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Jean-François Gonzalez, Marie-Christine Artru, Georges Michaud. Radiative accelerations on carbon, nitrogen and oxygen. *Astronomy and Astrophysics - A&A*, 1995, 302, pp.788-796. hal-03985557

HAL Id: hal-03985557

<https://hal.science/hal-03985557>

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Radiative accelerations on carbon, nitrogen, and oxygen

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Received 5 February 1995 / Accepted 21 March 1995

Abstract. Radiative accelerations acting on the elements carbon, nitrogen and oxygen are calculated over a large range of plasma parameters which covers the conditions of A-F star envelopes. The theoretical atomic data available from the OPACITY project (OP) have been extensively used to perform a detailed computation of radiative accelerations including the contribution of lines and photoionization for all ions of C, N and O. The present calculations apply the method developed in a recent related paper. It includes several improvements by comparison with the usual approximations adopted previously, in particular concerning the background opacity, the pressure broadening of lines, and the distribution of radiative acceleration between adjacent ions after photoabsorption.

Results are presented for models of stellar envelopes with effective temperatures ranging between 6 700 and 10 000 K. For each of the elements C, N, and O, the variation of the radiative acceleration through the envelope is obtained for 19 different abundances. A parameterization of these results is attempted, using a simple formula which gives the radiative acceleration, as a function of only two parameters for each ion. These parameters do not depend on plasma conditions. A greater accuracy of about 0.2 dex is possible by simple interpolation in the available tables of results. The radiative accelerations obtained for C, N, and O are used to estimate the equilibrium abundances of these elements in A and F-type stars, and the comparison with available observed abundances is discussed.

Key words: atomic processes – diffusion – radiative transfer – stars: abundances – stars: chemically peculiar

1. Astrophysical context

Carbon, nitrogen and oxygen (CNO) are among the most abundant elements heavier than helium in stars. As such, CNO are a

main source of opacity and play an important role as constraints for peculiar stars.

The standard evolutionary models generally neglect any process of chemical transport outside of convection zones, which is reasonable to obtain first order models. But if there is no turbulence below convection zones, atomic diffusion occurs and may produce significant effects on stellar structure. Even in stars with convection zones as massive as that of the sun, atomic diffusion has a significant influence on the pulsation frequencies (Brown et al. 1994; Christensen-Dalsgaard et al. 1992; Guenther 1994). To get internally consistent evolutionary models, it is necessary to calculate the atomic diffusion at the same time as the evolution. Chemical stratification could modify the stellar structure, since the mean opacity and the radiative accelerations are mutually coupled through the local concentration of abundant elements. At each evolutionary step, one must re-calculate the radiative accelerations for the species contributing most to the Rosseland opacity. It will lead to a self-consistent series of stellar evolution models to compare with observations. This is a necessary step before progressively introducing hydrodynamical processes competing with atomic diffusion.

The stellar models are further constrained by the observed superficial abundances, since anomalies are expected to result from the chemical transport. A general underabundance of CNO has been observed in chemically peculiar stars: Am, Fm, Hg-Mn and magnetic Ap stars (van't Veer et al. 1989; Gerbaldi et al. 1989; Roby & Lambert 1990; García López et al. 1993). There is an apparent dependence on T_{eff} : the CNO abundances tend to be smaller in cooler stars. Anomalies have also been observed in He-rich stars and these peculiarities put constraints on diffusion and mass loss (Michaud 1986). The CNO abundances have been suggested as a potential constraint in cooler stars where the Li-gap is observed (Michaud 1987). According to the explanation of the Li depletion by atomic diffusion, Li settles gravitationally in the deeper envelope, where it is ionized, since the bare nucleus Li^{3+} is not supported by the radiative force. In these layers CNO is present under different states of ionization and their superficial abundances are expected to show correlated anomalies, especially if their dominant ions belong to the

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He-like or H-like isoelectronic sequences at the bottom of the superficial convection zone. The CNO ions with 1 to 8 electrons have relatively simple electronic structures and hopefully they allow more accurate calculation of radiative accelerations than heavier elements.

