Diffusion and Chemical Transport in Stellar Atmospheres

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The current status of particle transport calculations in the atmospheres of ApBp stars is critically described. We emphasize the importance of the inner boundary condition, that is the time-dependent chemical flux and composition below the atmosphere which is determined by the interior evolution. For the non-magnetic HgMn stars a number of observed anomalies are explained with little arbitrariness, though isotope anomalies and observed variations from star to star are challenging. For the magnetic ApBp stars, detailed quantitative models of the observed mapping and size of anomalies are still lacking. Not all required hydrodynamical ingredients are currently included.

1 Astrophysical Context

The observed chemical composition of ApBp stars is the result of their initial chemical composition, the particle flux from the interior, the stellar wind and whatever mixing is present. This cannot yet be calculated uniquely from first principles: observations must be introduced to constrain models and each star becomes an experiment in stellar hydrodynamics.

We briefly describe (§ 2) how the flux being pushed into the atmosphere from the interior rapidly modifies atmospheric abundances, demonstrating the essential role of the inner boundary condition of the atmosphere. The critical link between HgMn and horizontal branch stars is shown to follow naturally by assuming that meridional circulation is the main process limiting abundance anomalies (§ 3). Then we present (§ 4) a few anomalies which can be explained by assuming simple static atmospheres followed (§ 5) by a discussion of the physical processes expected to play a role in the appearance of additional anomalies. A few examples of recent calculations (§ 6) are then briefly discussed, followed by the general conclusion in § 7.

2 Inner Boundary Condition

The inner boundary condition of the atmosphere is determined by the internal evolution of the star. Atomic diffusion is important in determining chemical abundances throughout an evolving star and so the boundary condition should be obtained using stellar models calculated including atomic diffusion throughout their evolution (Michaud et al., 2015). Radiative acceleration is a basic physical process that can now be calculated from first principles (Richer et al., 1998) and should always be included in atomic diffusion calculations. Given the number of chemical species that are included in the calculations, this requires solving a set of 56 linear differential equations at every stellar shell for each time step, considerably increasing the length of evolution calculations. Starting with the Sun (Turcotte et al., 1998) such evolution calculations have now been obtained for most types of stars.

To obtain realistic boundary conditions, the competing hydrodynamic processes must, however, also be included. Convection is routinely included in evolution models but mass loss, meridional circulation and turbulence should also be. To our knowledge no evolution models have been calculated with meridional circulation. This is an important gap to fill. A few models have been calculated with mass loss and series of models have been calculated with turbulence. We use these to give examples of the inner boundary condition that can be expected for atmospheres.

As a first example, two models of a $2.5\,\mathrm{M}_\odot$ star were evolved, one with mass loss and the other with turbulence. The evolution was calculated in detail for a mass loss rate of $10^{-13}\,\mathrm{M}_\odot\,\mathrm{yr}^{-1}$ as described by Vick et al. (2010). This model is similar to that used (Michaud et al., 2011) to understand Landstreet's critical assessment of the chemical composition of Sirius (Landstreet, 2011). For P, Mn and Fe, Fig. 1 compares the results of Vick et al. to those obtained in models of the same mass but calculated with turbulence from the surface to a depth where the temperature is $2 \times 10^5\,\mathrm{K}$ as described in Richer et al. (2000). From the model with turbulence a third model was generated by assuming turbulence to suddenly be present only from the surface to the bottom of the atmosphere at times of 20, 100 and 200 Myr. Very short time steps are required and abundance variations are very rapid so the evolution appears to be vertical in Fig. 1 for that experiment. Then surface abundance anomalies become much larger than observed anomalies in AmFm stars unless turbulence competes with atomic diffusion from the surface down to the depth of temperature of about $2 \times 10^5\,\mathrm{K}$ (Richer et al., 2000). For HgMn stars, however, many observed anomalies are compatible only with models calculated with the smaller turbulence such as those shown by the quasi-vertical lines. Computing models for HgMn stars with no mixing process imposed is currently prohibitive. Furthermore it would lead to the appearance of iron convection zones which mix regions around $2 \times 10^5\,\mathrm{K}$ so that computing complete models for the interior of HgMn stars is difficult unless one makes assumptions such as those done here for obtaining the vertical lines (which may also be seen more clearly in Fig. 2).

