Stars and their variability observed from space
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RECENT ADVANCES IN NUMERICAL MODELS THAT INCLUDE ATOMIC DIFFUSION IN STARS

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Abstract.
Atomic diffusion in stars is efficient in changing the distribution of elements slowly but strongly in any radiative zone. The process may produce detectable effects, over time-scales stretching from a few decades to star's lifetime, according to the depth of the radiative zones. The main consequences are that superficial abundances may depart from standard values, but also that internal structure and seismic diagnostics are affected owing to changes in local opacities. The main difficulty of including atomic diffusion in numerical models comes from radiation force (the dominant force acting on atoms within the layers concerned), which is specific to chemical species through their atomic properties, and which makes the process of abundance stratification strongly non-linear in usual situations (especially in atmospheres). This talk presented recent improvements that involve a fast method for calculating radiative accelerations in stellar interiors, and described progress in the modelling of stellar atmospheres.

Keywords: Processes: Diffusion, stars: abundances, chemically peculiar, magnetic field, mass-loss

1 Introduction

Atomic diffusion is a slow process that competes (with difficulty) with large-scale motions (mixing, mass loss, etc.). Separation of the chemical elements occurs inside stars in any stable (radiative) zone. Among the main difficulties of modelling these processes two can be emphasised: (1) calculating radiative accelerations that requires heavy computations of the total momentum acquired by atoms from the radiation field, and (2) estimating the strength of large-scale motions (convection and mass loss, for instance) that prevent element separation. Michaud et al. (2015) have given a detailed and exhaustive discussion on the subject. This talk presented some recent advances concerning the computation of radiative acceleration in a stellar interior, and numerical models of atmospheres including atomic diffusion and mass loss.

Even though the physics is basically the same, the calculation of atomic diffusion effects in stellar interiors and in stellar atmospheres is very different. That is mainly due to radiation transfer computation, which is carried out with very efficient approximations in stellar interiors but which are impossible to apply to stellar atmospheres, where the radiation transfer equation must be solved in detail. In addition, the characteristic time-scales are very different, since in the interior they are comparable to the stellar evolution time-scale, while they may be as short as a year in the atmosphere (Alecian 2013). Both cases were, until the present, considered separately in numerical codes. We should add that processes of atomic diffusion in stellar interiors concern the radiative zones of any type of star (for layers with diffusion time-scales smaller than the age of the star in question), while in an atmosphere they geneally concerns Ap/Bp chemically-peculiar stars (magnetic stars, HgMn, He-weak) and He-rich stars.

2 Improvement of SVP tables

There are several methods for computing radiative accelerations in stellar interiors: (i) the detailed method, which uses atomic transition tables directly, (ii) the opacity sampling method, which uses monochromatic opacity tables, and (iii) a parametric method. The first (i) is in principle the most accurate, but is rarely used because of its heaviness and the very large amount of data to handle (nevertheless, such an approach has to be used for atmospheres). The second approach (ii) is *widely* used (Vick et al. 2011; LeBlanc et al. 2000; Richer et al. 1998; Seaton 1997, 2007), but necessitates having monochromatic opacity tables for elements for which atomic

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diffusion is computed. The parametric method (iii) (*SVP*, for Singled-Valued Parameters) is less accurate than the other two methods but is extremely fast for numerical applications (Alecian & LeBlanc 2002; LeBlanc & Alecian 2004) and can be used for elements for which the usual opacity databanks do not provide any data (like Sc, for instance Alecian et al. 2013).

The *SVP* method can only be used in optically thick regions, and for stars with masses larger than, or equal to, approximately one solar mass. It has the advantage of calculating radiative acceleration ($g_{\rm rad}$) from pre-tabulated parameters (6 parameters per ion) without having to access complete atomic data or detailed monochromatic opacities. A first release of tables of parameters is available via the website `http://gradsvp.obspm.fr` for the computation of $g_{\rm rad}$ for various elements (C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca and Fe). A forthcoming release (early 2020) will extend the tables to other elements, and will support the computation of radiative accelerations for main-sequence stars with masses from $0.9 - 10\,M_{\odot}$. In addition, Fortran routines to help easy implementation into existing codes will be provided.

The parameters in this forthcoming release are also improved. An example of $g_{\rm rad}$ obtained by the improved *SVP* tables (though still provisional here) is shown in Fig. 1.

