# ON THE THEORY OF HELIUM DIFFUSION IN STELLAR OUTER LAYERS

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#### RESUMEN

Discutimos las aproximaciones que se hacen usualmente para el tratamiento de la difusión en las capas estelares externas. Analizamos analítica y numéricamente las hipótesis de difusión binaria y de difusión sobre un fondo que no se ve alterado por dicho proceso. Aplicamos los cálculos numéricos a ciertas estrellas centrales de nebulosas planetarias en las que se ha observado una abundancia de helio menor que la normal. Encontramos que, en este caso, la difusión puede ser tratada como un proceso binario pero no puede ser desacoplada del cálculo de estructura. Presentamos un método alternativo para estudiar la difusión y lo aplicamos a las estrellas centrales antes mencionadas. De este modo resolvemos el conjunto de ecuaciones hidrodinámicas estacionarias para un gas totalmente ionizado de hidrógeno y helio. Este modelo trata en forma consistente el comportamiento de todas las especies. Obtenemos abundancias de equilibrio muy diferentes de las obtenidas con el método del elemento de prueba mientras la densidad del helio y la de los electrones crecen hacia el interior de la estrella, la de los protones tiende a disminuir. Sin embargo, cálculos preliminares de estabilidad sugieren la posibilidad de que éstas no sean las distribuciones reales.

#### ABSTRACT

We discuss the approximations usually made in the different approaches to diffusion in stellar outer layers. We analyze the hypotheses of binary diffusion and diffusion over a non altered background both analytically and numerically. Numerical calculations are applied to central stars of planetary nebulae in which a depletion of helium is observed. We find that in this case helium diffusion may be considered as a binary process but cannot be decoupled from the structure computation. We present an alternative method for studying diffusion and apply it to the central stars. We thus solve a stationary hydrodynamic model for a completely ionized H-He plasma, which takes into account consistently the behavior of all the species. We find equilibrium abundance distributions very different from those obtained according to the trace element approaches while helium and electron densities increase with depth in the atmosphere, protons tend to decrease. However, preliminary studies of the stability show that these are not the actual distributions.

Key words: DIFFUSION - HYDRODYNAMIC MODELS - HELIUM ABUNDANCES

#### I. INTRODUCTION

The problem of diffusion in the context of anomalous abundances in stars has been extensively touched on (Chapman 1958; Michaud 1970; Vauclair and Vauclair 1979, 1982; Michaud et al. 1976; Vauclair and Reisse 1977; Vauclair, Vauclair, and Greenstein 1979; Fontaine and Michaud 1979). Generally the diffusion of a trace element is considered, decoupling this process from the structure equations. Moreover, the diffusion of the trace ions is treated as a binary process, neglecting the contribution of electrons (Aller and Chapman 1960; Vauclair and Vauclair 1982; Montmerle and Michaud 1976).

Structure models have been computed considering

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the effect produced by the modification of the diffusing species concentration during the evolution in Vauclair, Vauclair, and Pamjatnikh (1974) and Vauclair et al. (1978). However, in both cases, diffusion is treated in the binary approximation. Besides, there is one work (Noerdlinger 1977) in which the evolution of the structure is computed solving consistently the hydrodynamic equations for the elements present, considering diffusion in the multicomponent gas.

The assumption of binary diffusion has been also relaxed in a group of papers which mostly deal with the computation of transport coefficients. Noerdlinger (1978) uses multicomponent flow equations to obtain diffusion rates. A similar approach is applied to white dwarfs by Muchmore (1984). He also calculates the diffusion velocities in a multicomponent gas without taking the trace element approximation into account. A different treatment is carried out by Roussel-Dupré (1981) who computes the transport coefficients solving a Fok-

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ker-Planck equation for each component present in the mixture. Montmerle and Michaud also take electrons into account in order to compute the electric field, which finally affects the thermal diffusion coefficient, but neglect them in other processes. The equations derived in their paper have been extensively used in the literature for the study of chemically peculiar stars.

In the present work we are interested in the analysis of helium diffusion in central stars of planetary nebulae.

Recent studies of the atmospheres of central stars of planetary nebulae have revealed the existence of objects that have helium abundances significantly smaller than the solar one (Méndez et al. 1981; Méndez, Kudritzki, and Simon 1983). This effect is observed in the stars with higher surface gravities, which are presumably more advanced in their evolution, and it may be attributed to the gravitational settling of helium. This conclusion is supported by the fact that the outward radiation force is everywhere overcome by gravity and other thermodynamical forces. Indeed, we have computed the forces acting on helium using a grid of atmosphere models made available to us by Kudritzki (1983). A description of these models can be found in Kudritzki (1976), Kudritzki and Simon (1978) and Méndez et al. (1981). In Table 1 the stellar atmosphere parameters for the two models we analize in this paper are tabulated. We are interested in those regions where the optical depth is greater than unity. At this depth helium is mostly doubly ionized, therefore, the radiation force is expected to be weak. We have repeated the computation of the radiation force by two methods. The first one is the one used in Vauclair et al. (1979), the second one is that described in Montmerle et al (1979) (see Appendix C for more details). In Figure 1 we can see that in the deep atmospheric layers  $(\tau > i)$  the acceleration due to the pressure and temperature gradients averaged over all athe states of ionization of helium (g<sub>GT</sub>) is always greater than the radiative acceleration (g<sub>R</sub>) Therefore, one may conclude that the gravitational settling of helium indeed occurs. However, the underlying model which allows one to draw such a conclusion is based on assumptions, like binary diffusion on a background, which may not be valid in this case.

It is our aim to discuss the validity of the assumptions of binary diffusion and diffusion over a non-altered background. The analysis will not be completely general, and, in some cases, we will limit ourselves to the physical conditions that prevail in the central stars in which we are interested.

The organization of the paper is as follows. In Section

TABLE 1

	Model I	Model II
T <sub>eff</sub> (° K)	75 000	75 000
T <sub>eff</sub> (° K) log g (cm/seg <sup>2</sup> )	5.50	6.50
n <sub>He</sub> /n <sub>p</sub>	0.1	0.01

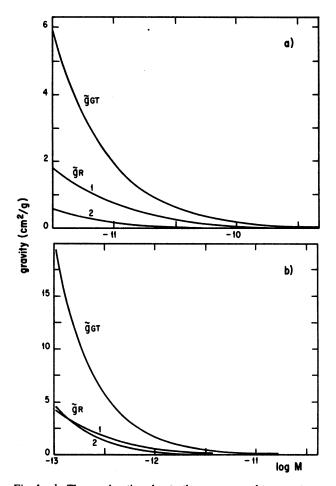


Fig. 1a, b. The acceleration due to the pressure and temperature gradient, conveniently scaled,  $\tilde{g}_{GT}$  and the radiative acceleration  $\tilde{g}_R$  computed by method 1 (curve labeled 1) and by method 2 (curve labeled 2) are compared. Fig. 1a corresponds to a model with normal helium abundance (Model I,  $n_{He}/n_p = 0.1$ ). Fig. 1b corresponds to a model with anomalous helium abundance (Model II,  $n_{He}/n_p = 0.01$ ). The differences between the radiative accelerations computed by the two methods considered are well within the uncertainty of the fitting formula used for method 2. This difference is smaller for Model II, due to the fact that the condition for using the fitting formula (eq. 10 of Michaud et al. 1979) is better satisfied. In both cases  $\tilde{g}_R$  is less than 30% of  $\tilde{g}_{GT}$ .

II we analyze under what conditions these assumptions may be valid and whether they may be applied to our case or not. We also discuss the simplifications usually made in the treatment of ionization and radiation. In Section III we describe the method for studying diffusion. We present a stationary hydrodynamic model for a gas of electrons, protons and ions and solve the equations for the central stars of planetary nebulae (Models I and II) in the equilibrium and in the case of non-vanishing diffusion velocitites. This hydrodynamic model is in the spirit of Noerdlinger (1977), but it is time-independent. We also describe some results concerning the stability of the distributions. Finally conclusions are summarized in Section IV.

