Element Stratification in Stars, 40 years of Atomic Diffusion
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DIFFUSION IN STELLAR ATMOSPHERES

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Abstract. A review of some of the most important studies of the past several decades pertaining to the study of atomic diffusion in stellar atmospheres is presented. A brief description of various studies of radiative accelerations and diffusion calculations in stellar atmospheres is given. Several physical phenomena such as ambipolar diffusion, light-induced drift and the effect of magnetic fields on diffusion are discussed. Results from recent self-consistent model atmospheres including elemental stratification are also reviewed. Particularities of radiative acceleration calculations in stellar atmospheres as well as difficulties and future challenges related to diffusion calculations in stellar atmospheres are also presented.

1 Introduction

During the past several decades, most of the diffusion studies have concentrated on the interior of stars. For example, most widespread calculations of radiative accelerations (e.g. Alecian & Artru 1990, Gonzalez *et al.* 1995, Seaton 1997, Richer *et al.* 1998 and LeBlanc & Alecian 2004) are only valid at large optical depths due to some of the approximations used. Meanwhile, evolutionary stellar models that include the effect of time-dependent atomic diffusion of the various elements have been constructed for stars such as the Sun (Turcotte *et al.* 1998) and for AmFm stars (Turcotte, Michaud & Richer 1998, Richer, Michaud & Turcotte 2000, Richard, Michaud & Richer 2001). These models have been relatively successful in reproducing the abundance anomalies observed. However, since the atmospheres of these stars are not stable enough to enable diffusion to take place, these diffusion studies do not explicitly include the atmospheres.

More recently, a mounting quantity of observational evidence (e.g. Ryabchikova 2005 these proceedings) has appeared that demonstrates the existence of vertical abundance stratification in several types of stars. Diffusion is suspected to be the main cause of many of these abundance anomalies.

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In this paper we shall first review some of the studies that have been published relating to diffusion in the atmospheres of stars. Although this review will certainly not include all of the work done in this field, it will however mention most of the more important studies. We will then discuss some of the physical phenomena related to diffusion which are important in the atmospheres of stars. We will also review recent results from modeling of stellar atmospheres while including stratification of the elements. Finally, a discussion, related to some of the difficulties that need to be surmounted in future modeling of diffusion in stellar atmospheres, will be presented.

2 Historical Perspective

2.1 Earlier studies

Since the breakthrough paper of Michaud (1970), a lot of studies pertaining to the diffusion of the elements in stellar atmospheres have been undertaken. Vauclair, Hardorp & Peterson (1979) was one of the first studies in which radiative accelerations were precisely calculated in the atmosphere. They showed that Si was more abundant at the surface of magnetic stars since the diffusion of the charged ion SiII, which diffuses inwards because of its weak radiative acceleration, is slowed when crossing magnetic lines (see further discussion about this phenomena below). This leads to an overabundance of Si in magnetic stars. Alecian & Vauclair (1981) repeated these calculations using more precise radiative forces, while including the SiII autoionization lines, and obtained the same qualitative results. It should be noted that in these studies, the radiative transfer equation was solved to obtain a precise value for the radiative flux. Borsenberger, Michaud & Praderie (1979) calculated radiative accelerations of the element B in ApBp and HgMn stars. In a follow-up study, Borsenberger, Michaud & Praderie (1981) also calculated the radiative accelerations of the elements Ca and Sr in ApBp stars. Meanwhile, Alecian & Michaud (1981) studied the diffusion of Mn in HgMn stars. They showed that overabundances of Mn could be supported in stars with $T_{eff} < 15000\ K$, while that element will be pushed out in hotter stars due to its large radiative acceleration.

