, carbon and oxygen at an effective temperature of $14\,000$ K. In the case of the EDTE approximation, the fixed profiles are represented by dotted lines. Profiles for models in which time-dependent element diffusion has been considered are represented by solid lines. q is the outer mass fraction defined by $q = 1 - M_r/M_*$.

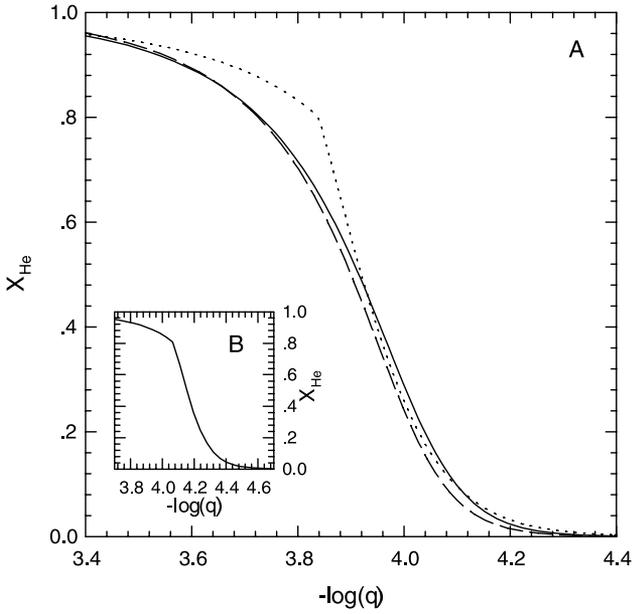


Figure 2. Panel A: the internal chemical profile for helium in terms of the outer mass fraction q at the hydrogen–helium interface. The solid line corresponds to a model at a temperature of 14 000 K in which time-dependent diffusion is considered. The long-dashed line means the same treatment but for a model at 10 000 K. Finally, the dotted line corresponds to the EDTE approximation prediction. Panel B: the chemical profile for helium as given by the EDTE approximation according to a $0.50\text{-}M_{\odot}$ model calculated by Bradley (private communication). Note that the shape of the profile in both models with diffusive equilibrium is the same.

4 RESULTS AND IMPLICATIONS

We begin by examining Fig. 2, in which we show the evolution of the chemical profile for helium resulting from time-dependent element diffusion together with the chemical profile arising from the EDTE approximation. Note that in the latter case, the profile remains unchanged throughout the evolution because, as we mentioned, ionization is complete at such deep layers.¹ By contrast, in the case with time-dependent diffusion, the chemical abundance distribution evolves appreciably during the ZZ Ceti evolutionary stages. Note that the shape of the profile in both treatments turns out to be markedly different, particularly at the centre of the transition. As we shall show below, this will have an appreciable influence on the P and \dot{P} values for some of the modes.

In Fig. 3, we depict the resulting Ledoux term (panel A) and the squared Brunt–Väisälä frequency (panel B) at two selected T_{eff} values. Let us remind the reader that the term B depends not only on the shape of the chemical profile but also on the thermal and mechanical structure of the star (see Brassard et al. 1991). Thus, even in the EDTE approach the term B changes with cooling. Because of the fact that the derivative of the chemical profile appears in the Ledoux term (see equation 35 of TFW), a slight change in the slope of the hydrogen–helium interface translates into a noticeable change in B . Thus, it is not surprising the B term exhibits a sharp peak in the case of the trace element treatment, in contrast to the more physical treatment as given by

¹ In the calculations presented here, the EDTE approximation has been applied only to the hydrogen–helium interface, which is the most relevant in the context of DA WD pulsations.