# II. DISCUSSION ON APPROACHES TO THE DIFFUSION PROBLEM

This section is devoted to the discussion of the validity of certain assumptions that are usually made in the study of diffusion in stars. They may be listed as:

i) diffusion as a binary process.

ii) test atom approximation.

iii) negligible concentration gradients for the computation of equilibrium abundances.

As we have already pointed out, there are some works in which these assumptions are relaxed. What we do in this section is to obtain the conditions that must be fulfilled for the assumptions i) and ii) to be valid, and check if the usual arguments that lead to these hypotheses are correct or not. In the computation of equilibrium abundances, we restrict our attention to the case of the central stars of planetary nebulae and analyze what may and may not be done in this particular case. However, some general conclusions may be obtained. We also discuss the problem of ionization and radiation connected with diffusion processes and give some qualitative ideas.

### a) Diffusion as a Binary Process

The diffusion problem has usually been treated as a binary process, neglecting the electron dynamics. (i. e., Montmerle and Michaud 1976). This assumption is based on the fact that the diffusion coefficients for electrons with respect to protons and ions are 40 times greater than the diffusion coefficients for ions with respect to protons. We will check this hypothesis for the simple case of a completely ionized gas formed of electrons, protons and ions in one state of ionization. We will assume one-dimensional geometry, which applies both to planar or spherical symmetry, and electrical neutrality. The analysis will be done as follows. We will start from the corresponding general equations, impose some restrictions, derive a "reduced" equation and compare it with the binary case (eq. 2.7). We will thus obtain sufficient conditions for the different hypothesis to be valid.

The general equations which relate the diffusion velocities are (see Chapman and Cowling 1970)

$$d_{i} + k_{i}^{T} \frac{d \ln T}{d r} =$$

$$= -(v_{i} - v_{p}) \frac{n_{i} n_{p}}{n^{2} D_{ip}} - (v_{i} - v_{e}) \frac{n_{i} n_{e}}{n^{2} D_{ie}}$$

$$d_{p} + k_{p}^{T} \frac{d \ln T}{d r} = -(v_{p} - v_{i}) \frac{n_{i} n_{p}}{n^{2} D_{i...}} -$$
(2.1)

$$-(v_{p}-v_{e})\frac{n_{p} n_{e}}{n^{2} D_{ne}}, \qquad (2.2)$$

$$d_{e} + k_{e}^{T} \frac{d \ln T}{d r} = -(v_{e} - v_{i}) \frac{n_{i} n_{p}}{n^{2} D_{ie}} - (v_{e} - v_{p}) \frac{n_{e} n_{p}}{n^{2} D_{ep}}$$
(2.3)

where

$$d_i + d_p + d_e = 0, k_i^T + k_p^T + k_e^T = 0,$$
 (2.4)

anc

$$d_{s} = \frac{d}{dr} \left(\frac{n_{s}}{n}\right) + \left(\frac{n_{s}}{n} - \frac{\rho_{s}}{\rho}\right) \times \frac{d\ln P}{dr} - \frac{f_{s}}{P} + \frac{\rho_{s}}{\rho n} \sum_{j} F_{j}, \quad (2.5)$$

Supposing that  $D_{ie}$   $n_p/D_{ip}$   $n_e >> 1$ , which holds for Coulomb interactions and for a non negligible proton abundance, after some algebra we obtain

$$- (v_{i} - v_{p}) = \frac{n^{2}}{n_{i} n_{p}} D_{ip} \times$$

$$\times \left[ \frac{d_{i} + k_{i}^{T} \frac{d \ln T}{d r}}{1 + \frac{D_{pe}}{D_{ie}} \frac{n_{i}}{n_{p}}} - \frac{d_{p} + k_{p}^{T} \frac{d \ln T}{d r}}{1 + \frac{D_{ie}}{D_{pe}} \frac{n_{p}}{n_{i}}} \right] . \quad (2.6)$$

At first sight this expression seems to be independent of the presence of electrons, since the ratio

$$\frac{D_{pe}}{D_{ie}} \approx Z_i^2 \left(\frac{m_i}{m_p}\right)^{3/2}$$

does not depend on electron variables. However, both  $d_i$  and  $d_p$  contain terms on the external forces acting on all the species present. From (2.4) we see that electrons also affect thermal diffusion. Thus, only when there are no external forces acting on the electrons or when thermal diffusion is not important, we can say that no electron term will appear in the expression for the diffusion of ions and protons. However, even in this case, equation (2.6) does not reduce to the corresponding one to a binary ion to proton diffusion which is

$$-(v_{i} - v_{p}) = \frac{n^{2}}{n_{i} n_{p}} D_{ip} \left( d_{i} + k_{i}^{T} \frac{d ln T}{dr} \right)$$
 (2.7)

Consequently the smallness of the  $D_{ie}/D_{pe}$  ratio does not suffice to reduce diffusion to the binary case.

Let us now suppose that the ion concentration is negligible,  $n_i/n << 1$ , and that ions do not affect electron to proton diffusion. This assertion is equivalent to saying that the electron and proton distributions are not altered by the ion diffusion (test atom approximation). For this last assumption to be valid it is necessary that the following conditions hold:

$$| v_{i} - v_{p} | \frac{n_{i} n_{p}}{n^{2} D_{ip}} << | d_{p} + k_{p}^{T} \frac{d \ln T}{d r} |,$$

$$| v_{i} - v_{e} | \frac{n_{i} n_{e}}{n^{2} D_{ie}} << | d_{e} + k_{e}^{T} \frac{d \ln T}{d r} |.$$

$$(2.8)$$

In this way the electron and proton velocities are related by

$$-(v_{p} - v_{e}) \frac{n_{e} n_{p}}{n^{2} D_{pe}} \simeq d_{p} + k_{p}^{T} \frac{d \ln T}{d r} \simeq$$

$$\simeq -\left(d_{e} + k_{e}^{T} \frac{d \ln T}{d r}\right) \quad (2.9)$$

where in this case is

$$n \simeq n_p + n_e$$
 .

Nevertheless, the ions affect these velocities through the external force terms which appear in  $d_p$  and  $d_e.$  Therefore, the ion contribution to  $\boldsymbol{v}_p-\boldsymbol{v}_e$  may be ignored only when  $F_i/P$  is negligible.

Substituting  $v_e$  obtained from (2.9) into (2.1) we obtain

$$-(v_i - v_p) = \frac{n^2 D_{ip}}{n_i n_p} \times$$

$$\times \left[ d_i + k_i^T \frac{d \ln T}{d r} - \frac{n_i}{n_p} \frac{D_{pe}}{D_{ie}} \left( d_p + k_p^T \frac{d \ln T}{d r} \right) \right] \cdot (2.10)$$

Provided that

$$D_{pe} n_i / D_{ie} n_p << I,$$
 (2.11)

we also obtain (2.10) from (2.6). However, in order to neglect the influence of ions on proton to electron diffusion it is necessary to also assume that

$$d_i + k_i^T \frac{d \ln T}{d r} << d_{p,e} + k_{p,e}^T \frac{d \ln T}{d r}$$
 (2.12)

Conditions (2.11) and (2.12) are equivalent to (2.8). We can see that further restrictions must be imposed to obtain (2.7). Binary diffusion is recovered supposing

$$\frac{n_{i}}{n_{p}} \frac{D_{pe}}{D_{ie}} \mid d_{p} + k_{p}^{T} \frac{d l n T}{d r} \mid << \mid d_{i} + k_{i}^{T} \frac{d l n T}{d r} \mid . \quad (2.13)$$