As a second example, Fig. 2 shows results for a $3.5\,\mathrm{M}_\odot$ star calculated with turbulence. The abundance evolution is very similar to that of the $2.5\ \mathrm{M}_\odot$ model with turbulence and of the model calculated with reduced turbulence giving the quasi vertical abundance variations. In the upper left hand corner, we have shown a zoom of the evolution of the Mn abundance around 103 Myr which leads to the quasi vertical evolution in the lower left hand panel. It shows clearly the rapid evolution once turbulence is reduced. If one imagined Mn stars to be periodically mixed by instabilities, this is an evaluation of the time scale to recover anomalies. Since the first layer of the model incorporates the whole atmosphere of an HgMn star, one needs to add a complete atmosphere model on top of the results given by the quasi vertical lines. These give the boundary conditions for diffusion calculations in model atmospheres as discussed in Section 6 below.

3 The Main-Sequence–Horizontal Branch Link

Most of the slowly rotating ($v \sin i < 100\,\mathrm{km\,s^{-1}}$) main-sequence and subgiant stars in the T_{eff} interval from 7000 to 16000 K show chemical abundance anomalies. On the main-sequence, when they have no large scale magnetic fields (not large enough to influence large scale hydrodynamics), they are mainly AmFm stars below 10000 K,

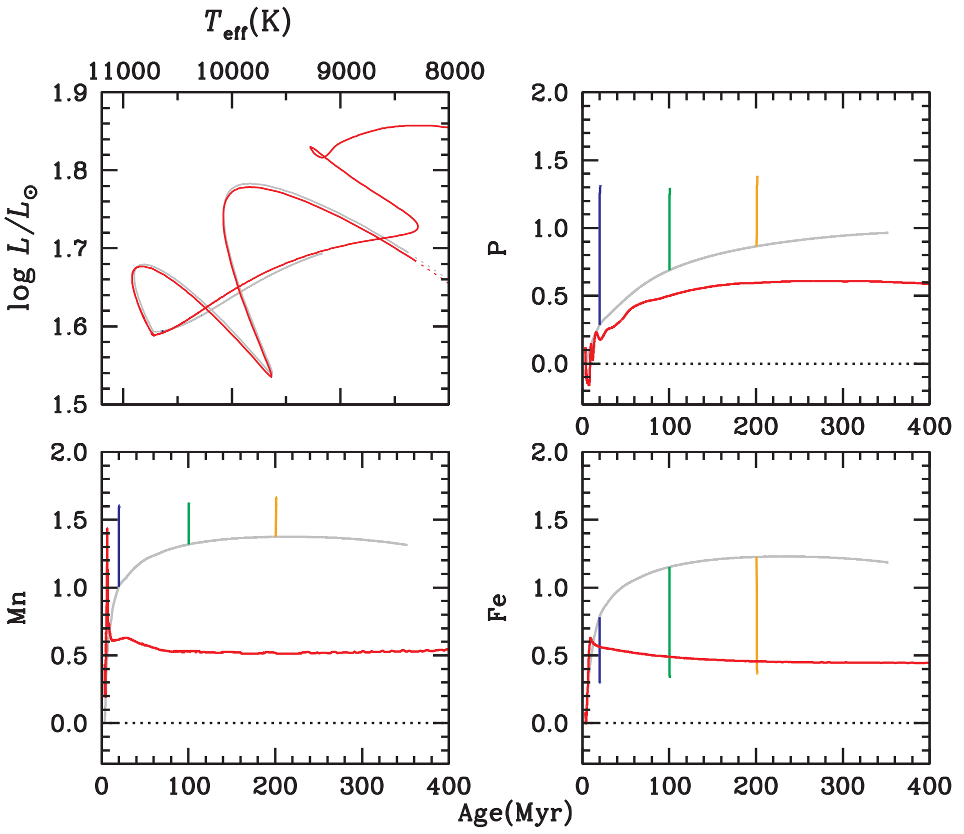

Fig. 1: Abundance evolution of P, Mn and Fe at the bottom of the atmosphere in a 2.5 $M_\odot$ star. The logarithmic vertical axis gives the abundance scaled to solar. The red line is from the evolution of a stellar model with a mass loss rate of $10^{-13}\,M_\odot\,yr^{-1}$ by Vick et al. (2010). The grey line comes from the evolution of a stellar model without mass loss but with turbulence as described in Richer et al. (2000). The turbulence model was parametrized for turbulence to drop rapidly above a temperature of 2×10^5K. The three nearly vertical lines were obtained by interrupting the evolution at 20, 100 and 200 $\times\,10^6$ yr, reducing the zone mixed by turbulence to include only the hydrogen convection zone and continuing evolution with smaller time steps. They are not vertical but correspond to an evolution over 3×10^5 yrs.

and HgMn stars, above that temperature. The models that reproduce the observations best include an atmospheric region stable enough for atomic diffusion to be important for the HgMn stars but a mixed outer region for AmFm stars. The transition at $T_{\rm eff} \simeq 10000\,$K is due to the surface hydrogen convection zone which, on the main-sequence, is present only in stars cooler than $T_{\rm eff} \simeq 10000\,$K. On the horizontal branch the situation could be expected to be more complex because of the strong dependence of log g with $T_{\rm eff}$. It turns out to be entirely predictable from the behavior on the main-sequence, if atomic diffusion, in competition with meridional circulation, is the physical mechanism responsible for the anomalies.