2.2 Some important physical processus

The presence of a magnetic field can strongly affect diffusion via several different processus. The first such process, which is described in Chapman & Cowling (1970), is related to the interaction of moving charged species with a magnetic field. The diffusion velocity is reduced when ions cross magnetic lines. Some studies mentioned above (e.g. Vauclair, Hardorp & Peterson (1979)) showed that this effect can be important for the vertical diffusion of the elements. Even though a horizontal velocity can appear when ions cross inclined magnetic field lines, Megessier (1984) showed that the related time scales seem too long for horizontal diffusion to play a role in Ap stars. Meanwhile, Hui-Bon-Hoa *et al.* (1996) showed that the effect of magnetic fields on the radiative accelerations of Al is important in the atmospheres of Ap stars.

The second physical process, that influences diffusion in magnetic stars, is the Zeeman effect. Following a paper by Babel & Michaud (1991a), which showed the potential importance of polarized radiative transfer on radiative diffusion, Alecian & Stift (2002 and 2004) developed an atmospheric code (CARAT) which can treat the polarized radiative transfer and calculate detailed radiative forces (see Stift 2005 in these proceedings for more details). Their results showed that both the intensity and the orientation of magnetic field lines influence the desaturation of atomic transitions. They found that the radiative accelerations, while including the Zeeman effect, can be amplified by up to approximately 0.4 dex for a field of 4 T, as compared to the nonmagnetic accelerations. Very recently, Kochukhov, Khan & Shulyak (2005) calculated model atmospheres with line-blanketing while including the Zeeman effect. These models produce a flux depression at 5200 Å for cooler Ap stars.

Another way that magnetic fields can play a role in stellar atmospheres, is the interaction between the ambipolar diffusion of hydrogen and magnetic fields (see below). This interaction can affect the atmospheric structure of stars. Babel & Michaud (1991b) studied the ambipolar of hydrogen in Ap stars and discussed its potential importance. Ambipolar diffusion of hydrogen occurs in the ionization transition zone of hydrogen. The proton density gradient in this zone causes a diffusion velocity of the protons in the outgoing direction, while neutral hydrogen diffuses inwards. Of course, the medium has to be hydrodynamically stable in order for such a process to take place, and thus, convection must not be present. Such a suppression of the convection zone in the atmosphere is commonly thought to be caused by the presence of a strong magnetic field.

The diffusing protons, caused by ambipolar diffusion, can drag the various charged species and thus affect their abundance in the atmosphere. Another physical effect, caused by ambipolar diffusion, is related to the Lorentz force acting on the diffusing protons when a strong magnetic field is present. LeBlanc, Michaud & Babel (1994) showed that this force can accentuate the effective gravity on the medium and can thus strongly affect the atmospheric structure of stars. They showed that for strong horizontal magnetic fields (several kG), the effective gravity in the hydrogen ionization zone can be amplified by up to approximately one order of magnitude. This compression can thus lead to a significantly different atmospheric structure in Ap stars, providing that the medium is stable enough to enable ambipolar diffusion of hydrogen.

Another physical process, called light-induced drift (LID), can also be important in stellar atmospheres. Atutov & Shalagin (1988) suggested that LID could be a possible source of isotopic anomalies observed in the atmospheres of certain chemically peculiar stars. For example, White *et al.* (1976) found that in the star χ Lupi, 99% of Hg was in the form of ^{204}Hg while it is only 7% in the Sun. LID can be important when the radiative flux is asymmetrical within the atomic line widths. If Doppler broadening dominates, the blue or red shifted side of the line sees a larger radiative flux than the other side. This then causes an asymmetry of atoms in the excited state traveling in the radial outgoing and ingoing directions, and thus, a spatial asymmetry in the average diffusion coefficients. This induces a drift of the species.

Since the corresponding lines of the isotopes, of a given element, are slightly shifted relative to one another, they can cause the needed flux asymmetry within the lines of their neighbouring isotopes. LeBlanc & Michaud (1993) calculated LID on ^{3}He in the atmospheres of stars with temperatures between 15000 and 21000 K. These calculations only included a single line (at 584 Å) of He and assumed similar effect for all of the other lines. Since the ^{3}He lines are red shifted as compared to the ^{4}He lines, LID causes an outgoing drift on ^{3}He and an ingoing drift for ^{4}He. It was shown that LID can accelerate the separation of ^{3}He and ^{4}He. When there is a large relative abundance of ^{4}He, it causes an outward drift of ^{3}He that can be more important than the diffusion velocity caused by regular radiative diffusion, in certain regions of the atmosphere. As the amount of ^{4}He diminishes, so does the LID effect. And eventually, a certain amount of He (with a relative overabundance of ^{3}He as compared to ^{4}He) will be supported by radiative pressure in the atmosphere.