This condition is not easily satisfied, since almost all the terms in  $d_i$  are proportional to  $n_i$ , except those on the external forces [see also that it must be satisfied together with (2.11) and (2.12)]. Let us consider the case for which the right hand side of (2.13) is mainly determined by  $F_i/P$ . If this term were of the order of  $d_p$  the diffusion velocity terms in (2.1) would be comparable to  $d_p$ , in contrast to condition (2.8). Consequently, a sufficient condition for (2.13) to be valid is to require that

$$\frac{n_i}{n_p} \frac{D_{pe}}{D_{ie}} |d_p + k_p^T \frac{dlnT}{dr}| << |d_i + k_i^T \frac{dlnT}{dr}| \sim$$

$$\sim \frac{F_i}{p} << |d_p + k_p^T \frac{dlnT}{dr}| . (2.14)$$

In the case for which thermal diffusion is dominant, similar reasoning may be applied, leading to the sufficient condition

$$\frac{n_{i}}{n_{p}}\frac{D_{pe}}{D_{ie}}\mid d_{p}+k_{p}^{T}\frac{dlnT}{dr}\mid << k_{i}^{T}\frac{dlnT}{dr} \sim$$

$$\sim |d_i + k_i^T \frac{d \ln T}{d r}| << |d_p + k_p^T \frac{d \ln T}{d r}|$$
 (2.15)

In summary, only if certain special conditions [such as (2.14) and (2.15)] are satisfied is it possible to describe the diffusion of ions as a binary process on a background of electrons and protons, whose state is not modified by the ion dynamics. This means that only in very special cases can we compute the stellar structure model and then study the ion diffusion in the test atom approximation, as it has been extensively done in the literature. Such a situation is not reached if only Coulomb interactions and a negligible ion concentration are assumed.

Besides the analysis we have made based exclusively on the general equations (2.1)-(2.3) we may also consider the influence of the dynamical constraints on the diffusion process. For instance, we may require hydrostatic equilibrium, which implies the absence of a net mass flux

$$\sum_{s} n_s m_s v_s = 0 \tag{2.16}$$

Moreover for a stationary model with no magnetic fields, the total electric current vanishes

$$\sum_{s} Z_{s} e n_{s} v_{s} = 0,$$
 (2.17)

which is satisfied due to the appearance of a small electric field. For the special case of a three component gas (2.13-14) relate the diffusion velocities as in equation (2.22) of Noerdlinger (1977) by

$$v_e = \frac{n_p}{n_e} = \frac{m_i - Z_i m_p}{m_i + Z_i m_e} v_p \simeq$$

$$\simeq \frac{n_p}{n_e} \left( 1 - \frac{m_p}{m_i} Z_i \right) v_p, \qquad (2.18)$$

$$v_i = -\frac{n_p}{n_i} \frac{m_p + m_e}{m_i + Z_i m_e} \quad v_p \simeq -\frac{n_p}{n_i} \frac{m_p}{m_i} v_p.$$
 (2.19)

Using (2.18) and (2.19) we may calculate

$$n_e \frac{D_{ip}}{D_{ie}} \quad \frac{v_i - v_e}{v_i - v_p} =$$

$$= \frac{m_p/m_i + (m_i - Z_i m_p)/m_i}{n_i/n_e + (n_p m_p/n_e m_i)} \frac{D_{ip}}{D_{ie}}, \qquad (2.20)$$

which gives much less than unity for Coulomb interactions. Therefore, in this case (2.1) yields (2.7). We then may conclude that under conditions of hydrostatic equilibrium and one-dimensional symmetry the ion to proton diffusion is binary, however it is not possible to decouple the ions from the dynamics of the other species: all the abundances  $(n_e, n_p \text{ and } n_i)$  must be computed together.

#### b) Ionization and Radiation

The hydrodynamic equations for a multicomponent gas may be obtained from Boltzmann equations by means of the Chapman-Enskog method. This method applies when it is possible to separate the collision processes into slow and fast ones. The fast processes determine the transport coefficients, while the slow processes appear as thermodynamical forces (Andersen 1969).

Ionizing interactions must be considered as fast processes under local equilibrium conditions, thus affecting only the transport properties of the medium. Therefore the problem arises in determining the form of the transport coefficients. A rather crude approximation can be made considering their expressions in terms of collision frequencies. In this case the ionization frequency  $\nu^{\rm I}$  must be added to the Coulomb one,  $\nu^{\rm c}$ . For instance, the diffusion coefficient between species i and j can be written as

$$D_{ij} = k T n_i / \mu_{ii} n (\nu_{ii}^c + \nu_{ii}^I)$$
 (2.21)

We see that the inclusion of this new frequency might lead to a reduction of the diffusion coefficients. As collisional ionization is most commonly produced by interactions with electrons, the ratios  $D_{ie}/D_{ip}$  and  $D_{pe}/D_{ip}$  may become of the order of unity, and treating diffusion as a binary process fails. However, for the cases we are interested in (T  $\sim$  8  $\times$  10<sup>4</sup>  $^{\circ}$ K, ionization of HeII) the ratio  $\nu^{I}/\nu^{c}$  is negligible. Therefore we shall work with the diffusion coefficient due to Coulomb collisions.

The interaction of radiation with matter also affects the hydrodynamic equations and the transport properties. In the deep atmospheric layers we are dealing with, the diffusion approximation for radiation is valid. This approximation leads to a modification of the total pressure and of the heat conduction coefficient. The question which arises is whether the radiation field can be treated as an external force in the relations that yield the diffusion velocities. In order to analyze this problem we will start from the Boltzmann equation for the s species. Let us first study bound-bound interactions, for which the collision term can be put as

$$\sum_{j < i} c \int d\nu \, dw \quad \left[ \sigma_{ji}^{A} f_{s}^{j} \left( v - \frac{h\nu}{m_{s}c} w \right) - \right.$$

$$\left. - \sigma_{ij}^{E} f_{s}^{i}(v) \right] F_{\nu} +$$

$$\sum_{j > i} c \int d\nu \, dw \quad \sigma_{ji}^{E} f_{s}^{j} \left( v + \frac{h\nu}{m_{s}c} w \right) -$$

$$\left. - \sigma_{ij}^{A} f_{s}^{i}(v) \right] F_{\nu} ,$$

$$(2.22)$$

where

$$f_s^j = (f_1 e^{-\epsilon} j^{/kT})/Z$$
,

and where we have used momentum conservation. As we shall see, spontaneous emission terms vanish. After a straightforward calculation sketched in Appendix A, (2.22) can be written as

$$-\frac{1}{n_s m_s c} \left( \int d\nu dw \, w \, \chi_{\nu}^s \, I_{\nu} \right) \, \frac{\partial f_s}{\partial v} \tag{2.23}$$

The coefficient which multiplies the velocity gradient of the distribution function in (2.23) represents the force per unit mass  $F^R$ , due to the spectral lines, acting on the species. Therefore, in the case of bound-bound transitions radiation interacts with each species as an external force, which can then be put at the left hand-side of the corresponding Boltzmann equation

$$\frac{\partial f_s}{\partial t} + v_s \frac{\partial f_s}{\partial x} + (F_s + F^R) \frac{\partial f_s}{\partial v} = L (f_s) \quad (2.24)$$

where bound-bound transitions are excluded in the collision term  $L(f_s)$  and  $F_s$  takes into account gravitational and electrical forces per unit mass. These results apply also to photon to atom scattering and to free-free collisions. However it is not clear that for bound-free transitions one can split the collision term in order to get an equation like (2.24). In the case of ionization and recombination processes the collision term summed over all states of ionization, yields contributions to both sides of the Boltzmann equation. There is a contribution to the external force, in which, besides radiation force, there appears an integral on the distribution function of electrons describing the force they exert on the atom of s species. On the other hand, such processes contribute to the transport coefficients, similar to other collisional processes, through their interaction cross-sections.

