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Atomic diffusion in G and F type stars and its impact on the asteroseismic determinations of stellar parameters

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Abstract

Atomic diffusion, including the effect of radiative accelerations on individual elements, leads to variations of the chemical composition inside the stars as well as the surface abundances evolution. Indeed the accumulation in specific layers of the elements, which are the main contributors of the local opacity, modifies the internal stellar structure and surface abundances. Here we show that the variations of the chemical composition induced by atomic diffusion in G and F type stars can have significant impact on their structure, stellar parameters and seismic properties. We will also discuss the effect of the coupling between rotation and atomic diffusion for such stars. These processes need to be taken into account in stellar evolution models as the observations are more and more precise, especially in the context of the space missions TESS and PLATO.

1 Introduction

In the last two decades the number of large surveys of stars has considerably increases. We have now access to a large amount of spectroscopic, photometric and asteroseismic data. A lot of effort has been put to improve the way we treat the data and they are now very precise. To understand these observations, we need to confront them to stellar models. But stellar models are for now not precise and accurate enough to use the full potential of observation and this is the reason why a lot of effort is put to improve them. We are clearly at a time where a new generation of stellar model (beyond the standard physics) is needed.

One key problem to be resolved in this new generation of stellar models is the transport of chemical elements. As this transport is not present in the four equations of stellar evolution (namely the equation of mass conservation, energy conservation, Poisson's equation and the equation of momentum conservation) it is mandatory to provide a theory to take it into account. We can split transport processes in two types of precesses: the microscopic ones (i.e. atomic diffusion) and the macroscopic ones.

Atomic diffusion comes from the first principles of physics and is naturally present in stars due to the internal pressure, temperature and density gradients. This produces a selective transport, which can deplete or accumulate elements inside stars. This process is studied for a long time (Chapman, 1917; Eddington, 1926) and we have now a lot of evidences of its occurrence inside stars.

The first evidence of atomic diffusion was for the chemically peculiar stars for which radiative accelerations are able to reproduce the surface abundances when coupled to a macroscopic transport process (e.g. Praderie, 1967; Michaud, 1970; Watson, 1970, 1971; Turcotte *et al.*, 1998a; Richer *et al.*, 2000; Richard *et al.*, 2001). The helioseismology opened a new area of observations of the Sun, and it has been possible to show that atomic diffusion is needed in the solar models (e.g. Bahcall & Pinsonneault, 1992; Bahcall *et al.*, 1995; Christensen-Dalsgaard *et al.*, 1996; Richard *et al.*, 1996; Ciacio *et al.*, 1997; Gabriel, 1997; Morel, 1997; Brun *et al.*, 1998; Elliott, 1998; Turcotte *et al.*, 1998b). This effect is visible in the sound speed profile and also in the surface abundances which are 10% lower than the initial ones.

There are also evidence of atomic diffusion in the age determination of old globular cluster with isochrones computed including atomic diffusion. The age determined for M92 goes from 15 Gyr with atomic diffusion to 13.5 Gyr with atomic diffusion (VandenBerg *et al.*, 2002), which is in better agreement with the age of the Universe determined by the cosmology community. This difference in age is also found in the M5 globular cluster. The abundance trends in globular cluster show also the presence of atomic diffusion in stars (e.g. Korn *et al.*, 2007; Nordlander *et al.*, 2012; Gruyters *et al.*, 2013, 2014; Dotter *et al.*, 2017; Souto *et al.*, 2018).

But in all these cases atomic diffusion alone produces too large over or under-abundances compare to observations which is also an evidence that atomic diffusion does not occur alone. There is a need of taking macroscopic processes into account too (Talon *et al.*, 2006; Michaud *et al.*, 2004, 2011). We can also find this aspect in F-type star model in which helium is very quickly depleted (which is not observed) in the models if atomic diffusion is taken into account alone. This is then important to study macroscopic transport processes as for example the mixing induced by the rotation. This process is studied also for a long time (e.g. Zahn, 1992; Talon & Zahn, 1997) and we are now able to study the combine effect of rotation and atomic diffusion in a consistent way for example with the CESTAM evolution code (Marques *et al.*, 2013; Deal *et al.*, 2018).