Since for ionized species, the Coulomb interaction is the dominating term for the diffusion coefficient, the difference between the diffusion coefficient of the initial and final states should be quite small, and thus, LID should be negligible. However, Proffitt *et al.* (1999) suggested that if the atom in the final state is quickly ionized, LID could then be important for charged species. The spatial anisotropy for the diffusion coefficients would then come from the difference of the values of their charge in the initial and final ionized states. More recently Aret & Sapar (2002) found that LID could be important for Hg in HgMn stars.

2.3 Model atmospheres with stratification

In the past, most spectroscopic and photometric studies have used model atmospheres with vertically homogeneous abundances. However, it is known that diffusion can cause stratification in stable stellar atmospheres, and thus, modify their physical structure. In such stars, one should calculate the atmospheric structure self-consistently, along with the predicted elemental stratification caused by diffusion. Dreizler & Wolff (1999) constructed model atmospheres of white dwarfs, while including the stratification of the elements predicted by the equilibrium solution of the diffusion equation (i.e. $v_{diff} = 0$). Their models can better reproduce a flux depression in the ultraviolet part of the spectrum of these stars than the homogeneous models.

Hui-Bon-Hoa, LeBlanc & Hauschildt (2000) constructed similar model atmospheres and applied these to blue horizontal branch (BHB) stars. Several observational clues seem to show that diffusion becomes dominant in the atmospheres of BHB stars with $T_{eff} \succeq 11500\ K$. Grundhal *et al.* (1999), and more recently Fabbian *et al.* (2005), found that elemental abundances observed in these BHB stars are very different from those of the clusters in which they are found. Moreover, Behr *et al.* (2000) found that the rotation velocity of BHB stars fall sharply for stars with $T_{eff} \succeq 11500\ K$. This suggests that diffusion could become dominant in the atmospheres of these stars. Photometric jumps (Grundhal et a. 1999) and photometric gaps (Ferraro *et al.* 1998) are also observed at this same critical value of T_{eff}. These cannot be reproduced with atmospheric models with vertically homogeneous abundances. A full review of observational anomalies of BHB is given in these proceedings (Recio-Blanco 2005).

The models constructed by Hui-Bon-Hoa, LeBlanc & Hauschildt (2000) are based on a modified version of the PHOENIX (e.g. Hauschildt, Allard & Baron 1999) atmospheric code. Their calculations included 39 elements and were done in LTE. The most important ingredient in the diffusion equation is the radiative acceleration (g_{rad}) of the various species. The accelerations in these models are calculated by sampling the radiative flux at a large number of frequency points. In order to have precise g_{rad}, a grid including approximately 240000 frequency points is generally used. The atmospheric code calculates the structure of the atmosphere self-consistently along with the stratification of the elements predicted by the equilibrium solution of the diffusion equation. It was shown that if diffusion becomes efficient in stars with $T_{eff} \succeq 11500\ K$, the models predict photometric jumps and gaps. These gaps and jumps are related to the differences between the homogeneous models (for stars with $T_{eff} \preceq 11500\ K$) and the models with elemental stratification (for stars with $T_{eff} \succeq 11500\ K$). These stratified models also reconcile the lower spectroscopic gravities found when using homogeneous models for BHB stars.