# c) Discussion of the Equilibrium Abundances Calculations

This paragraph is devoted to the analysis of the influence on the determination of equilibrium abundances. The importance of the d(lnc)/dr has been already pointed out in Vauclair et al. (1978), for the case in which turbulence is present and the diffusion coefficients are enhanced by a turbulent term. This is not our case where we work with the usual coefficients due to Coulomb interactions. Besides, we draw some conclusions about the

validity of studying diffusion on a pre-computed model. All numerical calculations present in this part are restricted to the case of the central stars of planetary nebulae (Models I and II).

Let us consider the expression for the binary diffusion velocity of an element (s) with respect to a given background (b)

$$v_{s} - v_{b} = D_{s} \left[ -\frac{d \ln c_{s}}{dr} + \overline{k_{p}^{s}} \frac{d \ln P}{dr} + \overline{k_{T}^{s}} \frac{d \ln T}{dr} + \overline{k_{T}^{s}} \frac{d \ln T}{dr} + \overline{k_{T}^{s}} \frac{d \ln T}{dr} + \overline{k_{T}^{s}} \right], \qquad (2.25)$$

where the quantities appear averaged over the ionization states of the given s atom

$$D_{s} \equiv \sum_{I} (D_{I}^{s} n_{I}^{s}/n),$$

$$\overline{k^{s}} = \sum_{I} (k_{I}^{s} D_{I}^{s} n_{I}^{s}/n D_{s})$$

and the indices b and I refer to the background and ionization state respectively.

When equilibrium is reached, (2.25) vanishes. In order to obtain the density distribution of the diffusing species one should solve the differential equation

$$\frac{d\ln c_s}{dr} - \frac{m_s}{kT(r)} \quad g_R(c_s) = \overline{k_p^s} \frac{d\ln P}{dr} + \frac{\overline{k_T^s}}{kT} \frac{d\ln T}{dr} \equiv \frac{m_s}{kT(r)} g_{GT}(r) \quad (2.26)$$

However, if we neglect the  $\mathrm{dlnc_s}/\mathrm{dr}$  term, as it is usually done (e. g. Vauclair et al. 1979, Montmerle and Michaud 1976), (2.26) reduces to an algebraic equation, which may be readily solved once  $\mathrm{g_R}(\mathrm{c_s})$  is given. In our case for both methods we get  $\mathrm{g_R}(\mathrm{c_s}) = \alpha (\mathrm{r)c_s}^{-1/2}$  (see Appendix C). Therefore, the solution of the algebraic equation is (Vauclair et al. (1979)]

$$c_{eq}^{s}/c_{o}^{s} = (g_{Ro}/g_{GT})^{2}$$
. (2.27)

where  $c_{eq}^{s}$  refers to the equilibrium concentration for the

s atom,  $C_o^s$  refers to the normal concentration of such atom and  $g_{Ro}$  is the radiative acceleration for  $C_o^s$  We have numerically solved the equation

$$2\frac{db_{s}}{dr} - \frac{m_{s}}{kT(r)} g_{GT}(r) b_{s} = \frac{m_{s}}{kT(r)} \alpha(r) , \qquad (2.28)$$

which is obtained from (2.26) by the substitution  $b_s^2 = c_s$  We have used a central finite difference scheme and selected as the outer boundary condition for  $c_s$  the value given by (2.27) at that point. We have taken the values of T(r),  $g_{GT}(r)$  and  $\alpha$  (r) from the Models I and II computed by Kudritzki. Solutions of (2.26) and (2.27) are compared in Figure 2. We can see that the density distributions are drastically different. This is a consequence of the appearance of an exponential term in the complete solution of (2.28), which comes from the homogeneous

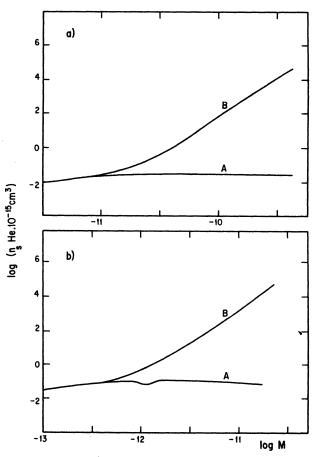


Fig. 2a, b. Helium equilibrium density is plotted against column mass. The curve labeled A refers to a solution obtained neglecting concentration gradients. The curve labeled B refers to a solution of the complete differential equation (2.26) taking as the outer boundary condition the value given by (2.27). Radiative acceleration  $g_R$  is computed by method 1.

solution, and which is not considered in (2.27). Besides, this behavior reflects the fact that the radiative acceleration is so small that ir cannot balance the effect of gravity. Therefore the equilibrium distribution is almost determined by the gravitational settling of helium [which corresponds to the homogeneous solution of (2.28)]. We then conclude that in this case it is not possible to neglect the derivative term in (2.26), no matter how small it may be: the solution obtained through (2.27) is unstable, in the sense that an infinitely small variation in the concentration will give a distribution which diverges exponentially from (2.27) (see Elszgoltz 1973). We may also conclude that, in general, when gravitational settling prevails it is imposible to neglect the dlnc<sub>s</sub>/dr term in the expression for the diffusion velocities.

We have also computed the density distributions taking the observed values as boundary conditions. In Figure 3, these distributions are compared with the proton and electron distributions. As the solutions of (2.28) increase exponentially, the helium concentration becomes much greater than the electron-proton density, violating the neutrality of the atmosphere. Therefore, the proposed model is not consistent: it is not possible to consider a background not affected by helium diffusion.

#### III. HYDROGEN-HELIUM DEEP ATMOSPHERE MODEL

The stellar structure equations (e. g. Chiu 1968; Cox and Giuli 1968) which describe the envelope regions, consider previously fixed abundances, that is, these abundances enter as parameters of the specific model. In this way the hydrodynamic equations reduce to those corresponding to a one-fluid model. Besides, in the cases where abundance anomalies appear, at certain stages of the stellar evolution, one way of explaining these phenomena is to invoke diffusion. The simplest way for describing diffusion is to assume that the diffusing species drift on a given structure. This background structure is computed according to a model without diffusion. Moreover, further approximations are posed in order to compute diffusion velocities and determine equilibrium abundances. As we have discussed in the previous section, the neglect of electron dynamics, or the neglect of concentration gradients, may lead to erroneous results. On the other hand, to decouple diffusion from the structure of the atmosphere may become inconsistent with the basic assumptions of the model, for instance, the neutrality condition may be violated. Therefore, one can improve the analysis of diffusion by means of a structure model which allows one to deduce all the abundances simultaneously. As it has already been pointed out in the introduction, works in this direction are those of Vauclair et al. (1974), Vauclair et al. (1978) and Noerdlinger (1977). The basic equations of a consistent structure model should be the set of hydrodynamic equations for the species present. The most complete description would be given by the solution of an evolutionary model which

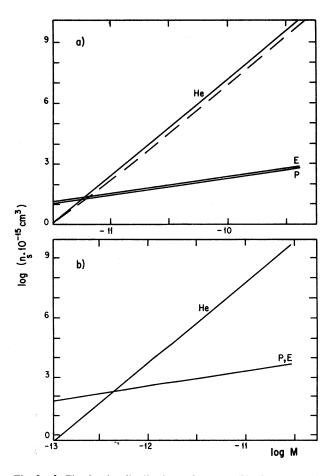


Fig. 3a, b. The density distributions of protons (P), electrons (E) and helium (He, dashed line corresponds to method 2 and solid line to method 1, these two curves cannot be distinguished for Model II) are compared. Helium density is computed by solving the differential equation obtained setting the helium diffusion velocity equal to zero. (eq. 2.26). The outer concentrations are taken equal to the observed values. The distribution of helium differs from case B of Figure 2 due to the different boundary conditions: while in Figure 2 these conditions imply that the derivative of  $c_s$  vanishes at the boundary, in Figure 3 it is different from zero. Neutrality is clearly violated when one computes helium abundances without taking into account the possible modification of the background model (an electron-proton plasma) Fig. 3a corresponds to Model I  $(n_{\text{He}}/n_p = 0.1; \log g = 5.50)$  and Fig. 3b corresponds to Model II  $(n_{\text{He}}/n_p = 0.01; \log g = 6.50)$ .

takes into account, the effect of diffusion as in Noerdlinger (1977). However, this program is beyond the scope of this work and so we propose a simpler, two step analysis: (i) the computation of a consistent stationary structure model, (ii) the stability analysis of the structure, which in turn may yield the characteristic growth rates of the instabilities. In this way we can also obtain the equilibrium distributions, which may not be the actual ones if the structure turns out unstable.