Asteroseismology offers now the possibility to test such physics by probing the internal structure of stars with a high precision thanks to CoRoT, *Kepler* and in a more or less close future with TESS and PLATO. In the following sections we will show how seismology allows us to probe the effects of atomic diffusion and the mixing induced by rotation in solar-like oscillating main-sequence stars. The theory of atomic diffusion and rotation will be described and some study cases will be presented.

2 Theory

2.1 Diffusion velocity

Atomic diffusion is the result of internal pressure, temperature and density gradients. The diffusion velocity V_E of a trace element E can be expressed as shown Fig. 1. In this

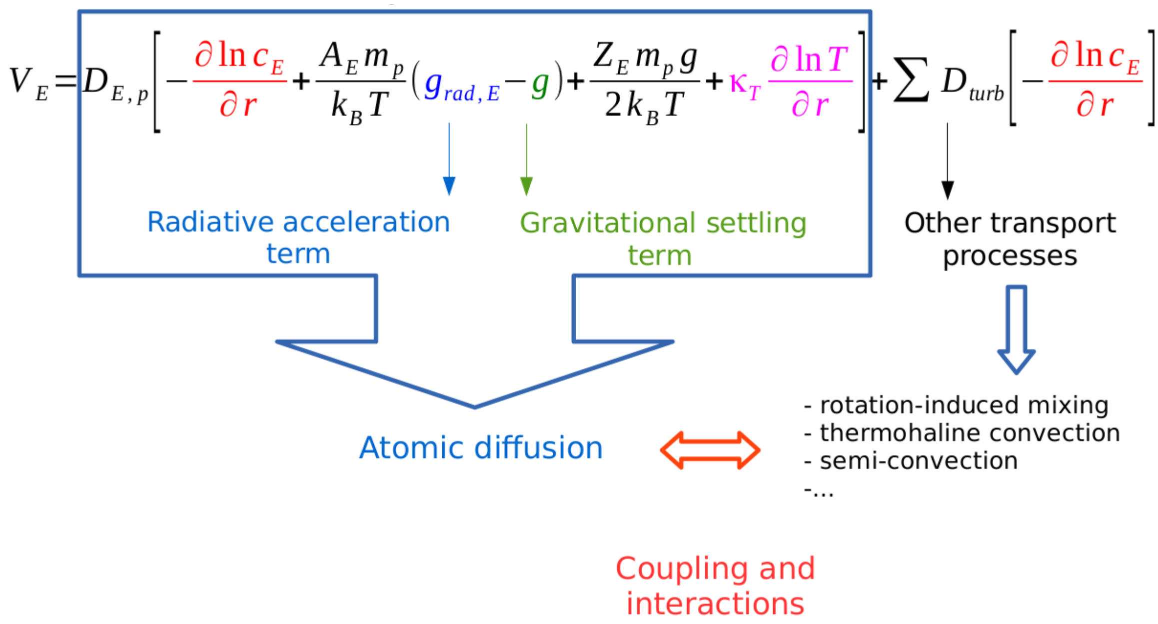

Figure 1: Diffusion equation of a trace element E.

figure we see that atomic diffusion (left part of the equation, blue rectangle) is composed of different processes. There is the impact of the concentration gradient (red term) with c_E the concentration and r the radius, the impact of the temperature gradient (pink term) with κ_T the thermal diffusivity and T the temperature. There is the effect of the electric field (black term) with Z_E the charge of the element, m_p the proton mass, g the acceleration of the gravity and k_b the Boltzmann constant. The two main terms of the equation are the effect of the gravity (green term) with A_E the mass of the element, which makes the element move toward the center of the star. And the other one is the radiative accelerations term (in dark blue) which is a transfer of momentum between photon and ions and make the element statistically move toward the surface of the star. Radiative acceleration on an element E is given by (Richer *et al.*, 1998):