A more recent version of the models of Hui-Bon-Hoa, LeBlanc & Hauschildt (2000) have recently been applied to Ap stars (LeBlanc & Monin 2004). Several improvements were brought to the models. The treatment of diffusion in the partially ionized hydrogen zone was improved, as was the convergence method used to obtain a self-consistent atmospheric structure while calculating elemental stratification. The possibility of having a convective mixing zone was also included. Even though no convection is observed in Ap stars, we cannot at this point exclude the possibility of having a slow convective mixing zone which could dominate diffusion in the hydrogen ionization zone. The reason being that the lower observationnal limit of the mixing velocities, that can be detected, are larger than the typical diffusion velocities. No magnetic effects were included in these models.

Figure 1 shows the stratification of Fe predicted by the stratified models in a $T_{eff} = 7700\ K$ star. Two theoretical models are shown: one assuming a stable atmosphere and another with a convective mixing zone. These theoretical stratification profiles are compared to an empirical one step profile, found by fitting the wings and the centre of Fe lines from observations of the Ap star β CrB (Wade *et al.* 2001). These observations and theoretical results should be interpreted with caution due to the high complexity of Ap stars. It should be noted that the upper plateau in the stratified models, with convective mixing, depends strongly on the position of the convective mixing zone and on mass-loss (e.g. Babel 1992, LeBlanc & Monin 2004). LeBlanc & Monin (2004) showed (see their Figure 2) that the physical structure of the stratified models without convective mixing is strongly modified (as compared to its homogeneous counterpart). Since convective mixing

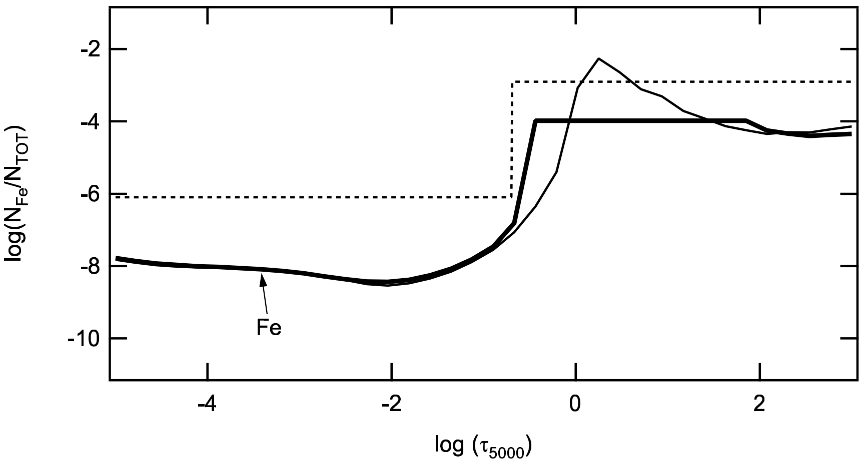

Fig. 1. Abundance at equilibrium of Fe (thin solid curve) supported through the various layers of a $T_{eff} = 7700\ K$ stratified model. The thick solid curve represents the abundance of Fe supported in a model assuming convective mixing. The dotted curve represents the abundance Fe inferred from observations assuming a one step abundance distribution in β CrB.

diminishes the abundance supported in certain parts of the atmosphere, the structure of models with convective mixing is not as strongly modified. These stratified models can also better reproduce the observed UV excess of β CrB (see Fig. 5 of Ryabchikova, Wade & LeBlanc 2003).

The models assuming no convective mixing actually give the maximum amount of matter for each element, that can be supported by radiative pressure at each depth. However, time-dependent phenomena in a real star could prevent this state from being achieved. Models are now being developed with constraints on the reservoir of matter available to accumulate in the atmosphere. To illustrate this, Figure 2 shows the abundance of the element S that can be supported in a homogeneous $T_{eff} = 8000\ K$ atmospheric model. In the simplest time-dependent diffusion scenario; excluding all other competing physical processus and assuming as initial condition an homogeneous solar abundance; the sulphur form the outer atmosphere would sink towards the interior and accumulate in the region $log(\tau_{5000}) \approx 0.6$. The sulphur above $log(\tau_{5000}) \approx 1.1$ would be pushed out and also accumulate there. The sulphur below $log(\tau_{5000}) \approx 1.1$ should sink inwards until equilibrium is reached. In this simple scenario, the amount of sulphur that could accumulate below the region $log(\tau_{5000}) \approx 0.6$ will be limited and will depend on the initial conditions. Constraining the total amount of matter of each element that can accumulate in the atmosphere should give more realistic models than those presented in Figure 1.