In the subsequent paragraphs we describe the basic

equations of the model and show the results obtained for the central stars of planetary nebulae (Models I and II).

### a) Model Equations

In what follows we shall write the stationary model equations for the subatmospheric layers  $(\tau > 1)$  where radiation can be treated in the diffusion approximation. We consider an ideal non-degenerate gas composed of electrons, protons and helium nuclei, electrically neutral, with spherical symmetry and hydrostatic equilibrium. We treat the relative motion of the three species as a diffusion process, and suppose that all three species are at the same temperature. We do not make any assumption on the helium to proton concentration, but rather obtain it as a result of the model computation. Therefore, the general hydrodynamical equations read as continuity

$$\frac{d}{dMr} (r^2 n_p v_p) = 0, (3.1)$$

hydrostatic equilibrium

$$4 \pi r^2 \rho \frac{d}{dM_r}$$
  $nkT + \frac{a}{3} T^4 = -\frac{G\rho M_r}{r^2}$ , (3.2)

energy balance

$$\frac{d}{dM_r}$$
 (r<sup>2</sup> q) = 0 , (3.3)

Poisson's formula

$$\frac{dr}{dM_{\rm r}} = \frac{1}{4 \pi r^2 \rho} , \qquad (3.4)$$

Maxwell equation

$$J = e n_p v_p + 2e n_{He} v_{He} - e n_e v_e = 0.$$
 (3.5)

In this set of equations there is only one continuity equation, because the diffusing fluxes are all proportional [see (2.17)-(2.18)]. In order to obtain a closed set of equations the following relations must be satisfied (i) electrical neutrality

$$n_{\rm p} = 2 \left( 1 + \frac{\text{me}}{2 \, \text{mp}} \right) n_{\rm e} \, \frac{\rho}{m_{\rm p}} , \qquad (3.6)$$

$$n_{He} = \frac{\rho}{2m_p} - \frac{n_e}{2} \left( 1 + \frac{m_e}{m_p} \right);$$
 (3.7)

(ii) constitutive relations for the diffusion velocities (Chapman and Cowling 1970)

$$V_{s} = -4 \pi r^{2} \rho - \sum_{t} \frac{\Delta_{st}}{nkT} \left[ \frac{d}{dM_{r}} (n_{s} kT) - \frac{Fs}{4 \pi r^{2} \rho} \right] - D_{s} \frac{dlnT}{dM_{r}} ; \quad (3.8)$$

the explicit form of the diffusion coefficient  $\Delta_{sT}$  is given in Appendix B.  $F_s$  includes electrical and radiative forces. As we are dealing with a completely ionized gas, in which no transformation of the species takes place, we can suppose that radiation affects diffusion as an external force. Besides, as the radiation force on protons and helium nuclei is much less than the radiation force on electrons  $F_R^e$ , we take  $F_R^e$  equal to the total radiation force. Thus, we put

$$F_{\rm R}^{\rm e} = -\frac{a}{12 \pi r^2 \rho} \frac{dT^4}{dM_{\rm r}}$$
 (3.9)

This is a crude estimation, but does not introduce errors greater than 1%.

(iii) the relation defining the energy flux q (which we suppose to be due to radiative and electron heat conduction) is

$$q = \frac{1}{4\pi r^2 \rho} (\lambda_e + \lambda_R) \frac{dT}{dM_r}$$
 (3.10)

where  $\lambda_R$  is related to the Rosseland mean opacity  $\overline{\chi}_R$  by

$$\lambda_{R} = \frac{4}{3} \frac{acT^{3}}{\frac{7}{\chi_{R}}}$$

For a detailed description of the transport coefficients and the atomic processes considered see Appendix B.

Further simplifications may be done. First, we can eliminate (3.5) by obtaining an expression for the electric

field in terms of the other thermodynamical forces. The calculation is straightforward, as the electric field enters linearly in the diffusion velocities. Moreover, (3.1) and (3.3) can be immediately integrated, leading to

$$r^2 n_p v_p = \text{const.} \equiv K$$
 (3.11)

$$r^2 q = const. \equiv U$$
 (3.12)

With all the assumptions and simplifications described above, we have reduced the original set of equations to another system of four equations (3.2, 3, 11, 12) on the variables  $n_e$ ,  $\rho$ , T and r.

Furthermore, as we have obtained a set of first order differential equations, we must state the boundary conditions by imposing values at one point for the four independent variables and for the two constants K and U. K is a free parameter which determines the values of the diffusing fluxes. For the first calculations we will take K equal to zero (equilibrium case). This means that the species do not diffuse. U is simply related to the luminosity L by

$$U = \frac{L}{4\pi} \qquad .$$

As we are not solving the complete structure of the star, we do not have reliable conditions to impose at the inner boundary of the envolope. If we could do so, we would obtain the density distributions at the surface as a result of the model and would be able to compare them with the observed ones. On the contrary, we take the values given by an atmosphere model (Kudritzki 1983) which adjust the observations, as boundary conditions and integrate the equations towards the center of the star.

## b) Equilibrium Distributions

The models we have computed differ substantially from those which are based on the assumption of chemical homogeneity, that is, those which take main results in Figure 4 (for a normal surface helium abundance in Figure 4a and for an anomalous one in Figure 4b), where the species densities are plotted. In both models, computed with vanishing diffusion velocities (K = 0), we observe that the star envelope is stratified. While helium and electron densities increase with depth protons tend to decrease in the inner layers of the atmosphere. This behavior of the helium density is similar to the one obtained in Section 2.3, when we solved the differential equation (2.26) determined by the expression of the helium diffusion velocity. In that case neutrality was clearly violated due to the fact that the helium density was computed independently from the background model. In this case, as all the distributions are computed

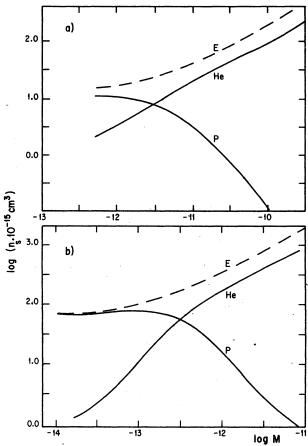


Fig. 4a, b. The density distributions of protons (P), electrons (E) and helium nuclei (He), solutions of a consistent hydrodynamic model with vanishing diffusion fluxes, are plotted against the column mass. Fig. 4a corresponds to Model I ( $n_{He}/n_P = 0.1$ ; log g = 5.50) and Fig. 4b corresponds to Model II ( $n_{He}/n_P = 0.01$ ; log g = 6.50). For both models, the envelope structure is clearly stratified showing the occurrence of a kind of gravitational settling.

simultaneously, the neutrality condition determines that the increasing of the helium density must be compensated by a depletion of the proton density. That is why we obtain such a stratified structure. We could not continue the computation for deeper layers because, as the proton density became so small, it would be necessary to include metals in the model. Besides, some numerical problems appeared at those layers. What we have obtained is the equilibrium structure compatible with the observations and the assumptions of the model. We must remember that it may not correspond to the actual one because of instabilities. Besides there is no reason for supposing that diffusion has already ceased at these stages. Moreover there are some simplifications (such as considering a gas of protons, ions and electrons) which finally affect the results. In spite of these limitations, it is interesting to compare it with the equilibrium concentrations derived in Section II. These stratified models show that diffusion of helium in the central stars of planetary nebulae cannot be analyzed in the test atom approximation; it must be studied together with the evolution.

