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A. Siebert, K. Baillié, M. Béthermin, F. Cantalloube, E. Josselin, N. Lagarde, J. Malzac, J. Richard, L. Selliez, O. Venot (eds)

ATOMIC DIFFUSION: A TRANSPORT PROCESS THAT SEPARATES CHEMICAL SPECIES

A. Hui-Bon-Hoa[1]

Abstract. While most transport processes act on the stellar material as a whole and originate from intrinsic parameters of the star or from global quantities of the stellar matter (e.g. opacity, mean molecular weight), the effects of atomic diffusion depend on quantities related to each chemical species. In turn, the properties of each species (e.g. atomic mass, collisional cross-sections, absorption properties) are involved in the calculation of atomic diffusion. If the mixing processes are weak enough, the chemical composition then varies from place to place in the star, giving rise to superficial abundance anomalies and to structural changes, which can be detected by asteroseismology.

Keywords: transport processes – stellar interiors – stellar atmospheres – atomic diffusion – radiative accelerations

1 Introduction

Most transport processes at play in the stellar medium induce motions of particles regardless of their kind. Some depend only on global properties of the star, such as rotational mixing (Zahn 1992). Other are triggered by bulk quantities of the medium, like the mean molecular weight for fingering instability (e.g. Vauclair 2004, and references therein). They act on the stellar material as a whole, either mixing it and/or moving it from one place the another (e.g. meridional circulation).

Atomic diffusion is the only transport process that acts differently on each chemical species, inducing motions depending on properties pertaining the species under consideration. The main forces that drive the motion are gravity and radiative accelerations, which describe the momentum transfer between the radiation field and each kind of particles. As time goes by, elements separate, each having an abundance varying with depth, provided that the mixing processes are weak enough. The velocities induced by diffusion are actually very small and, as an illustration, Michaud (1970) stated that the velocity of the mixing processes should be less than 10^{-3}cm.s^{-1} in A-type star atmospheres for diffusion to be efficient. The departures from the initial abundances are observable at the surface and atomic diffusion was historically first invoked to understand the observation of abundance anomalies at stellar surfaces, like the absence of metal signatures in the spectra of white dwarfs (Schatzman 1945), and the strong abundances anomalies observed in Am stars (Watson 1970; Smith 1971) or Ap stars (Michaud 1970), among other Chemically Peculiar (CP) stars. More subtle effects can be detected through asteroseismology, the variation of the internal mixture changing the propagation of the pulsation modes (e.g. Deal et al. 2018).

We first describe the basic properties of atomic diffusion (Sect. 2) and then show some recent improvement in its implementation in stellar evolution codes (Sect. 3). We proceed with some recent applications (Sect. 4).

2 Basics on atomic diffusion

Transport by atomic diffusion appears when inhomogeneities are present in a given medium, e.g. concentration or temperature gradients, or when external forces act on it. The process is described in the framework of kinetic theories, in the present case by solving the Boltzmann equation. The motion of the different chemical species is determined by a diffusion velocity, expressed with respect to another species. In the formalism of

[1] IRAP, Université de Toulouse, CNRS, UPS, CNES, Toulouse, France

Burgers (1969), no species has a particular role, whereas the Chapman & Cowling (1970) approach requires to define a background species in which the species of concern, whose number density is negligible (test atom approximation), moves. In stellar applications, this most convenient background species is the major component of the medium, e.g. hydrogen for main sequence stars. We write below a simplified expression from Chapman & Cowling (1970)'s formalism showing the main terms involving the species i we consider:

$$V_{\rm diff}(i) \simeq D_{\rm diff}(i) \times \left[\frac{M_i}{\mathrm{k}T}(-g + g_{\rm rad}(i)) - \nabla \ln c_i + \frac{(Z_i+1)m_p g}{2\mathrm{k}T} + ...\right] \tag{2.1}$$

where $V_{\rm diff}(i)$ is the diffusion velocity of ions i, $D_{\rm diff}(i)$ their diffusion coefficient, M_i their mass, Z_i their ionisation degree, and c_i their concentration. m_p is the proton mass, k the Boltzmann constant and T the temperature. Gravity acceleration g and the radiative accelerations $g_{\rm rad}(i)$ yield the external forces.

3 Implementation in stellar codes

The diffusion coefficients $D_{\rm diff}(i)$ can be obtained through numerical estimates of the coupling of ions during collisions as in Paquette et al. (1986). The radiative acceleration g_{rad} on element i writes

$$g_{\rm rad}(i) = \frac{1}{c}\frac{1}{M_i}\int \sigma_\nu^{\rm mta}(i)\mathcal{F}_\nu \mathrm{d}\nu \tag{3.1}$$

where c is the speed of light. The cross-section $\sigma_\nu^{\rm mta}(i)$ describes the momentum transfer to the atom at frequency ν (thus the superscript 'mta') and contains the contributions of bound-bound transitions, photoionisation, and free-free absorption. The last two processes are three-body interactions and part of the momentum of the photon is granted to the electron. $\sigma_\nu^{\rm mta}(i)$ includes only the part taken away by the atom. $\mathcal{F}_\nu$ is the radiation flux at frequency ν and is obtained by solving the radiative transfer equation (RTE). In optically thin media, like stellar atmospheres, the RTE has to be solved numerically.