It was first shown that meridional circulation, using the analytic solution of

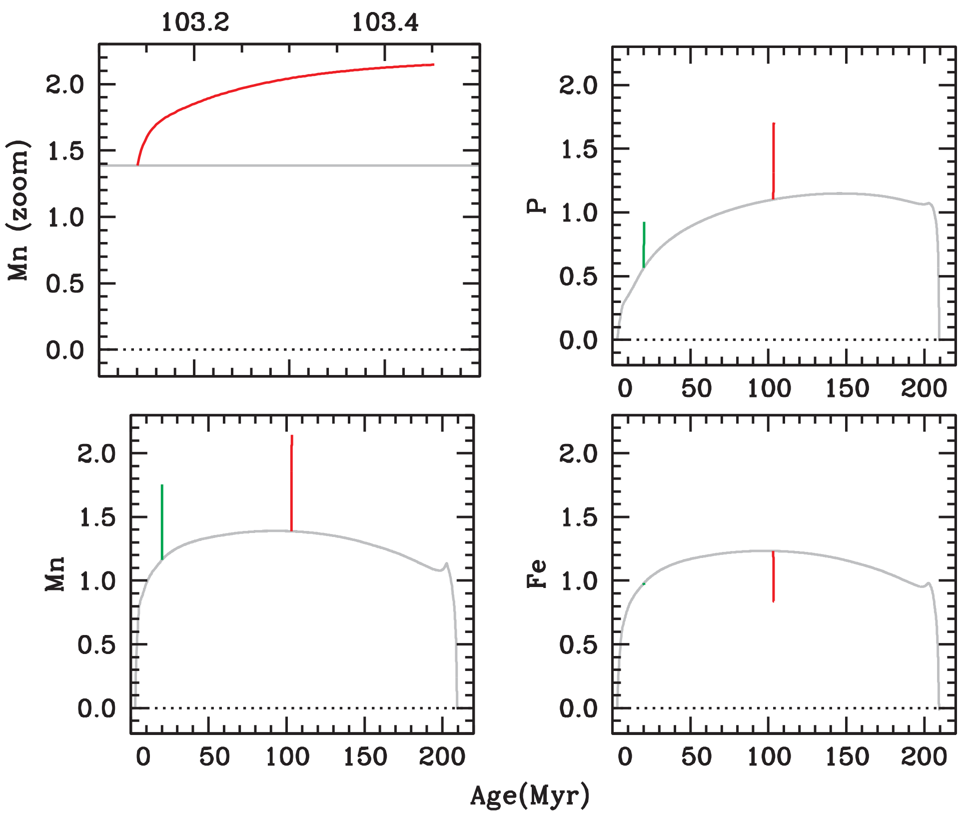

Fig. 2: Abundance evolution of P, Mn and Fe at the bottom of the atmosphere in a 3.5 $M_\odot$ star and, in the upper left panel, zoom of the Mn abundance variation slightly after 103 Myr. The vertical axis is logarithmic and gives the abundance scaled to solar. The solid grey line comes from the evolution of a stellar model without mass loss but with turbulence as described in Richer et al. (2000). The mixed zone was assumed to extend to a temperature slightly larger than 2 $\times 10^5$ K by using a turbulence model that drops rapidly above that temperature. The two nearly vertical lines were obtained by interrupting the evolution at 20 and 100 $\times 10^6$ yr, reducing the mixed zone to include only the hydrogen convection zone and continuing evolution with smaller time steps. They are not vertical but correspond to an evolution over 3×10^5 yr, as may be seen in the upper left panel for Mn slightly after 100×10^6 yr.

Tassoul & Tassoul (1982), prevented the settling of He II in HgMn stars rotating at more than $\simeq 90\,\mathrm{km\,s^{-1}}$ at $\log g = 4.4$ and at more than $\simeq 5\,\mathrm{km\,s^{-1}}$ at $\log g = 3.5$ (Michaud, 1982; Charbonneau & Michaud, 1988, 1991). At higher rotation velocities the He II convection zone is not eliminated by He settling and the atmosphere is not expected to be stable enough for anomalies to develop.