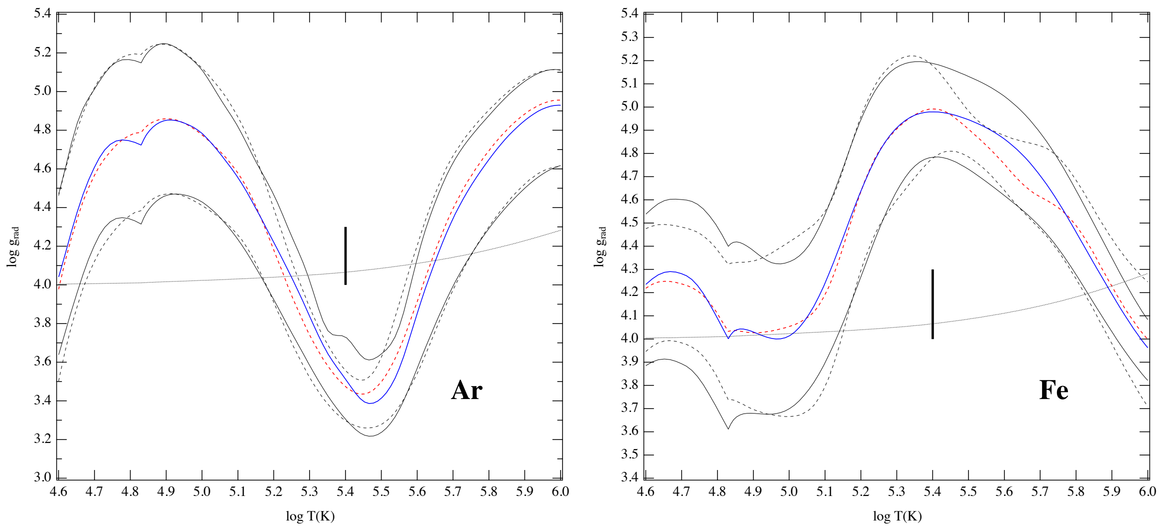

Fig. 1. Radiative accelerations obtained using the *SVP* method. This work is still in progress (see text). **Left**: Argon, radiative acceleration with respect to depth [in $\log T(K)$] in a $2-M_{\odot}$ model obtained through the *SVP* method (dashed lines), and through the procedure proposed by the Opacity Project (OPCD 3.3, solid lines) for three concentrations of Ar from 10^{-1} (the upper curves) to 10 times the solar value. The blue and red lines are for solar abundances. The vertical bar represents 0.3 dex (the maximum error above which we decided to reject the parameters), and the pointed curve is the local gravity. **Right**: Same as the left panel but for iron.

3 Recent results for atmospheres of CP stars

Among chemically-peculiar (CP) main-sequence stars, Ap/Bp stars (including roAp) often have very strong magnetic fields. Atomic diffusion is very efficient in their atmospheres, and produces non-uniform distributions of chemical elements (element spots and/or abundance stratification). To compute how diffusion works in those atmospheres, one needs first to compute a detailed solution of the polarized radiation transfer equation, and then compute element stratification build-up. We have developed the Carat family numerical codes (in collaboration with M. Stift), starting from the calculation of radiative accelerations in magnetic atmospheres (Alecian & Stift 2004) to the recent model of 3D abundance distributions (Alecian & Stift 2017) and additional physical processes (Alecian & Stift 2019).

Up to now, all calculations of the distribution of elements in stellar atmospheres (see for instance LeBlanc et al. 2009; Alecian & Stift 2010) were obtained assuming equilibrium solutions; concentrations of elements were such that $g_{\rm rad} = g$ (the gravity) in all layers. However, it is not yet known to what extent such equilibria obtain in real atmospheres. The best approach is to solve the time-dependent continuity equation for concentrations, which is a strong numerical challenge. However, since Alecian et al. (2011), it is being used increasingly.

Recent progress in modelling atomic diffusion in atmospheres includes the first calculation by Alecian & Stift

(2017) of a theoretical 3D map of chromium and iron, assuming a magnetic geometry inspired by an observed magnetic map (non-strictly dipolar). That calculation is shown in Fig. 2, and is still obtained for equilibrium solutions, but a time-dependent calculation is in preparation.

Another recent improvement in modelling atomic diffusion is the addition of a missing physical process in our numerical codes: the global outgoing flow of material caused by mass loss. It is accepted, at least from the work of Vauclair (1975) on helium-rich stars, that mass loss (if present) competes with atomic diffusion. It has certainly been taken into account in evolution codes that include atomic diffusion (Vick et al. 2010), but not for atmospheres. That has now been done, in time-dependent calculations, by Alecian & Stift (2019), as shown in Fig. 3 (left panel). The main result that can be drawn from this calculation is that the observed Mg abundances in HgMn stars cannot be explained without assuming a mass loss of about $5.0\,10^{-14}\,M_{\odot}.y^{-1}$. A second result obtained from such a calculation (right panel of Fig. 3) is that to recover the stratification for phosphorus as observed by Ndiaye et al. (2018) in the atmosphere of HD 53929, one needs to assume that this HgMn star, hitherto generally considered as non-magnetic, should have a small magnetic field (around 100 Gauss).