$$g_{rad,E} = \frac{1}{4\pi r^2}\frac{L^{rad}\kappa_R}{cX_E}\int_0^\infty \frac{\kappa_{u,E}}{\kappa_u(\text{total})}P(u)du \qquad (1)$$

where u is the dimensionless frequency variable $u = h\nu/k_bT$, P(u) the normalized blackbody flux and $L^{rad}/4\pi r^2$ is the total radiative momentum flux. κ_u is the monochromatic opacity at u. All these terms are multiplied by the diffusion coefficient $D_{E,p}$ between the element E and the protons (trace element case).

The contribution of atomic diffusion to the diffusion velocity mainly comes from the competition between the gravity and radiative accelerations. To atomic diffusion is added all the contribution of macroscopic transport processes. In the equation (Fig. 1) all the D_{turb} are added but this is an approximation. It is not possible to add two turbulent diffusion coefficients because processes are coupled and the prescriptions are generally determined in studies of only one process. These macroscopic transport processes are for example the mixing induced by the rotation (e.g. Zahn, 1992), the fingering convection (e.g. Brown *et al.*, 2013), ... etc. Both microscopic and macroscopic processes are coupled with each other and this is only when taking both types of processes that we can hope to get consistent surface abundances and internal structure in the models with observation.

2.2 Effect of atomic diffusion on abundance profiles

Atomic diffusion occurs in radiative zones of stars because the mixing in convective zones is too important to allow microscopic motions. In the case where radiative accelerations are larger than the gravity for a given element and at a given place in the star, the elements will be accumulated. These accumulations occur where the elements are main contributors to the opacity, e.i. where it absorbs most of the photons. If is occurs at the bottom of the surface convective zone, the elements are accumulated at the surface. On the other hand, if the gravity dominates, the elements move toward the center of the star and are depleted. There are in some type of stars region where gravity dominates in the upper part and radiative accelerations in the lower part. This leads to local accumulations (e.g. Richard *et al.*, 2001). This kind of accumulation can lead to hydrodynamical instabilities as fingering convection (Théado *et al.*, 2009; Deal *et al.*, 2016).

As accumulations occur where the element is the main contributor to the opacity, it induced a local increase local of the opacity and then influence the structure of the star. These effects are different for each element. It depends on the abundance of the element. The more abundant is the element the less it is supported due to saturation effects. The effects are also different depending on the ionisation state of the elements.

2.3 Implementation of atomic diffusion in stellar evolution codes

The computation of atomic diffusion in stellar evolution codes needs three main ingredients. The first one is the computation of the diffusion velocity of chemical elements. The four main methods are the one described in Burgers (1969),Chapman & Cowling (1970) (hereafter C&C), Michaud & Proffitt (1993) (hereafter MP93) and Thoul *et al.* (1994). The two last methods are approximations of the Burgers (1969) equations. The four methods have their advantages and disadvantages. The most precise one is the Burgers' formalism, but this is also the more time consuming. Note that the easiest to implement, one of the fastest to be computed and the one recommended in Michaud *et al.* (2015) is the MP93 for-

Table 1: List of evolution codes including atomic diffusion computation with radiative accelerations

Codes	Diff. eq.	$g_{\rm rad}$	Opacities	references
Montréal/Montpellier	Burgers	Opacity sampling	OPAL monochromatic	Richer *et al.* (2000)
TGEC	C&C	SVP	OPCD	Théado *et al.* (2012)
CESTAM	MP93	SVP	OPCD	Deal *et al.* (2018)
MESA	Thoul94	OPCD	OPCD	Paxton *et al.* (2018)

malism. In addition to the resolution of diffusion equations the diffusion coefficient is generally derived from the Paquette *et al.* (1986) study. It is crucial for these computations to take partial ionisation into account in the evolution code and to be able to follow elements individually.