Michaud et al. (2004) suggested that one may, for HB stars, use the same critical equatorial velocity as in HgMn stars where the HB crosses the main-sequence in the HR diagram; that is at the T_{eff} where main-sequence and HB stars have the same gravity. Then, applying the scaling expected from the results of Michaud (1982), one can determine the expected critical rotational velocity on the HB. In this way they obtained (see their Eq. (2)):

$$v_e^l \propto g^{1.75}/{T_{\rm eff}}^2 \ . \tag{1}$$

By using the observed $100\,{\rm km\,s^{-1}}$ limit for HgMn stars of $T_{\rm eff} = 15000$ K and $\log g = 4.4$ one can anchor Eq. (1) and predict the limiting rotational velocity on the HB where both gravity and $T_{\rm eff}$ change along the branch. This prediction is compared to observations and to a more complete solution of the meridional circulation patterns in fig. 4 of Quievy et al. (2009). One sees there that Eq. 1 agrees with both the more complete calculations of circulation in HB stars and with the observations in clusters. Calculations predict that meridional circulation cannot stop He settling nor strong abundance anomalies for $T_{\rm eff}$ greater than 11500 K, while the observations suggest a limit of 11000 K with an uncertainty of 500 K.

This parameter-free link between the two classes of objects strongly suggests that meridional circulation plays a role in both HgMn and HB stars. The detailed calculation of evolutionary models taking atomic diffusion and meridional circulation into account will certainly shed additional light on the mixing processes in the interior of those stars. It would be very interesting to calculate evolutionary models with both meridional circulation and atomic diffusion (calculated including radiative accelerations). But this is not easy.