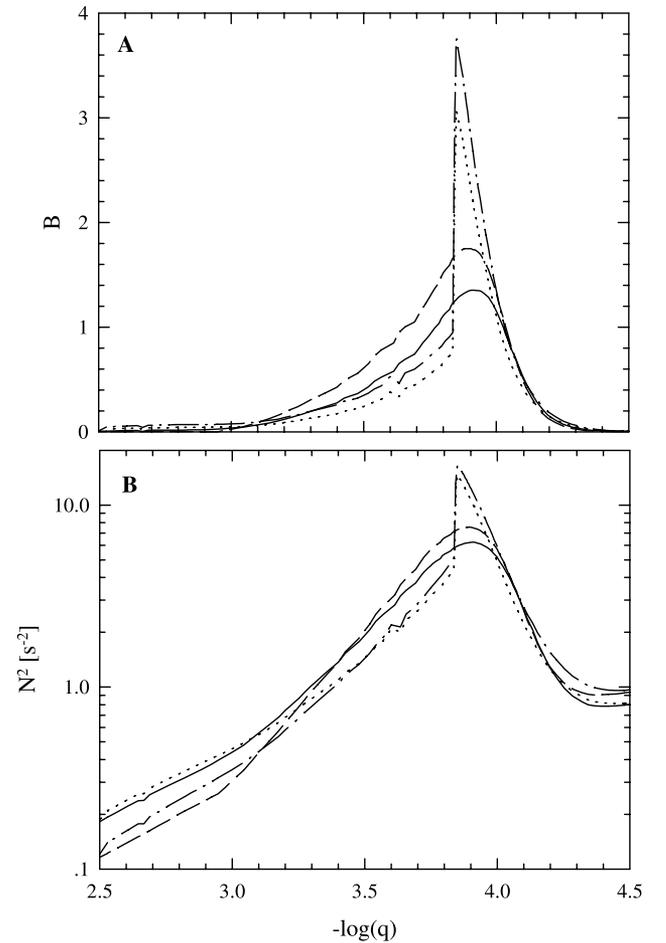


Figure 3. In the upper panel is shown the Ledoux term B at the hydrogen–helium interface in the case of time-dependent diffusion at the T_{eff} values of 14 000 and 10 000 K, given by solid and long-dashed lines, respectively. Dotted and dot-dashed lines correspond to the same temperature values but for the EDTE approximation. In the lower panel the square of the Brunt–Väisälä frequency is shown for the same cases analysed in panel A. For details, see text.

non-equilibrium diffusion. In turn, this feature is reflected in the Brunt–Väisälä frequency. As it has been exhaustively shown by Brassard et al. (1992a,b), the shape of the Brunt–Väisälä frequency at the chemical interfaces plays a key role in fixing the structure of the period pattern (e.g. mode trapping) of ZZ Ceti stars.

Now let us turn our attention to the computed pulsational modes. In Figs 4 and 5 we show P and \dot{P} corresponding to modes with $\ell = 1$, $k = 1, \dots, 6$ for models with time-dependent element diffusion and with the EDTE approximation at the hydrogen–helium interface as a function of T_{eff} . From a close inspection of these figures, it can be realized that the effects of time-dependent element diffusion are indeed non-negligible in P and \dot{P} , although for some modes the results are very similar. We want to mention that the same trend has been found in modes of higher radial order (not shown here for brevity). Note that for the modes analysed in these figures the greatest relative differences encountered are ≈ 20 per cent for \dot{P} and ≈ 5 per cent for P .

It is worth mentioning that the differences cited above arise mainly from the very different shape of the interface profile resulting from the two treatments of diffusion investigated here. In particular, the differences in the helium profile for $X_{\text{He}} \geq 0.5$ (see Fig. 2) in these treatments are the main reason why the periods and