The second ingredient is a method to compute radiative accelerations. There are three methods which are more or less time consuming. The most precise, but time consuming one is the OPCD package (Seaton, 2005) method which computes the radiative accelerations directly from atomic data. The second one which is faster is the opacity sampling methods (Richer *et al.*, 1998) which compute the equation 1 from monochromatic opacity data. The last method and the faster one is the Single-Valued Parameter (SVP) method (Alecian & LeBlanc, 2000, 2002; LeBlanc & Alecian, 2004). This method splits the atomic data contribution to the abundance contribution in the radiative acceleration equations. It is then possible to tabulate the atomic data contribution which is relatively constant for a given stellar mass. The computation is then very fast and the results are comparable to the two other methods.

The last ingredient is opacity tables which allows to compute the Rosseland mean opacity at each mesh point and each time step in order to consistently take into account the abundance variations in the computation of the structure of the stellar models. Two sets of this kind of opacity tables exist. The OPAL monochromatic tables which are not public (Richer *et al.*, 1998) and the OP data with the OPCD package (Seaton, 2005). The computation of the Rosseland mean opacity with these tables is very time consuming and is the more problematic ingredient if you aim to compute a large number of models taking into account atomic diffusion (including radiative accelerations).

All these methods are used in different evolution codes. Some of them are listed Table 1 with the different methods used by each code.

3 Impact of atomic diffusion on stellar properties

3.1 The case without radiative accelerations

Atomic diffusion without radiative accelerations has been shown to be important for the modelling of the Sun (see Section 1). There are a lot of evidence of its effect in star and some recent studies studied the impact of atomic diffusion on the stellar parameters. The study of Nsamba *et al.* (2018) for example, shows that neglecting atomic diffusion (without radiative accelerations) induced internal systematics in the model up to 0.5% on the density, 0.8% on the radius, 2.1% on the mass and 16% on age for models between 0.7 to 1.25 $M_\odot$. These systematics are not negligible, especially for the age and this shows that atomic diffusion (without radiative accelerations) cannot be neglected in stellar models.

3.2 The case with radiative accelerations

3.2.1 94 Ceti A

The first study of the impact of atomic diffusion (including radiative accelerations) on the stellar parameters determination with asteroseismology was done on the 94 Ceti A star (Deal *et al.*, 2017). This is an F-type star and the mass determined by this study was 1.44 $M_\odot$. The aim of the study was to determine the difference in age obtained when the determination is done with models including or not radiative accelerations. The result of the study was an age difference of 4%. This seems to be negligible, but the 94 Ceti A star undergoes small effects of radiative accelerations according to the models which means that for stars with larger effects the age difference should be larger.

3.2.2 A larger sample

A more general study was made on a larger number of models at different metallicity (Deal *et al.*, 2018). The aim of this study was to determine at what mass and metallicity is it important to include radiative accelerations in the models in order to get precise enough stellar parameters. Two sets of three grids of models were computed with the CESTAM evolution code (Morel & Lebreton, 2008; Marques *et al.*, 2013), one including radiative accelerations and the other not. Each grid has a different metallicity, [Fe/H]=-0.35,0.035 and +0.25. For more detail on the input physics of the model see the article. These models were computed including only atomic diffusion, which means that the abundance variations are upper-limits because rotation was not included for example.

The first impact of radiative accelerations is on the surface abundances (see Fig. 2). Some elements are not supported by radiative accelerations (C, N and O), some are weakly supported which reduces the depletion (Ne, Mg, Ca) and some are strongly supported which produces an accumulation at the surface (Al, Fe). This is the reason why elements should be followed individually in stellar evolution codes if one want to compute models with an accurate transport of chemical elements by atomic diffusion.

As some elements accumulate at the surface it means that they are the main contributors to the opacity at the bottom of the surface convective zone. This accumulation then leads to a local increase of the opacity. The difference in opacity reaches up to 60% in the 1.4 $M_\odot$ and shows the importance of taking into account the abundance variations in the Rosseland mean opacity computation.