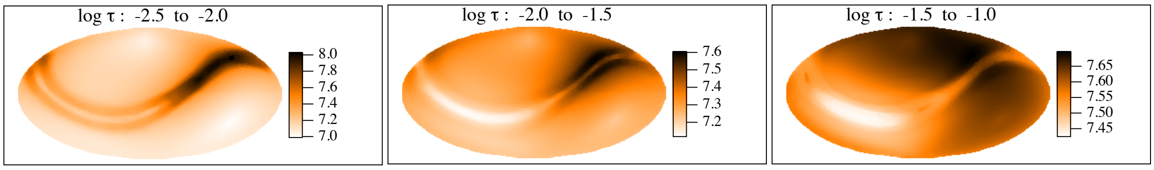

Fig. 2. Tomographic view of the abundance of Cr (Hammer equal-area projection). Three slabs corresponding to three contiguous optical depth ranges (indicated above each projection) are shown. Note that the relation between abundances and colour scale differs from one slab to the other. The solar abundance of Cr is 5.67. See Alecian & Stift (2017) for details.

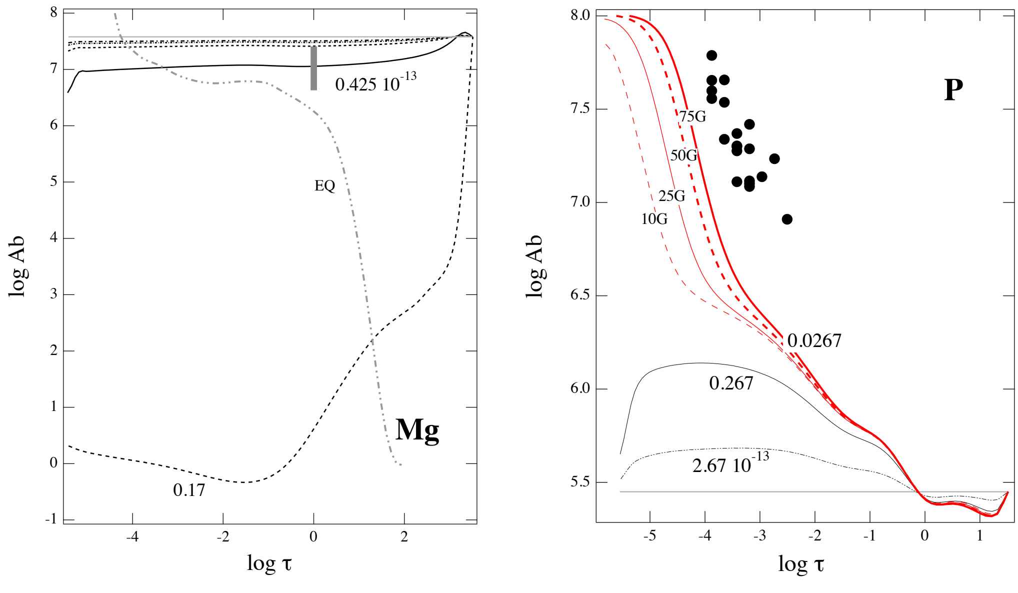

Fig. 3. Left: Stratification of Mg abundance (stationary solutions) *vs.* the logarithm of the optical depth at $\lambda\,5000\,\text{Å}$ as a function of various mass-loss rates (model with $T_{\rm eff} = 12000\,\text{K}$, and $\log g = 4.0$). The Mg stratification is shown for 5 different mass-loss rates (1.7, 1.28, 0.85, 0.425, 0.17 in units of 10^{-13} solar masses per year). The vertical thick grey bar corresponds to observations of Mg overabundances in HgMn stars having approximately the same $T_{\rm eff}$ and $\log g$. The equilibrium solution (EQ) (heavy dash-dot-dot grey line) is also shown. See Alecian & Stift (2019) for details. **Right:** Stratification of P in the atmosphere of HD 53929. Filled circles show the abundances determined empirically by Ndiaye et al. (2018) from observations. The solid grey line is the solar abundance; the thin solid and dash-dot-dot curves are our stationary non-magnetic solutions for mass-loss rates of 2.67 and $0.267\,10^{-13}$ solar mass per year, respectively. The group of red curves labelled 10 G, 25 G, 50 G and 75 G are the solutions obtained by assuming a weak horizontal magnetic field, and for the lowest mass-loss that ensures convergence of this model ($0.0267\,10^{-13}$). See Alecian & Stift (2017) for details.

4 Conclusions

Recent improvements in the parametric *SVP* method for calculating radiative accelerations for stellar interiors will be available shortly (foreseen for the beginning of 2020), together with Fortran routines, at `http://gradsvp.obspm.fr`.

For stellar atmospheres (with and without magnetic fields), this talk presented the first theoretical 3D calculations of the distribution of elements (at equilibrium), and calculations of time-dependent stratification build-up with mass loss. Two main results can be drawn from those time-dependent calculations; first, mass loss could be considered systematically for all types of CP stars, and secondly, we can justify considering that weak magnetic field may exist in HgMn stars. As a concluding remark, one must admit that numerical models are not yet able to describe detailed abundance distributions modified by atomic diffusion in the atmospheres of individual stars. However, there is a reasonable hope that we will succeed in overcoming this challenge fairly soon through 3D numerical simulations, as long as we also succeed in taking into account all physical processes that make a significant contribution.

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