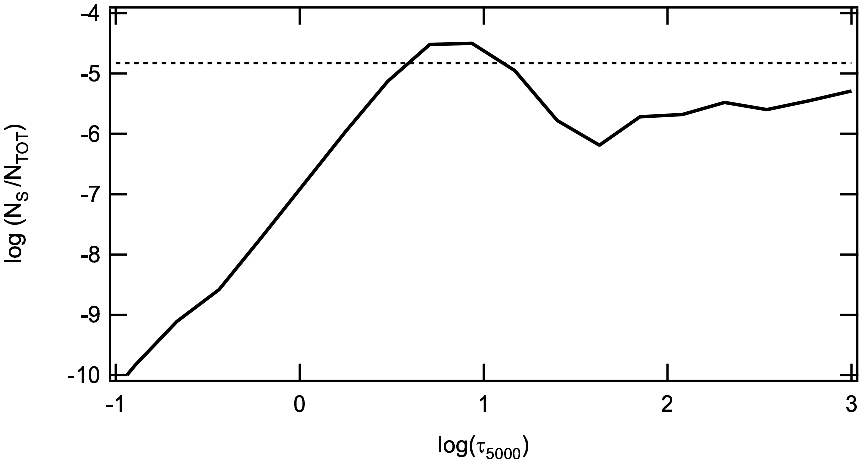

Fig. 2. Abundance at equilibrium of S (solid curve) supported through the various layers of a $T_{eff} = 7700\ K$ homogeneous model. The dotted curve represents the solar abundance of S.

3 Future challenges

Diffusion calculations in stellar atmospheres are particularly difficult for several reasons. These will be discussed in this section. Since the line widths in the atmosphere are much narrower than in stellar interiors, to properly sample the opacity of each species, a large number of frequency points must be used in the integration of the radiative acceleration equation (which depends on opacity of the species times the radiative flux, see Alecian 2005 in these proceedings for more details concerning the properties of radiative accelerations). Typically, approximately 200000 frequency points are needed to obtain precise g_{rad} in the atmosphere. However, this number depends inversely on the abundance of the element under consideration.

Another factor, that differentiates the calculation of g_{rad} in the atmosphere as compared to stellar interiors, is that the flux must be calculated in detail. In interiors, the commonly called diffusion approximation of the flux (Milne 1927) which is however only valid at large optical depths, is sufficient. Hui-Bon-Hoa *et al.* (2002) showed that, as expected, g_{rad} becomes inaccurate at depths of $\tau_{5000} < 1$ (see their Figure 1) when using this approximation. Having to solve the radiative transfer equation at such a large number of frequency points is numerically expensive.

A major uncertainty in the g_{rad} in atmospheres is related to the redistribution of the momentum among the various ions of a given element (see for instance Alecian 2005 in these proceedings and Montmerle & Michaud 1976). Since the diffusion coefficient of the neutral species is much large than that of charged ions, redistribution of momentum to and from the neutral state can greatly modify the