The increase of the opacity close to the bottom of the surface convective induce the increase of its size. In the 1.4 $M_\odot$ at solar metallicity the difference in the mass of the surface convective zone reaches up to 70%. It is 120% for the 1.2 $M_\odot$ at lower metallicity. These differences are important and need to be taken into account when trying to determine the position of surface convective zones with glitch studies. The 70% of the 1.4 $M_\odot$ translates in 160s in acoustic depth which is larger than the uncertainties of the determination made for the F-type stars of *Kepler* (Verma *et al.*, 2017). As the struc-

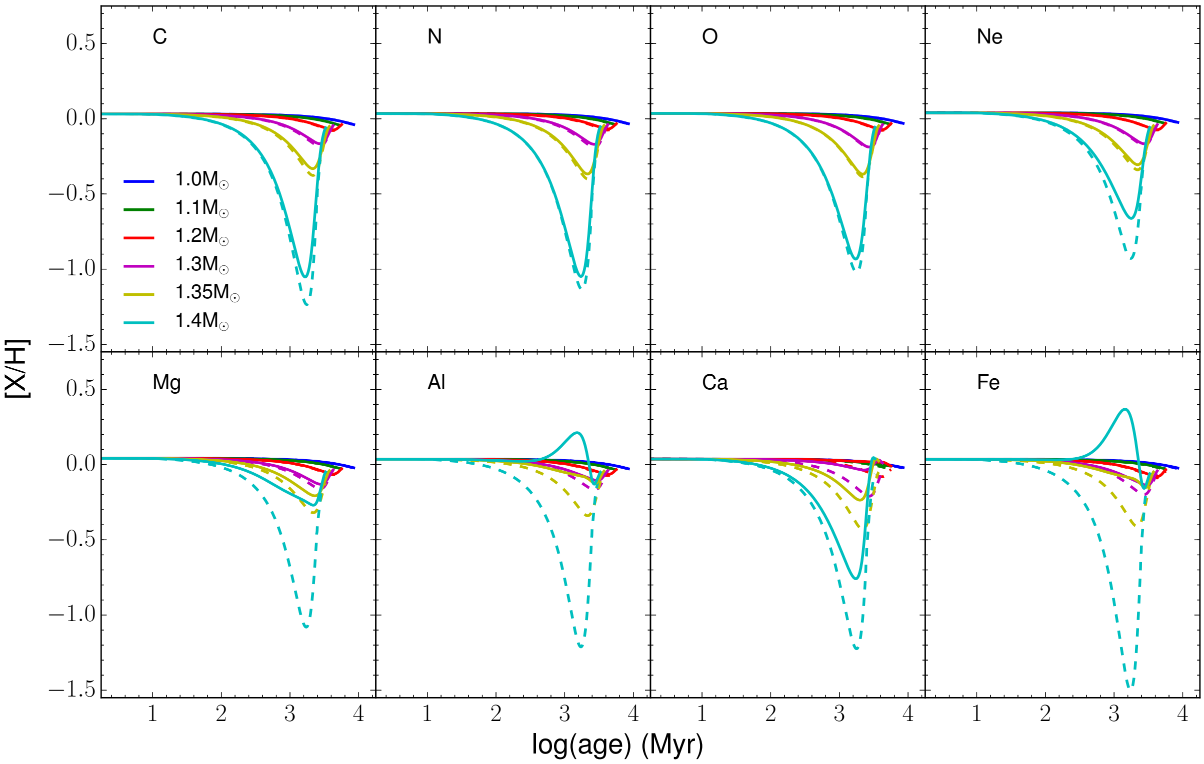

Figure 2: Evolution of surface abundances with time for eight elements of models at solar metallicity. The solid and dashed curves respectively represent models with and without $g_{\rm rad}$. Adaptation of Fig. 3 of Deal *et al.* (2018).

ture of the star in impacted it has also an influence of the radius. The difference in radius reaches 2% for the 1.4 $M_\odot$ at solar metallicity.