4 Abundance Anomalies From Parameter-free Calculations

Few NLTE calculations of radiative accelerations are currently being done. Around 1980 however, detailed NLTE model atmospheres were calculated (Borsenberger & Gros, 1978) for main-sequence stars from 10000 to 15000 K. They included only H, He and C I as opacity sources. They were then used to calculate NLTE radiative accelerations for B (Borsenberger et al., 1979), Ca and Sr (Borsenberger et al., 1981) and Be, Mg and Ba (Borsenberger et al., 1984). For instance for Ca, it was shown that the radiative acceleration could support a cloud in the atmosphere. The Ca would not leave the star because $g_{\rm rad}$(Ca) is smaller than gravity for $\log \tau \le -4$ (see fig. 2 of Borsenberger et al. 1981) and furthermore $g_{\rm rad}$(Ca) supports an abundance of Ca leading to the Ca II line at 3934 Å of approximately the observed strength (see fig. 9 of that paper). The agreement is not as good for the Ca line at 3159 Å which is thought to be a blend.

These NLTE calculations are of special interest because they lead to the formation of traps for some elements when radiative accelerations become smaller than gravity outside the atmosphere as described here for Ca. LTE calculations only rarely lead to the formation of traps because they emit at least the black body flux at line center of absorption lines formed in LTE. Similar success in comparing to observations with NLTE calculations was obtained for Mn (Alecian & Michaud, 1981). For Hg it would be interesting to do calculations similar to the NLTE calculations Proffitt et al. (1999) carried out for homogeneous distributions of Hg but to carry them out for distributions of Hg in layers. These NLTE calculations are however very demanding once complex atoms are involved. For a more complete discussion of simple models for HgMn stars, see Sections 8.2.1.2 and 8.2.1.3 of Michaud et al. (2015).

5 The Required Physics

Landstreet's observations have strongly contributed to establishing which physical processes are important in magnetic stars. In general, one should consider meridional circulation, turbulence, mass loss (including magnetic confinement), magnetic geometries (beyond dipolar), ambipolar diffusion, the effect of abundance variations on atmospheric structure and line formation, and NLTE effects. One cannot currently include all of them simultaneously so one must proceed in steps. In this section we briefly describe 53 Cam and mass loss and in the next section, a few of the more recent models.

Landstreet (1988) carried out a careful study of 53 Cam, and in particular the periodic time variability of the star's abundances. These were found to be most simply explained by the presence of mass loss (Babel & Michaud, 1991). These authors concluded that mass loss had to be involved in particular to explain the Ca, Mn, Cr and Sr relative overabundance in the polar region compared to the equatorial region.

Using Ca line profiles to model the wind and how it varies over the surface, Babel (1992) then calculates how the abundances vary over the surface as well as the line profiles and obtains agreement for spectral line profiles and time variations of Ca, Cr, Fe and Sr. The mass loss rate required is $3 \times 10^{-15}\,\mathrm{M}_{\odot}\,\mathrm{yr}^{-1}$. Babel & Lanz (1992) use IUE high resolution spectra to test the diffusion model with mass loss for 53 Cam. They confirm the stratification that the wind model predicts for chromium. Babel (1994) further showed that Ca stratification was observed in a large sample of Ap stars cooler than 9000 K. Missing from these papers is an evolving atmosphere with an interior boundary condition caused by the evolving stellar interior. The analysis of Ap stars requires stratified model atmospheres taking diffusion into account, as some of the models described in the next section are now attempting.

6 Recent Models

There are currently LTE stratified model atmospheres being converged incorporating diffusion of the main species, so leading to a self-consistent analysis of observations. However numerous steps are needed in practice to arrive at satisfactory models to analyze the observations. We mention only a few of those which have been taken, indicating some of their limits.

LeBlanc et al. (2009) calculated LTE model atmospheres using the PHOENIX code and letting the 39 included elements converge to diffusive equilibrium between gravity and the radiative accelerations calculated using opacity sampling. While using opacity sampling limits the accuracy for species with few lines in the calculated spectrum, these are not expected to contribute strongly to the model structure which is the main aim of this study. They took redistribution of momentum between ions into account since it affects the temperature structure at a level of 10% (see their fig. 5). The effect of the diffusion of metals on the structure of the atmosphere can approach 20% of the local temperature.