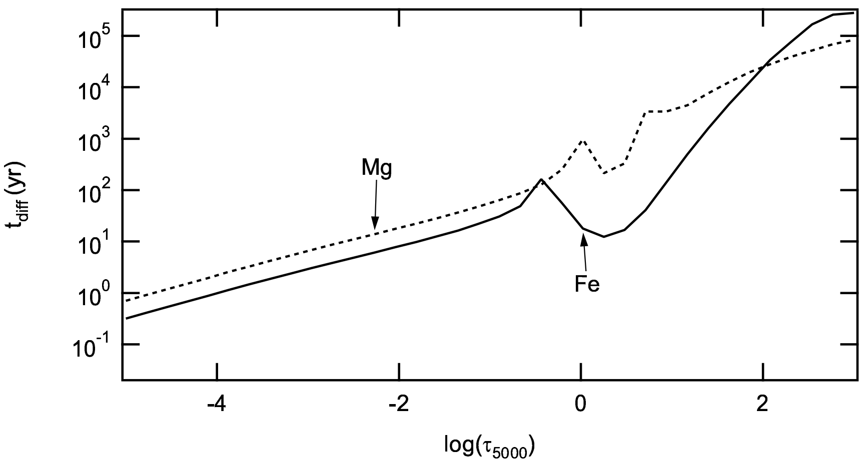

Fig. 3. Diffusion times for a solar abundance of Fe (solid curve) and Mg (dotted curve) through the various layers of a $T_{eff} = 8000\ K$ homogeneous model.

g_{rad} in the atmospheres.

Calculations of g_{rad} have been performed while including the Zeeman effect for a large number of elements (Alecian & Stift 2004). Other g_{rad} calculations have been done in NLTE, but for a somewhat more limited number of elements (e.g. Vauclair, Hardorp & Peterson 1979, Borsenberger, Michaud & Praderie 1979 and 1981, Budaj & Dworetsky 2002). All of the factors mentioned above that affect g_{rad} (redistribution, Zeeman effect and NLTE), should be taken into account simultaneously in future atmospheric studies. This, once again, will demand large computational resources.

The modeling of magnetic stars is particularly difficult. As is commonly known, these stars exhibit abundances patches on there surface. One dimensional models, of vertically stratified atmospheres, can then only have limited success in reproducing the observations of these stars.

Physical effects such as ambipolar diffusion or LID should also be included in future modeling in stars where these phenomena can be important. Since ambipolar diffusion can influence the abundances at the surface of magnetic stars, and that this physical effect can only be present in stable atmospheres, its careful study could give us some information on the stability of the hydrogen ionization zone in Ap stars. Proper treatment of competing physical processus; such as mass-loss, convection and turbulence; should also be included in future modeling. Efforts towards including more elements, specially rare-earths, should also be undertaken, since these are observed to be strongly overabundant in certain stars.

As discussed in the previous section, a time-dependent diffusion model would optimally be needed in order to better reproduce physical reality. However, as shown in Figure 3, we see that the characteristic diffusion times in stellar atmospheres are much shorter than evolutionary time scales. Typical time steps used in evolutionary models, such as those of Turcotte *et al.* (1998), are at a minimum of the order of 10000 yr. While the characteristic times shown in the line forming region can be several orders of magnitude lower. A huge number of time steps would then have to be done in such time-dependent calculations, along with interfacing with the stellar interior. These sorts of calculations are presently outside the bounds of possibilities, due to extremely large CPU time needed for such modeling.

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References

Alecian, G. 2005, these proceedings

Alecian, G. & Stift, M. J. 2004, A&A, 416, 703

Alecian, G. & Stift, M. J. 2002, A&A, 387, 271

Alecian, G. & Artru, M.-C. 1990, A&A, 234, 323

Alecian, G. & Michaud, G. 1981, ApJ, 245, 226

Alecian, G. & Vauclair, S. 1981, A&A, 101, 16

Aret, A. & Sapar, A. 2002, AN, 323, 21

Atutov, S. N. & Shalagin, A. M. 1988, Sov. Astron. Lett., 14, 284

Babel, J. 1992, A&A, 258, 449

Babel, J. & Michaud, G. 1991a, A&A, 241, 493

Babel, J. & Michaud, G. 1991b, A&A, 258, 155

Behr, B. B., Djorgovski, S. G., Cohen, J. G., McCarthy, J. K., Côté, P., Piotto, G. & Zoccali, M. 2000, ApJ, 528, 849

Borsenberger, G., Michaud, G. & Praderie, F. 1979, A&A, 76, 287

Borsenberger, G., Michaud, G. & Praderie, F. 1981, ApJ, 243, 533

Budaj, J. & Dworetsky, M. M. 2002, MNRAS, 337, 1340

Chapman, S. & Cowling, T. G. 1970, The Mathematical Theory of Non-uniform Gases, Cambridge University Press, 3rd ed.