We saw that the structure of the models was strongly impacted by radiative accelerations. This impact can be translated into variations in the asteroseismic parameters. The $\nu_{\rm max}$ and $\Delta_\nu 0$ can be obtained by scaling relations (Kjeldsen & Bedding, 1995). Figure 3 shows the difference in $\Delta_\nu 0$ between models including or not radiative accelerations. We see that with the two uncertainties considered for $\Delta_\nu 0$ (see Table 2) the difference between models including or not radiative accelerations is obtained for quite low mass stars. The limit mass are listed Table 2.

The impact of radiative accelerations on the seismic parameters occurs for masses we thought not affected. This is because these are the maximum effect of atomic diffusion as no other transport processes is taken into account. These limit masses have to be considered as upper-limits. It means that atomic diffusion can be neglected for masses lower that these limits without causing an error in the parameter determination with asteroseismology. For larger masses, it depends on the efficiency of the other transport processes.

3.2.3 *Impact for Kepler and PLATO stars*

With the models presented in the last section we can try to determine the maximum number of stars affected by radiative accelerations in the *Kepler* and PLATO field of observation. We used the limit masses determined in Table 2. Figure 4 shows the number of affected stars (right side of solid curves). It corresponds to 33% and 59% depending on the uncertainty set (A for the blue curve and B for the red curves). The number of affected stars is quite large and indicate that a specific attention needs to be put on the treatment of transport processes (especially atomic diffusion) in the models in order to be able to provide accurate stellar parameters from asteroseismic data.

We tested to determine stellar parameters with models including atomic diffusion (with radiative accelerations) using the code AIMS **?**. The first result shows that the error on the mass can reach 4% and the age 20% for a 1.4 $M_\odot$ star if radiative accelerations are neglected. These are preliminary results, but it indicates that it in not possible any more to neglect atomic diffusion in the models.

4 Coupling between atomic diffusion and rotation

The rotation in star induced a transport of chemical elements which is often invoked to justify to neglect atomic diffusion in the model. In this section we determine in what condition it is true and we show what happened if it is not.

4.1 Transport of chemical elements by rotation

The aim of this section is not to give a detailed description of the transport of angular momentum and chemical elements in stars (see e.g. Zahn, 1992; Talon & Zahn, 1997; Maeder, 2009, for more details). The transport of chemical elements by rotation is given by (Chaboyer & Zahn, 1992):

$$D_{turb,rota} = D_v + \frac{(rU_2)^2}{30D_h} \quad (2)$$

where D_v is the vertical component of turbulent diffusivity, D_h the horizontal component of turbulent diffusivity , U_2 the vertical component of the velocity of the meridional circulation. This term can be added to the diffusion velocity (multiplied by the concentration gradient).