3.1 Computations of radiative accelerations in stellar interiors

We will now focus on stellar interiors where the medium is optically thick so that an analytical solution for the radiative flux (the photon diffusion approximation, Milne 1927) can be used. $g_{\rm rad}(i)$ is then written as

$$g_{\rm rad}(i) = \frac{1}{c}\frac{\mu}{\mu_i}\mathcal{F}\kappa_{\rm R}\gamma_i \tag{3.2}$$

with μ and μ_i the mean atomic mass and the atomic mass of species i, respectively,

$$\gamma_i = \int \frac{\sigma_\nu^{\rm mta}(i)}{\sigma_\nu}\frac{\frac{\mathrm{d}B_\nu}{\mathrm{d}T}}{\frac{\mathrm{d}B}{\mathrm{d}T}}\mathrm{d}\nu \tag{3.3}$$

where σ_ν is the total opacity of the mixture at frequency ν, and $\mathcal{F}$, the integrated flux,

$$\mathcal{F} = \pi B(T_{\rm eff})\left(\frac{R_*}{r}\right)^2 \tag{3.4}$$

$B(T_{\rm eff})$ is the Planck function at effective temperature $T_{\rm eff}$. r and R_* are the local and stellar radii, respectively.

3.1.1 Optimised computations from monochromatic cross-sections

According to Eq. 3.3, integrations over the whole frequency range are required for each element in each layer of the stellar model, which could be time-consuming. However, Hui-Bon-Hoa (2024) implemented in the Toulouse-Geneva Evolution Code (TGEC, Hui-Bon-Hoa 2008) a method to reduce the computing time by performing as few calculations as possible. This aim is reached by computing once for all the γ_i's for all the elements with their initial abundances and store them in an array. Then, for each layer of the star, $g_{\rm rad}(i)$ is computed as in the Opacity Project (OP) OPCD v.3.3 routines (Seaton 2005): 16 grid points (4 temperatures T, by 4 electronic densities $N_{\rm e}$) are selected around the (T, $N_{\rm e}$) of the current layer, providing 16 γ_i values. The γ_i for the layer of concern is then obtained by a bi-cubic interpolation of the logarithms of the 16 grid point γ_i's (see

Hui-Bon-Hoa 2024 for the handling of negative γ_i's). If the abundances in a given layer are the same as the initial ones, the 16 γ_i's are excerpted from the array. If not, new γ_i's are computed with the current abundances using a parallelised routine. As we go from a layer to the next, if the mixture is the same, some if not all of the previous set of 16 γ_i's can be reused. Only γ_i's that were not considered for the previous layer are calculated. Figure 1 shows the case where one new temperature and one new electronic density are required, implying the computation of only 7 new grid point γ_i's.

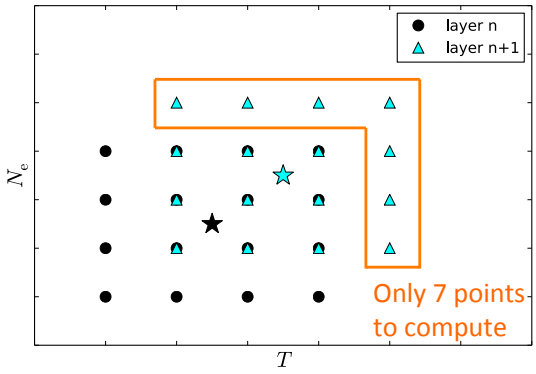

Fig. 1. Grid points (black dots) in the (T,N_e) plane involved in the computation of the γ_i's of layer n (black star) and those (blue triangles) needed for layer $n+1$ (blue star). Nine grid points overlap so that only 7 new γ_i's are computed.

Calculation from OP monochromatic data is also implemented in MESA (see Jermyn et al. 2023, and references therein), first with the Hu et al. (2011) method, which is an optimisation of that of OP. Mombarg et al. (2022) introduced further optimisation steps, including an approximation for the dependence of $g_{\rm rad}$ with respect to the abundances. To save computing time, they split the envelope in two areas and used a mean abundance in each part for each element. Their $g_{\rm rad}$ thus depart from the values obtained with the actual abundances, and this optimisation procedure cannot be used in stars in which the abundances vary in a large interval in the envelope (Hui-Bon-Hoa 2024). The Montpellier-Montréal evolution code (Turcotte et al. 1998) also computes $g_{\rm rad}$ by integrating monochromatic data (Richer et al. 1998), but with OPAL cross-sections.