## c) Calculations with Non-Vanishing Diffusion Velocities

We have also computed envelopes with  $K \neq 0$ . We have fitted our model distributions for the deep regions of the atmosphere with Kudritzki (1983) outer atmosphere with Kudritzki (1983) outer atmosphere models, at  $\tau = 1$ . The results are shown in Figure 5. In these models the depletion of the proton concentration is slower than in the former ones, but the tendency to deposit helium in the deep envelope is still maintained. Therefore, for both cases, a kind of gravitational settling is observed. For non-vanishing diffusion velocities the stratification is less severe. One might therefore suppose that trying different values for the diffusing fluxes would yield a structure where all the densities increase together. Let us try to determine under what conditions this situation will occur.

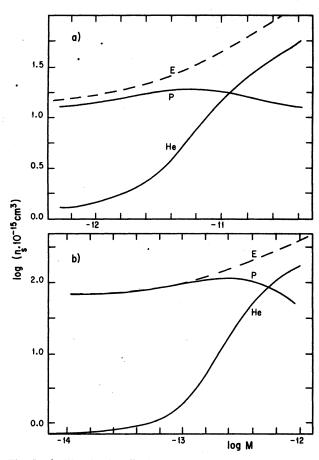


Fig. 5a, b. The density distributions of protons, electrons and helium nuclei, solutions of a consistent hydrodynamic model with non-vanishing diffusion velocities are plotted Fig. 5a which corresponds to Model I ( $n_{He}/n_P = 0.1$ ; log g = 5.50) and Fig. 5b corresponds to Model II ( $n_{He}/n_P = 0.01$ ; log g = 6.50). In this case the depletion of the proton density is slower than in Figure 4. A kind of stabilization of this density may also be seen.

As all the densities are related by the condition of neutrality (3.6-3.7), the density gradients are also interrelated. In this case the condition

$$\frac{dn_e}{dM_r} < 0 \qquad \qquad \frac{dn_{He}}{dM_r} < 0$$

$$\frac{\mathrm{dn}_{\mathrm{p}}}{\mathrm{dM}_{\mathrm{r}}} < 0 \qquad \qquad \frac{\mathrm{d}\rho}{\mathrm{dM}_{\mathrm{r}}} < 0$$

is similar to require that

$$\frac{1 + m_e/2m_p}{1 + m_e/m_p} > 
\left(1 + \frac{m_e}{2m_p}\right) m_p \frac{dn_e}{dM_r} / \frac{d\rho}{dM_r} > \frac{1}{2}$$
(3.13)

Condition (3.13) is clearly a severe restriction which is always satisfied for the chemical homogeneous structure models. However, it is easily violated when one is dealing with the solution of a consistent set of hydrodynamic equations. It is always possible to choose initial conditions which satisfy (3.13) in order to obtain monotonically increasing distributions. However, this behavior is only locally guaranteed. In some sense, the density distributions in the deep layers are weakly sensitive to the boundary conditions. We must also remember that condition (3.13) applies to a model composed of electrons, protons and helium nuclei; this fact limits the applicability of its consequences.

### d) Stability

We have studied how the structure would evolve if the electron density and the temperature were altered. maintaining the other conditions of the model (hydrostatic equilibrium, electrical neutrality, spherical symmetry) invariant. We have only analyzed the linear stability as follows: we have taken the complete set of hydrodynamic equations for the non-stationary case and imposed the restrictions of spherical symmetry, electrical neutrality and hydrostatic equilibrium. Further, we have written the electron density and the temperature as:  $n_e = n_e^{\circ} + \delta n_e$ ;  $T = T^{\circ} + \delta T$ , (where  $n_e^{\circ}$  and T correspond to the stationary distributions previously computed) and have linearized the equations in the small variations  $\delta n_a$ and  $\delta T$ , while considering also the variation of the transport coefficients due to their dependence on ne and T. Finally we have proposed an  $e^{\hat{w}t}$  dependence for  $\delta n_c$ and  $\delta T$  and obtained the characteristic growth frequencies  $\omega$ , which determine if the stationary structure is stable  $(\omega < 0)$  or not  $(\omega > 0)$ . In our case we have obtained positive frequencies. Consequently we may say that, according to these results, the equilibrium distributions of III. 2 are not the actual ones. Therefore, a non-linear analysis is needed in order to obtain the stable structure. However, this is not a complete study since it does not consider the possibility of the appearence of convection (the condition of hydrostatic equilibrium is still maintained). Besides these results are not the definitive ones, due to the limitations of both the model and the method. We think that they must be confirmed by another method, if possible, by an analytical one.

#### IV. CONCLUSIONS

We have discussed the main assumptions of the usual approaches to the study of diffusion. We have first analyzed the consequences of the smallness of the  $D_{\rm ip}/D_{\rm pe}$  ratio and of a negligible ion concentration for a three component gas. We have also obtained sufficient conditions for treating diffusion as a binary process and for neglecting the ion dynamics in the structure computation. Electrons may be neglected only in the case of very restrictive dynamical conditions, and their importance is due to their influence on the external forces and thermal diffusion.

Further, we have briefly studied the effect of ionization and radiation on diffusion. Ionization and radiation processes in which three or more species are involved are difficult to treat in the hydrodynamic approximation. For local chemical equilibrium conditions, ionization only affects the diffusion coefficients. This effect may only be important when the ionization and Coulomb frequencies are comparable. Nevertheless, detailed studies of the Boltzmann collision term are needed in order to determine the expressions of these new coefficients. Radiation affects diffusion velocities through an external force term for bound-bound and free-free transitions or electron scattering. For processes which involve a transformation of the species (bound-free transitions) radiation also modifies the transport coefficients. Also in this case a deeper analysis is needed. However, the difficulties encountered in these topics may be overcome by the construction of specific models for each case.

We have then discussed the computation of the equilibrium density distributions. The determination of equilibrium abundances may be erroneous when one neglects the concentration gradient in the expression of the diffusion velocity. If we take it into account and solve the complete differential equation we obtain a completely different equilibrium concentration. Moreover, this distribution does not satisfy the neutrality condition. In this way we may see that the equilibrium abundance of the diffusing species cannot be determined independently from the model computation.

We have therefore presented a method for the analysis of diffusion. It consists of the computation of a stationary structure model and the study of its stability. For the calculation of the structure we have proposed a consistent hydrodynamic model which determines all the densities simultaneously and which is adequate for the physical conditions prevailing in the central stars of planetary nebulae. The main feature of the model is the fact that it does not take the concentrations as parameters but obtain them as results of the computation. We have solved the equations for two central stars of planetary nebulae. The structure obtained in both cases is completely stratified: while the helium density increases rapidly into the star, a depletion of the proton density is observed. We have also found that only under very restrictive conditions can the densities increase simultaneously. Even if these conditions are satisfied for the boundary distributions, the solutions of the hydrodynamic equations may evolve in such a way that these conditions are then violated. The stratification we obtain is due to the fact that helium sinks, as gravity overcomes the outward radiation force everywhere. Therefore, in order to maintain a neutral envelope, the proton density decreases (as it is stated in Noerdlinger 1977). The occurrence of this stratification is also a strong argument against the study of helium diffusion over a non altered background. Returning to the case of the central stars of planetary nebulae, preliminary studies of the stability of these stratified envelopes show that they are thermally unstable. This means that the structures obtained do not correspond to the actual ones and that other phenomena must be considered in order to obtain a reliable description. An improvement of the stability analysis together with the study of the possible appearance of convection is needed. Convective and turbulent motions may mix the stellar matter competing with diffusion processes. In such a case the envelope structure would be completely different from the stratified one.