In the models we present in the next section, we used D_V

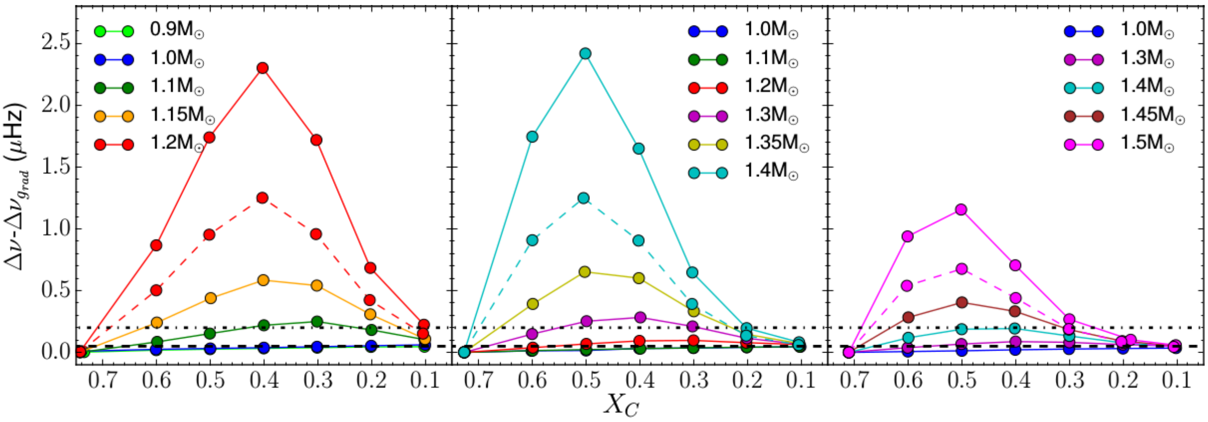

Figure 3: Evolution with the central hydrogen content of the differences of the average large separation $\Delta\nu_0$, between models without and with $g_{\rm rad}$ for the three grids. The dashed lines represent the same models but without the effect of partial ionisation. The horizontal black dash-dotted lines indicate the adopted A uncertainty set, and the horizontal black dashed lines indicate the adopted B uncertainty set. Adaptation of Fig. 7 of Deal *et al.* (2018).

Table 2: Considered uncertainties on observed $\Delta\nu_0$ (μHz) and determined limit masses ($M_\odot$).

	$\delta\Delta\nu_0$	masses at [Fe/H]=-0.35	masses at [Fe/H]=0.035	masses at [Fe/H]=+0.25
A	0.05	0.9	1.1	1.2
B	0.2	1.05	1.25	1.4

from Talon & Zahn (1997), D_h from Mathis *et al.* (2004) and the prescription of extraction of angular momentum at the surface due to magnetised wind from Matt *et al.* (2015).

4.2 Impact of rotation on element accumulation/depletion by atomic diffusion

We computed models at three different masses (1.3, 1.4 and 1.45 $M_\odot$) including the effect of rotation ($v_{\rm ini}$ = 30km/s, maximum rotation speed find in the *Kepler Legacy* sample Benomar *et al.* (2015)) and atomic diffusion, and compare them to models without atomic diffusion. The evolution of [Fe/H] is shown Fig. 5 for these three models. For the 1.3 $M_\odot$ model, radiative accelerations make no difference in the iron surface abundance. The effect of atomic diffusion is strongly reduced in this model because the mixing induced by rotation is very important. The efficiency of the mixing is reduced when the mass increases because the extraction of angular momentum by magnetised wind depends on the size of the surface convective zone (to generate a magnetic field with dynamo). And this extraction is driving efficiently the meridional circulation, and then the mixing. This is why at 1.45 $M_\odot$, iron is nevertheless accumulated at the surface

In the case of the 1.4 $M_\odot$, rotation prevents the accumulation of iron at the surface (compare to what was obtained without rotation Fig. 2). The mixing is large enough to reduce the effect of atomic diffusion, but not to suppress it. There is still a different of 0.1 dex between the model with and the model without radiative accelerations. This indicates that even in this case this is not possible to neglect radiative accelerations.

It is possible in this case to determine a limit mass (as in Section 3.2.2) not with the seismic parameters, but with the difference in [Fe/H]. We choose a criteria of 0.1 dex as the limit difference which need to be reached in order to affirm that radiative accelerations cannot be neglected in rotating stellar models models. These limit mass a represented as the green curve in Fig. 4. We determine in this case that the number of stars affected by radiative accelerations reaches 14%. This is less stars than in the other cases, because rotation reduces the efficiency of atomic diffusion, but this is still not negligible. Note that the current theory probably neglect the transport of angular momentum in stars, which means that the transport of chemical elements is probably overestimated. A lot of work needs to be done before we can hope to obtain a definitive answer to this problem.

It is important to note that even in the 1.3 $M_\odot$, even if the surface abundances remain close to constant, a model without atomic diffusion and without rotation is not equivalent to a model including both processes. Rotation cancels the effect of atomic diffusion, but the mixing inside the star affects its evolution. Some material is brought to the core and modifies the available combustible for nuclear reactions. The work on rotating stars and atomic diffusion is in progress and a more detailed paper is in preparation.