In Alecian (2015) a 10000 K a model stellar atmosphere consistent with equilibrium concentration gradients of 16 species is presented. Most species are not fully converged at the magnetic equator (see his fig. 1). The equilibrium is assumed throughout the atmosphere of a 10000 K star, irrespective of the flux from below.

He takes the effect of concentration on the structure of the atmosphere into account and as such this is an important self-consistent result which is a useful step towards a solution.

The time-dependent calculations of Stift & Alecian (2016) should be viewed as a step in the direction of a model based on time-dependent diffusion calculations. It is not a complete model ready to be compared with observations of all species in a given star. It contributes, however, to our understanding by showing how some species (those that satisfy the strict condition of the calculation) develop a constant flux. Their fig. 1 is a very interesting presentation of the difference between equilibrium distribution of Fe and its time-dependent distribution in the presence of mass loss. These calculations are in LTE while radiative accelerations at very small optical depths may well not be in LTE. They are, however, interesting solutions to have.

In a recent paper (Alecian & Stift, 2019) calculate the time-dependent diffusion of Fe and Mg in the presence of mass loss in two stellar atmospheres with $T_{\rm eff}$ and gravity appropriate for HgMn stars. This is an important step since weak mass loss is probably present in HgMn stars and solving the atmosphere consistently with mass loss is important. But it seems that a number of additions to their model are required if it is to be complete. They assume, for instance, constant solar abundances at the bottom of their model ($\tau \sim 1000$) and from the results of the evolution with mass loss presented in Fig. 1 above for a somewhat cooler star, this is unlikely.

They conclude that to support the observed abundance of Mg, a small mass loss is unavoidable, otherwise the Mg abundance would be much smaller. But consider the cloud equilibrium calculation of Borsenberger et al. (1984) leading to their fig. 4 for a cloud formation and their fig. 9 for the prediction that such a cloud formation gives for the observed strength of one Mg line. This is the result of the parameter-free calculations described in Section 4. There is no mass loss and no adjustable parameter in the calculation. We do not argue that this should be considered proof that there is no mass loss in this star, but only that it is premature to claim that mass loss is the only possible explanation for a Mg abundance similar to that observed.

Alecian & Stift (2017) study the type of three-dimensional patterns that non-axisymmetric magnetic geometries can lead to.

In a critical look at the results of diffusion calculations, Kochukhov & Ryabchikova (2018) have concluded that the existing detailed diffusion calculations did not improve agreement with Doppler Imaging maps when compared to equilibrium diffusion calculations. According to them the equilibrium atmospheric diffusion models of LeBlanc et al. (2009) and LeBlanc & Monin (2004) agreed reasonably well with observed overabundances but could not address the horizontal variations since they did not include magnetic fields. They emphasize that observations do not agree with a model predicting that all overabundant chemical elements are concentrated at the same place, for example where the magnetic field lines are horizontal as in Alecian & Stift (2010) or Alecian (2015). This is true and shows that the approach of Alecian and Stift needs to take a few more steps towards realistic models, as they certainly realize. The problem is that each step requires a big effort.

7 Conclusion

One may find it surprising that nearly fifty years after atomic diffusion processes were suggested as responsible for the ApBp phenomenon (Michaud, 1970) the models are still unable to reproduce all of the observed anomalies for a given star. The problem is that many processes potentially play a role, the relative importance of each is not evident, and the problem involves the three space dimensions and that of time. Progress requires considerable interaction between observers and modellers.

The first step of such an iterative process started between John Landstreet and G.M. on a plane between Montreal and Vienna on our way to the Ap stars meeting of 1975. It has continued ever since and has been quite enjoyable, but it needs some intensification by a more systematic data assimilation approach such as used for the Sun (Schad et al., 2015). Our problem is not easier than theirs.

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