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# APPENDIX A

# CALCULATION OF THE BOLTZMANN COLLISION TERM FOR BOUND-BOUND TRANSITIONS

The collision term for bound-bound interactions between the s particles in the i-state of internal energy and radiation can be put in the form:

$$\begin{split} \sum_{j < i} \left| \int d\nu \, dw \, c \, F_{\nu} \right| \left( \sigma_{ji}^{A} \, f_{s}^{j} \left( v - \frac{h\nu}{m_{s}c} \, w \right) \right. \\ &\left. - \sigma_{ij}^{E} \, f_{s}^{i} \left( v \right) \right) \right. + \end{split}$$

$$+ \sum_{j>i} \int d\nu \, dw \, c \, F_{\nu} \left( \sigma^{E}_{ji} \, f^{j}_{s} \left( v + \frac{h\nu}{m_{s}c} \, w \right) \right) -$$

$$- \sigma^{A}_{ij} \, f^{i}_{s} \left( v \right) \right) , \qquad (A-1)$$

where only induced emission is considered,

$$f_s^j(v) = f_s(v) e^{-\epsilon j/kT} / Z$$

and w is the direction of the interacting photon.

Imposing the momentum conservation condition, which reads

$$v_s^j + \frac{h\nu}{m_s c} \quad w = v_s^i \tag{A-2}$$

for the first summatory (i + v = i transitions), and

$$v_s^i + \frac{h\nu}{m_s c} \quad w = v_s^j \tag{A-3}$$

for the second summatory  $(i + \nu \neq j \text{ transitions})$ , and making an expansion of f<sub>5</sub> around v<sup>i</sup> (small particle momentum variation), we obtain

$$\sum_{j>i} \left| \int d\nu \, dw \, c \, F_r \left[ \frac{h\nu}{m_s c} \, w \, \frac{\partial f_s}{\partial v} \, \sigma_{ji}^E - f_s \, (v_s^i) \right] \right| \times$$

$$\times (\sigma_{ij}^{A} e^{-(\epsilon_{i} - \epsilon_{j})/kT} - \sigma_{ji}^{E}) e^{-\epsilon_{j}/kT}/Z$$
 (A-4)  $\chi_{s}^{L}$  is the opacity in the lines for the  $\nu$  frequency. Therefore, the collision term can be put in the form

where we have introduced the definition of the specific intensity

$$I_{\nu} = h\nu c F_{\nu}$$

The energy difference  $\epsilon_i - \epsilon_i$  is equal to  $h\nu$ .

Taking into account that for the Boltzmann distribution of internal states the number density of s particles in the i-state ni is related to the total number of s particles (in the same state of ionization) by:

$$n_s^i = \frac{n_s e^{-\epsilon_i/kT}}{Z}$$
 (A-5)

and that for the diffusion approximation is

$$\sum_{i,j} n_s^i \sigma_{ij}^E = \sum_{\substack{i,j\\i>i}} n_s^i \sigma_{ji}^A e^{-h\nu/kT}$$
(A-6)

The collision term is reduced to

$$-\frac{1}{n_s} \int \frac{w}{m_s c} \frac{\partial f_s}{\partial v} I_{\nu} (1 - e^{-h\nu/kT}) X$$

$$\times X_s^L(v) d\nu dw , \qquad (A-7)$$

where we put

$$\chi_s^L(\nu) = \sum_{\substack{i,j\\i>j}} n_s^j \sigma_{ji}^A \qquad ; \qquad (A-8)$$

$$-\frac{\partial f_s}{\partial v} F^R \qquad (A-9)$$

with

$$F^{R} = -\frac{1}{n_{s} m_{s} c} \int \chi_{\nu}^{s} w I_{\nu} d\nu dw$$
 (A-10)

It is not necessary to consider the spontaneous emission processes, because for isotropic opacities the integral over the photon directions (dw) is zero.

# APPENDIX B EXPRESSIONS USED FOR THE TRANSPORT COEFFICIENTS AND THE OPACITY

a) Diffusion Coefficients The diffusion coefficients  $\Delta_{st}$  are calculated by

$$\Delta_{\rm st} = \frac{a \left( n_{\rm s} \, n_{\rm t} / n^2 \, D_{\rm st} \right)}{\Delta} \tag{B-1}$$

where

$$\Delta = \begin{bmatrix} \left(\frac{n_e}{n}\right)^2 & \frac{1}{D_{ee}} & \frac{n_e \, n_p}{n^2} & \frac{1}{D_{pe}} & \frac{n_e \, n_{He}}{n^2} & \frac{1}{D_{e \, He}} & \rho_e \\ \frac{n_e n_p}{n^2} & \frac{1}{D_{pe}} & \left(\frac{n_p}{n}\right)^2 & \frac{1}{D_{pp}} & \frac{n_p \, n_{He}}{n^2} & \frac{1}{D_{p \, He}} & \rho_p \\ \frac{n_e \, n_{He}}{n^2} & \frac{1}{D_{e \, He}} & \frac{1}{n^2} & \frac{n_p \, n_{He}}{n^2} & \frac{1}{D_{p \, He}} & \rho_{He} \\ \rho_e & \rho_p & \rho_{He} & 0 \end{bmatrix}$$

$$\lambda_e = \frac{15}{4\sqrt{2\pi}} \frac{n_e \, k^{3/2}}{m_e^{1/2} e^4} \frac{T^{3/2}}{\sum_i \ln\left(\frac{kTd}{Z_i \, e^2}\right) n_i Z_i^2}$$

and  $a(n_s n_t/n^2 D_{st})$  is the cofactor of the  $n_s n_t/n^2 D_{st}$  term in the determinant  $\Delta$ . The  $D_{st}$  are the binary coefficients for Coulomb interactions

$$D_{st} = \frac{3}{16n} \left( \frac{2 k T}{\pi} \frac{(m_s + m_t)}{m_s m_t} \right)^{1/2} \times \left( \frac{2 k T}{e^2 Z_s Z_t} \right) \frac{1}{\ln \left[ 1 + \frac{4 k T d^2}{Z_s Z_t e^2} \right]} , \quad (B-2)$$

where d is the Debye length  $d = \left(\frac{kT}{4\pi e^2 \sum_{i} n_i Z_i^2}\right)^{1/2}$ .

$$\sum_{s} n_{s} m_{s} \Delta_{st} = 0 \quad . \tag{B-3}$$

b) Thermal Diffusion Coefficients

We calculate D<sub>c</sub><sup>T</sup> by (see Chapman and Cowling 1970)

$$D_s^T = \sum_j \frac{n_s n_j}{n^2} \alpha_{sj} , \qquad (B-4)$$

where  $\alpha_{ep} = -1.608$ ,  $\alpha_{Hep} = 10.61$ .