3.1.2 Computations with an analytical approximation

Aimed to gain time by avoiding the frequency integrations, the approximation developed by G. Alecian and F. LeBlanc (see Alecian & LeBlanc 2020, and references therein) uses analytical functions (the so-called Single-Valued Parameter method, SVP) that separate the atomic properties of the ion under consideration and the stellar local and global quantities. For each stellar mass of a given mass grid, six coefficients are computed for each ionisation stage of each chemical species. Three of them are calculated from atomic data, the three other being determined through fits to the $g_{\rm rad}$ coming from the OPCD v.3.3 data and codes (Seaton 2007). $g_{\rm rad}$ due to bound-bound transitions are evaluated with an expression involving four of these coefficients whereas the absorptions through photoionisations are estimated with a two-coefficient function. For masses out of the grid points, $g_{\rm rad}$ is obtained using a linear interpolation of the coefficients for the surrounding mass grid points. The SVP tables are publicly available*, and are used to date in TGEC, CESAM2k20 (Deal et al. 2018) and Moedas et al. (2025)'s version of MESA.

4 Recent applications

4.1 Evolution of the surface abundance of scandium in Am stars

Scandium is a key element in Am stars because its surface underabundances is one of the signature of this group of CP stars, along with the deficiency of calcium and overabundances of heavy elements (Conti 1970). The case of some of these other elements have been addressed by Richer et al. (2000) with stellar models including *ad hoc* turbulent mixing, and by Vick et al. (2010) using models with mass loss. Hui-Bon-Hoa et al. (2022) used the SVP

*https://voparis-gradsvp.obspm.fr/

approximation in TGEC to compute $g_{\rm rad}$ for Sc and the time evolution of its surface abundance with various mixing prescriptions. The Sc abundance evolution tracks were compared to observed cluster stars values and they concluded that their results were in line with previous studies with other elements: the turbulent mixing model of Richer et al. (2000) was the only mixing prescription that could reproduce the observations, and the mass loss rates of Vick et al. (2010) allowed to match the observations, though smaller values could be adopted.

4.2 Comparison between direct integration method and analytical approximation

Using TGEC, Hui-Bon-Hoa (2024) compared the $g_{\rm rad}$ obtained through the 2004 and 2020 versions of the SVP approximation with those coming from direct integration of the monochromatic data. This exercise has been done for Am star models and showed that the three methods agree within a typical abundance uncertainty of 0.2 dex, except for some elements of the 1.5 $M_{\odot}$ wind model. The gain in computing time with SVP depends on the number of $g_{\rm rad}$ calculations between two structural convergences and is generally small if the Rosseland means are also computed from monochromatic data, which ensures consistency between abundances and stellar structure. In a test with mean opacities obtained through interpolations in OPAL opacity tables, the gain is much greater with SVP, though some abundance differences exceed marginally the typical error.

5 Conclusions

Atomic diffusion is included nowadays more and more often in stellar modelling thanks to the availability of efficient computers and to numerical strategies developed to optimise the calculations of the radiative accelerations. Derived from first principles, atomic diffusion allows to constrain the free parameters of competing transport processes, with the aid of the insight on the stellar structure provided by asteroseismlogy.

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References

Alecian, G. & LeBlanc, F. 2020, MNRAS, 498, 3420
Burgers, J. M. 1969, Flow Equations for Composite Gases (Academic Press)
Chapman, S. & Cowling, T. G. 1970, The Mathematical Theory of Non-uniform Gases. an Account of the Kinetic Theory of Viscosity, Thermal Conduction and Diffusion in Gases, 3rd edn. (Cambridge: University Press)
Conti, P. S. 1970, PASP, 82, 781
Deal, M., Alecian, G., Lebreton, Y., et al. 2018, A&A, 618, A10
Hu, H., Tout, C. A., Glebbeek, E., & Dupret, M.-A. 2011, MNRAS, 418, 195
Hui-Bon-Hoa, A. 2008, Ap&SS, 316, 55
Hui-Bon-Hoa, A. 2024, A&A, 691, A266
Hui-Bon-Hoa, A., Alecian, G., & LeBlanc, F. 2022, A&A, 668, A6
Jermyn, A. S., Bauer, E. B., Schwab, J., et al. 2023, ApJS, 265, 15
Michaud, G. 1970, ApJ, 160, 641
Milne, E. A. 1927, MNRAS, 87, 697
Moedas, N., Deal, M., & Bossini, D. 2025, A&A, 695, A9
Mombarg, J. S. G., Dotter, A., Rieutord, M., et al. 2022, ApJ, 925, 154
Paquette, C., Pelletier, C., Fontaine, G., & Michaud, G. 1986, ApJS, 61, 177
Richer, J., Michaud, G., Rogers, F., et al. 1998, ApJ, 492, 833
Richer, J., Michaud, G., & Turcotte, S. 2000, ApJ, 529, 338
Schatzman, E. 1945, Annales d'Astrophysique, 8, 143
Seaton, M. J. 2005, MNRAS, 362, L1
Seaton, M. J. 2007, MNRAS, 382, 245
Smith, M. A. 1971, A&A, 11, 325
Turcotte, S., Richer, J., & Michaud, G. 1998, ApJ, 504, 559
Vauclair, S. 2004, ApJ, 605, 874
Vick, M., Michaud, G., Richer, J., & Richard, O. 2010, A&A, 521, A62
Watson, W. D. 1970, ApJ, 162, L45
Zahn, J. P. 1992, A&A, 265, 115