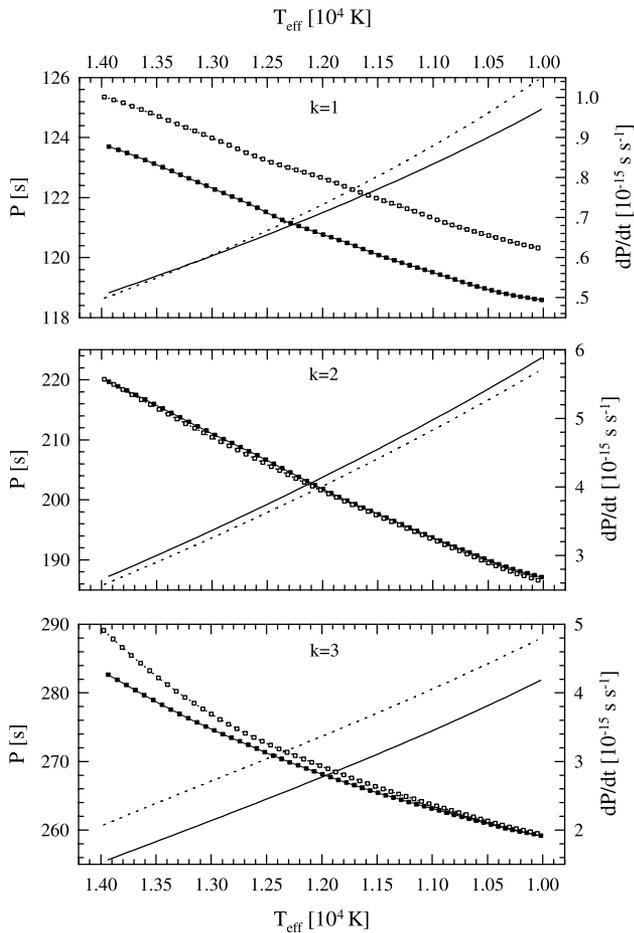


Figure 4. Period and period derivative for $\ell = 1$, $k = 1, 2, 3$ modes for a $0.55\text{-}M_{\odot}$ carbon–oxygen WD model in at a T_{eff} interval containing the DAV instability strip. Solid lines (filled squares) correspond to periods (period derivatives) computed considering equilibrium diffusion while dotted lines (empty squares) depict periods (period derivatives) computed according to the EDTE approximation at the hydrogen–helium interface. For discussion of the results, see text.

period derivatives become different. In addition, there is a small contribution to the differences in P and \dot{P} due to the evolution of the profiles of each chemical interface in response to non-equilibrium diffusion.

Thus, as models with time-dependent element diffusion are more physically plausible, these should be taken into account when an asteroseismological fit to observed periods is performed. Also, as \dot{P} is modified, this approach should also be taken into account when using observed \dot{P} values to infer the composition of the WD core.

Before closing the paper, we would like to discuss at some length a major issue raised by our referee. Indeed, in their report, our referee asked us to look for the underlying physical reasons for the differences between the standard treatment of EDTE approximation and our full treatment of time-dependent element diffusion. To be specific, the referee asked us whether such differences are due mostly to the relaxation of the trace element approximation or the equilibrium hypothesis.

In order to find the answer, we decided to perform a simple numerical experiment: we simulate the equilibrium diffusion conditions with our full code. Equilibrium diffusion would be a good approximation if the diffusion time-scale were much shorter