5 Conclusion

The problem of the transport of chemical elements is far from simple and it will need a lot of effort to improve our current theory. Some crucial processes are already studied (atomic diffusion, rotation, fingering convection,...) but we probably still miss processes which could be important.

Atomic diffusion remain an important piece of that puzzle and it is crucial for stellar evolution code to be able to take it into account including the radiative accelerations. The impact of atomic diffusion is not only on the surface abundances, it has a strong impact on the internal structure due to the local opacity increase. It leads to an increase the size of surface convective zones and to a modification of radii. The structure variations are visible in the seismic indicators as $\Delta\nu$ and $\nu_{\rm max}$ and the difference in the models including or not radiative accelerations are larger than the uncertainties on these parameters for low mass stars.

We saw that atomic diffusion can be efficient to reduce

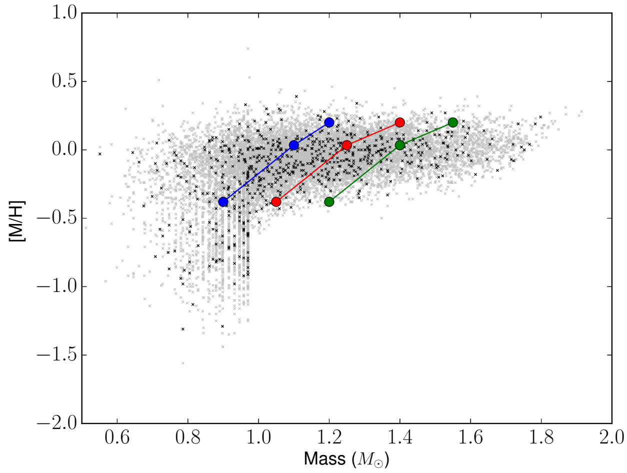

Figure 4: Metallicity according to the mass of a population simulation (Annie Robin, private comm., Besançon code Czekaj *et al.* (2014)) of the PLATO (grey crosses) and *Kepler* (black crosses) core programme stars. The selected stars are from K7 to F5 with magnitudes in the range 4 < V < 11, effective temperature in the range 4030 < $T_{\rm eff}$ < 6650 K, and luminosity classes between IV and V. The blue, red and green points correspond to the models listed in Table 2 and in Section 4.2, which represent masses when $g_{\rm rad}$ needs to be taken into account. Adaptation of Fig. 9 of Deal *et al.* (2018).

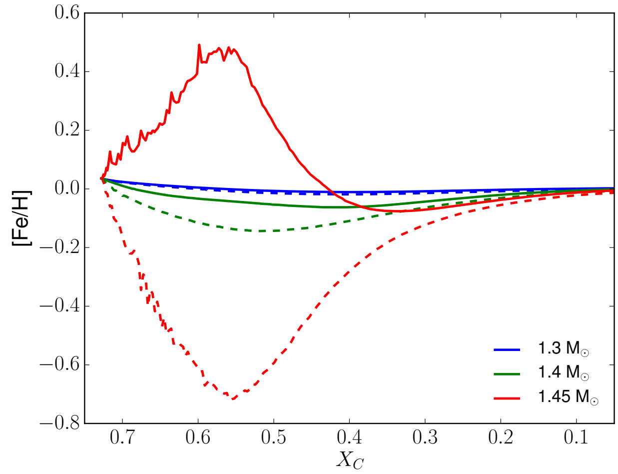

Figure 5: Variations of [Fe/H] according to the hydrogen mass fraction in the core X_C. The solid curves are models including radiative accelerations and dashed models which does not include it. The initial [Fe/H] is 0.035.

the effect of atomic diffusion but not in all cases. When the extraction of angular momentum is not efficient enough to drive the meridional circulation, accumulations of elements at the surface become possible. The coupling between rotation and atomic diffusion needs to be more investigates. There is still a lot of work to do understand the transport of chemical elements in stars, but the generation of models which is developed at this moment is going in the good direction.

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