Dreizler, S. & Wolff, B. 1999, A&A, 348, 189

Fabbian, D., Recio-Blanco, A., Gratton, R. G. & Piotto, G. 2005, A&A, 434, 235

Ferraro, F. R., Paltrinieri, B., Fusi Pecci, F., Dorman, B. & Rood, R. T. 1998, ApJ, 500, 311

Gonzalez, J.-F., LeBlanc, F., Artru, M.-C. & Michaud, G. 1995, A&A, 297, 223

Grundahl, F., Catelan, M., Landsman, W. B., Stetson, P. B. & Andersen, M. I. 1999, ApJ, 524, 242

Hauschildt, P. H., Allard, F. & Baron, E. 1999, ApJ, 512, 377

Hui-Bon-Hoa, A., LeBlanc, F., Hauschildt, P. H. & Baron, E. 2002, A&A, 381, 197

Hui-Bon-Hoa, A., LeBlanc, F. & Hauschildt, P. H. 2000, ApJ, 535, L43

Hui-Bon-Hoa, A., Alecian, G. & Artru, M.-C. 1996, A&A, 313, 624

Kochukhov, O., Khan, S. & Shulyak, D. 2005, A&A, 433, 671

LeBlanc, F. & Alecian, G. 2004, MNRAS, 332, 1329

LeBlanc, F. & Monin, D. 2004, in The A-star Puzzle, eds. J. Zverko, J. Ziznovsky, S. J. Adelman and W. W. Weiss, IAU Symp., 224, 193

LeBlanc, F., Michaud, G. & Richer, J. 2000, ApJ, 538, 876

LeBlanc, F., Michaud, G. & Babel, J. 1994, ApJ, 431, 388

LeBlanc, F. & Michaud, G. 1993, ApJ, 408, 251

Michaud, G. 1970, ApJ, 160, 641

Milne, E. A. 1927, M. N., 87, 697

Megessier, C. 1984, A&A, 138, 267

Montmerle, T. & Michaud, G. 1976, ApJS, 31, 489

Proffitt, C. R., Brage, T., Leckrone, D. S., Wahlgren, G. M., Brandt, J. C., Sansonetti, C. J., Reader, J. & Johansson, S. G. 1999, ApJ, 512, 942

Recio-Blanco, A. 2005, these proceedings

Richard, O., Michaud, G. & Richer, J. 2001, ApJ, 558, 377

Richer, J., Michaud, G. & Turcotte, S. 2000, ApJ, 529, 338

Richer, J., Michaud, G., Rogers, F., Iglesias, C., Turcotte, S. & LeBlanc, F. 1998, ApJ, 492, 883

Ryabchykova, T. 2005, these proceedings

Ryabchykova, T., Wade, G. & LeBlanc, F. 2003, in Modelling of Stellar Atmospheres, eds. N. Piskunov, W. W. Weiss and D. F. Gray, IAU Symp., 210, 301

Seaton, M. J. 1997, MNRAS, 289, 700

Stift, M. J. 2005, these proceedings

Turcotte S., Richer, J. & Michaud, G. 1998, ApJ, 504, 559

Turcotte S., Richer, J., Michaud, G., Iglesias, C. A. & Rogers, F. J. 1998, ApJ, 504, 539

Vauclair, S., Hardorp, J. & Peterson, D. M. 1979, ApJ, 227, 526

Wade, G. A., Ryabchikova, T. A., Bagnulo, S. & Piskunov, N. 2001, in Magnetic Fields across the Hertzsprung-Russell Diagram, ed. G. Mathys, S. K. Solanki & D. T. Wickramasinghe, ASP Conf. Series 248, 373

White, R. E., Vaughan, A. H., Preston, G. W. & Swings, J. P. 1976, ApJ, 204, 131