We calculate the electronic conduction coefficient by

$$\lambda_{e} = \frac{15}{4\sqrt{2\pi}} \frac{n_{e} k^{3/2}}{m_{e}^{1/2} e^{4}} \frac{T^{3/2}}{\sum_{i} \ln\left(\frac{kTd}{Z_{i} e^{2}}\right) n_{i} Z_{i}^{2}}$$
(B-5)

d) Radiative Heat Conduction Coefficient

We calculate the radiation heat conduction coefficient by

$$\lambda_{R} = \frac{8\pi}{3} \left( \frac{h}{C} \right)^{2} \frac{1}{kT^{2}} \times \left( \frac{8}{(e^{h\nu/kT} - 1)(1 - e^{-h\nu/kT}) \chi(\nu)} \right) . \quad (B-6)$$

e) Opacity and Radiation Force Calculations

The atomic processes considered for the opacity and radiation force calculations are

- i) bound-bound transitions for H I and He II.
- ii) bound-free transitions for H I and He II.
- iii) free-free for H II and He II.
- iv) electron Thomson scattering.

For the computation of the H I opacity we consider an atomic model with four bound states and the continuum and for the He II opacity a model with six bound states and the continuum. We compute these coefficient according to Cox (1968).

# APPENDIX C **CALCULATION OF RADIATION FORCES**

The calculation of the radiative acceleration g is performed by two methods. The first one is the method used in Vauclair et al. (1979). The only suppositions involved in the derivation of their equation (10) which we use, are:

i) Lorentzian line profiles.

ii) Smooth behavior of  $B_{\nu}$  and  $\chi_{\nu}(R)$  (part of the total opacity not due to the diffusing element) at the vicinity of the line frequency. Here we only consider the line frequency. Here we only consider the contribution due to the force on the lines of He II. Therefore the final average over the states of ionization reads:

$$g_R (He) = g_R (He II) D_{He II,p} / n_{He} D_{He} (C-1)$$

The second method is the one described in Michaud et al. (1979). We use their fitting formula (17) along with their equation (7). This expression is already averaged over all the states of ionization and also takes into account the effect of ionization in the momentum transfer. It applies to a wide range of stellar parameters and different helium to proton concentrations.

From Figure 1 we can see that the second method gives a higher g value than method 1. The origin of this difference may be the same that the one described in Michaud et al. (1979): method i does not consider the photoionization of He II which is responsible, among other things, for the overestimation of the radiation force in method 2.

Concerning the variation of  $g_R$  with concentration, we see that the expression given by method 2 has an explicit  $c_s^{-1/2}$  dependence. As stated in Michaud *et al.* (1979), this behavior may be understood by saturation

effects (though they also note that, for higher temperatures,  $g_R$  is less sensitive to  $c_s$ ). The  $c_s$  dependence of  $g_R$  for method 1 is more complicated, though it may be simplified in certain cases. We have compared the opacity due to the line of interest  $\chi_L$  with  $\chi_{\nu}$  (R) at the center of the line and see that the ratio  $\chi_L/\chi_{\nu}(R)$  is not always much greater than unity. Nevertheless, the condition  $\chi_L/\chi_{\nu}$  (R) applies for those lines which determine the total radiation force. We have compared  $g_R$  obtained by adding equation 10 of Vauclair et al. (1979) over all the lines of interest with the simplifying formula

$$g_{R} = \sum_{L} \frac{1}{m_{L} n_{L}} \left( \frac{8\pi^{2} k^{3}}{3 h^{2} c^{3}} \right) T^{2} - \left( -\frac{\partial T}{\partial r} \right) \frac{(h\nu/kT)^{4} e^{h\nu/kT}}{(e^{h\nu/kT} - 1)^{2}} \left( \frac{\chi_{L}}{\chi_{\nu}(R)} \right)^{1/2}$$
 (C-2)

and found a very good agreement: they differ in a 10% at most, the major differences appearing at the deepest layers. Therefore we may consider a  $c_s^{-1/2}$  dependence for both methods.

## **GLOSSARY**

a Wien's law constant;  $a = 8\pi^5 k^4/15 h^3 c^3$ .

c light velocity.

 $c_s$  s species concentration;  $c_s = n_s/(n_e + n_p)$ .

 $D_{st}$  binary diffusion coefficient between species s and t.

D<sub>I</sub> binary diffusion coefficient between the s atoms in the I state of ionization and protons.

D<sub>s</sub> binary diffusion coefficient for the s particles averaged over all the states of ionization.

D<sub>s</sub><sup>T</sup> thermal diffusion coefficient.

 $\Delta_{s\,t}$  diffusion coefficient between the s and t species.

e electronic charge.

 $\epsilon_i$  internal energy for the j state.

f<sup>i</sup><sub>s</sub> (v) distribution function of the s particles in the internal energy state.

 $f_s$  (v) distribution function for the s species;  $f_s$  (v) =  $\sum_i f_s^i$  (v) where the sum must be performed over all the bound states.

F,, photon distribution function.

 $\boldsymbol{F}_{\mathrm{S}}$  external force per unit volume acting on the s species.

F<sub>s</sub> external force per unit mass.

$$\begin{split} g_{GT} \ \ \text{acceleration due to the pressure and temperature} \\ \text{gradients;} \ g_{GT} = \frac{kT}{m_s} \left( \begin{array}{c} \overline{k_p^s} \, \frac{d \ln P}{dr} \, + \overline{k_T^s} \, \frac{d \ln T}{dr} \end{array} \right) \, . \end{split}$$

 $g_{R,I}^{s}$  radiative acceleration on an s particle in the I state of ionization.

 $g_R^s$  radiative acceleration averaged over all the states of ionization;  $g_R^s = \sum\limits_I g_{e,I}^s \ D_I^s \ n_I^s/n \ D_s$ .

 $g_R^s = (m_{He}/\rho kT) g_R^s$ .

 $\widetilde{g}_{GT} = (m_{He}/\rho kT) g_{GT}$ .

 $I_{\nu}$  specific intensity;  $I_{\nu} = h \nu c F_{\nu}$ .

J electric current.

 $k_{I,p}^{s}$  pressure diffusion coefficient for the s atoms in the I state of ionization;  $k_{I,p}^{s} = \frac{2m_{s}}{mp} - Z_{I} - 1$ .

 $k_{I,T}^{s}$  temperature diffusion coefficient for the s atoms in the I state of ionization;  $k_{I,P}^{s} = 2.65 Z_{I}^{2} + 0.805$   $(Z_{I}^{2} - Z_{I}^{2})$ .

k<sub>p</sub> averaged pressure diffusion coefficient;

$$\overline{k_p^s} = \sum_{l} \frac{n_l^s}{n} D_l^s k_{l,p}^s / D_s$$

 $\overline{k_T^s}$  averaged temperature diffusion coefficient;

$$\overline{k_T^s} = \sum_{l} \frac{n_l^s}{n} D_l^s k_{l,T}^s / D_s.$$

 $\boldsymbol{k}_s^T$  thermal diffusion coefficient related to  $\boldsymbol{D}_s^T$  by

$$D_s^T = \sum_j \Delta_{sj} \ k_j^T.$$

 $\lambda_e$  electronic heat conduction coefficient.

 $\lambda_R$  radiative heat conduction coeffcient.

m<sub>s</sub> s species mass.

 $\mu_{ii}$  reduced mass.

$$M_r = 4\pi \int_0^r dr \ r^2 \rho \ .$$

$$M = 1 - M_r/M_*$$

n<sub>s</sub> number density of the s species.

 $n_{\,I}^{\,s}$  number density of the s atoms in the I state of ionization.

n total number density of particles.

w photon direction.

P total pressure.

q energy flux.

r radial spherical coordinate.

 $\rho$  total density.

 $\rho_s$  density of the s species.

 $\sigma_{ii}^{A}$  absorption cross section for i j transitions.

 $\sigma_{ii}^{E}$  induced emission cross section for  $i \rightarrow j$  transitions.

T total temperature.

v<sub>s</sub> s species diffusion velocity.

Z partition function for the s particles.

Z<sub>s</sub> electric charge of s species.

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