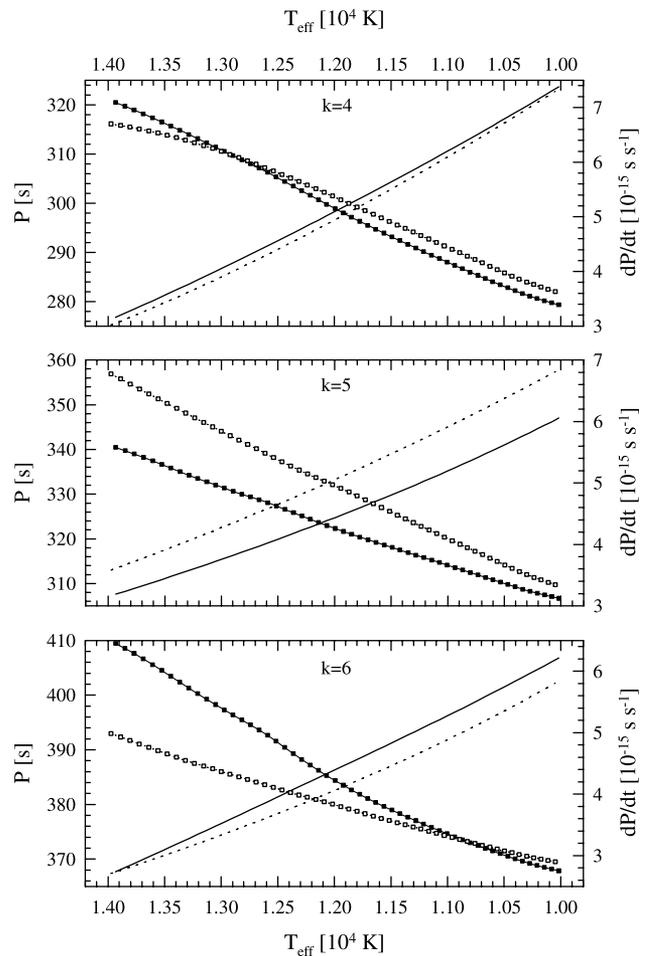


Figure 5. Same as Fig. 4, but for modes with $\ell = 1$, $k = 4, 5, 6$.

than the evolutionary one. Then, in order to simulate this situation, we simply assumed the diffusion time-step to be several times the evolutionary one.² This is equivalent to assuming that the whole diffusive process occurs several times faster. We computed the evolution of our WD model under this hypothesis. The result was that the WD *did not* evolve along the cooling branch, *but instead* suffered from a hydrogen thermonuclear flash. Physically, the reason for this behaviour is that if diffusion had plenty of time to evolve to equilibrium profiles, then the tail of the hydrogen profile would be able to reach hot enough layers to be ignited in a flash fashion. The fact that when equilibrium diffusion conditions are imposed the star undergoes a hydrogen thermonuclear flash, while in the detailed, self-consistent time-dependent diffusive treatment the star cools down quiescently, clearly shows the incorrectness of the hypothesis of equilibrium. In view of this, we are forced to conclude that there is no alternative other than to abandon the idea that the shape of the internal profiles in the WD is determined by equilibrium diffusion. This conclusion is valid at least for massive hydrogen envelopes. We think that the only physically sound way to compute such profiles, a key ingredient in asteroseismological studies, is to calculate the WD evolution in a self-consistent way with time-dependent element diffusion and nuclear burning.

In addition, some words are in order about the standard

² Here, because of numerical reasons, we assumed a diffusive time-step of 100 times the evolutionary one.

treatment of equilibrium diffusion, which is based on the work of Arcoragi & Fontaine (1980). Recent asteroseismological studies of DAV WDs (Clemens 1994; Bradley 1998, 2001) seem to favour large values for the thickness of the hydrogen envelope ($M_H/M_* \approx 10^{-4}$). At the thermodynamical conditions relevant to DAV WD models, we find that most of the hydrogen–helium interface occurs at degenerate conditions. Because the Arcoragi & Fontaine (1980) equations are valid for *non-degenerate* conditions, we should remark that this treatment cannot be applied to the modelling of the hydrogen–helium interfaces in DA WDs with massive hydrogen envelopes.

We should also remark that, in the case of the trace element approximation, we have found that the object does not undergo any thermonuclear flash. This is another artefact of the approximation, due to the ad hoc truncation of the profile at some low density (see the Appendix). Indeed, in our numerical experiments, we have found that the stellar model evolves along the WD cooling track if we truncate the hydrogen profile at $X_H = 10^{-3}$. However, if we allow the equilibrium hydrogen profile to extend to slightly lower abundances (e.g. $X_H = 10^{-4}$) the model experiences a thermonuclear flash!

The results presented in this paper indicate that a more extensive and systematic exploration of asteroseismology of DAV in the frame of detailed evolutionary models considering time-dependent element diffusion is worth being done, and it will be the subject of further papers. While the present paper was in process of reviewing, some interesting results about the effects of diffusion on mode trapping have been presented in Córscico et al. (2001b).

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APPENDIX A

For the sake of completeness, we describe here the equations employed to include diffusion processes in most of WD pulsational studies. This approximation is based on the work of Arcoragi & Fontaine (1980; see also Tassoul et al. 1990). Here we limit ourselves to comment on the most important aspects involved in this treatment.

To begin with, Arcoragi & Fontaine (1980) assume a stellar plasma made up of two-ionic species with average charges Z_1 and Z_2 and atomic weight A_1 and A_2 . In addition, thermal diffusion is neglected and an ideal gas equation of state is considered under the assumption that the plasma is sufficiently diluted. Under these approximations, the diffusion velocity w_{12} reads

$$w_{12} = D_{12}(1 + \gamma) \times \left[-\frac{\partial \ln c_2}{\partial r} + \frac{A_2 - A_1}{A_1 + \gamma A_2} \frac{\partial \ln p}{\partial r} + \frac{A_2 Z_1 - A_1 Z_2}{A_1 + \gamma A_2} \frac{eE}{k_B T} \right]. \quad (\text{A1})$$

D_{12} is the diffusion coefficient, and c_i , the number concentration of ions of species i , is defined by

$$c_i \equiv \frac{n_i}{n_1 + n_2} = \frac{p_i}{p_1 + p_2} \quad (\text{A2})$$

where p_i is the partial pressure. E is the electric field, given by

$$eE = m_p g \frac{A_1 Z_1 + A_2 Z_2 \gamma}{Z_1(Z_1 + 1) + Z_2(Z_2 + 1)\gamma}, \quad (\text{A3})$$

and γ is defined as

$$\gamma \equiv \frac{n_2}{n_1} = \frac{p_2}{p_1} = \frac{c_2}{c_1}. \quad (\text{A4})$$

The remainder of the symbols have the usual meaning. Notice that

equations (A2) and (A4) are valid in an isothermal medium, i.e. we are neglecting temperature gradients.

Now we impose equilibrium diffusion, by assuming $w_{12} = 0$, and from equations (A1)–(A4) we get the ordinary differential equation for the equilibrium profile (equation A5 of Arcoragi & Fontaine 1980). In the trace element approximation ($\gamma \ll 1$), for the species 2 considered as a trace, we get

$$\frac{\partial \ln c_2}{\partial r} = \alpha_2 \frac{\partial \ln q}{\partial r}, \quad (\text{A5})$$

where

$$\alpha_2 = \frac{A_2}{A_1}(1 + Z_1) - Z_2 - 1. \quad (\text{A6})$$

For the purpose of application, Tassoul et al. (1990) divide the transition zone into two parts: an upper one in which element 1 is dominant and element 2 is a trace, and a lower one in which the roles of the respective elements are reversed. For the upper region the abundance profile of element 2 considered as a trace is given by equation (A5) and for the lower part of the transition zone the abundance of element 1 (considered as a trace) is given by

$$\frac{\partial \ln c_1}{\partial r} = \alpha_1 \frac{\partial \ln q}{\partial r}, \quad (\text{A7})$$

where

$$\alpha_1 = \frac{A_1}{A_2}(1 + Z_2) - Z_1 - 1. \quad (\text{A8})$$

q is the mass fraction ($1 - M_r/M_*$). The integration of equations (A5) and (A7) gives the equilibrium abundance profiles:

$$c_2 = k_2 q^{\alpha_2} \quad (\text{upper region of interface}) \quad (\text{A9})$$

and

$$c_1 = k_1 q^{\alpha_1} \quad (\text{lower region of interface}) \quad (\text{A10})$$

By invoking the condition of continuity in the middle point of the interface, we obtain the relation

$$k_2 q_m^{\alpha_2} = k_1 q_m^{\alpha_1} = \frac{1}{2}, \quad (\text{A11})$$

where q_m is the mass fraction where the abundances of two species are equal; the q_m value is obtained by forcing the mass conservation of element 1. Thus, in the case of the hydrogen–helium transition region, the outer mass fraction of hydrogen ($q_{\text{H}} = M_{\text{H}}/M_*$) is employed for computing q_m . Note that possible changes in the equilibrium profiles result only from slight changes in the ionization states of the elements present at the interfaces, i.e. variations in the exponents α_1 and α_2 (Tassoul et al. 1990).

To implement this approach to the modelling of the hydrogen–helium transition zone, it is necessary to set small abundances to zero in order to avoid having a tail of hydrogen in regions deep enough where carbon is abundant (for this case we should generalize the above treatment for three species). Moreover, if we did not do this, hydrogen would be present at layers hot enough to force the star to undergo a thermonuclear flash. This is the case at least for thick hydrogen envelopes like those we have treated here, which in turn are the ones favoured by current asteroseismological studies (see the main text).

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