A complete set of theoretical atomic data for all states of ionization of CNO is now available thanks to the OPACITY project (Seaton 1987,1993). Its database, TOPbase, accessible at CDS, Strasbourg, France (Cunto et al. 1993a,b), yields all needed bound-bound and bound-free cross-sections. In this paper we use these data to calculate radiative accelerations in detail, as described in Gonzalez et al. (1995, hereafter Paper I). Section 2 briefly recalls the methods used in this study. The results, presented in Sect. 3, are estimated to be accurate within about 50 percent in most of the stellar envelopes. Tables of radiative accelerations as well as an approximate formula (see Sect. 4) are presented to make the use of the results possible in stellar evolutionary models. Equilibrium abundances are derived from these radiative accelerations through a simple diffusion model and are compared to existing observations in Sect. 5.

2. Methods

The radiative accelerations presented here are computed using the diffusion approximation, assuming local thermodynamical equilibrium (LTE, see Sect. 2 of Paper I), in stellar envelope models with T_{eff} ranging from 6700 K to 10000 K, and with $\log g = 3.8$ or 4.2 . These models are calculated with the procedure described in Richer & Michaud (1993), but using the latest version of OPAL Rosseland mean opacities (Iglesias et al. 1992, hereafter noted $\bar{\kappa}_{\text{OPAL}}$), with a metallicity $Z = 0.02$ and a value $\alpha = 1.767$ for the ratio of the mixing length to the pressure scale height. The relative abundances for the metals are taken from Grevesse & Noels (1993).

The contribution of bound-bound (b-b) and bound-free (b-f) transitions to the radiative accelerations are calculated using the oscillator strengths and the photoionization cross-sections provided in the OP database for each ion. For the latter, the fraction f_{ion} of the momentum transferred to the photoelectron is roughly approximated by assuming the same behaviour as for the fundamental state of hydrogen (Sommerfeld 1939; see Sect. 6 of Paper I). Calculations of f_{ion} for any nl orbital in a central potential are in progress (Massacrier 1995).

The atomic populations are obtained from the formalism of Hummer & Mihalas (1988). The modified semi-empirical (MSE) method developed by Dimitrijević & Konjević (1980,1986,1987) is used to compute the pressure widths of the b-b transitions (see Sect. 4 of Paper I). The distribution of the radiative acceleration among the different ionization states after a photoabsorption is taken into account through a simple model comparing the rates of excitation, de-excitation, ionization, recombination, and scattering processes (see Sect. 5 of Paper I for details).

The monochromatic opacity $\kappa(\nu)$ is computed at 4000 equally spaced frequency points in the $0 \leq u = \frac{h\nu}{kT} \leq 20$ domain, and on a grid containing 21 values of

$$R_e = \frac{N_e}{T^3} \quad (1)$$

(where N_e is the electron density and T the temperature in cgs units) within the range $-3.0 \leq \log R_e \leq 7.0$, and for the same 50 temperature values used by the OPAL group (Rogers & Iglesias 1992). These opacities are calculated separately for the elements H, He, C, N, O, and Fe, and can then be combined to give opacities for a mixture consisting of these six elements, whatever their proportion (see Sect. 3 of Paper I). Figure 1 shows at three points in a stellar envelope the contributions of carbon, nitrogen, and oxygen to the opacity spectrum, together with the total monochromatic opacity of a mixture with solar abundances. As can be seen, these elements are important contributors to the opacity, especially oxygen, which is the most abundant. Its contribution is particularly large at high frequencies, where photoionization dominates. The contribution of iron is not shown since, at the temperatures used in Fig. 1, it does not contribute a large fraction to the total opacity.

To obtain the radiative acceleration at each layer of the model envelope, one must know the value of the background opacity $\kappa_b(\nu)$ (which is the total monochromatic opacity $\kappa(\nu)$ minus the contribution of the transition being processed, see Sect. 2 of Paper I) for each layer. It is then necessary to interpolate its value on the (T, R_e, u) grid defined above. However, if one interpolates between two points of adjacent temperatures on this grid to obtain $\kappa_b(\nu)$, the position of a line or of a photoionization resonance will be different on our discrete $u = \frac{h\nu}{kT}$ scale; this position may be on one side of a u grid point or the other, which may lead to errors in the interpolated value of $\kappa_b(\nu)$, and so cause artificial irregular variations of the radiative acceleration with respect to depth. To fix this problem, we performed the integration of the differential radiative acceleration over the frequencies on the u grid (and not on the interpolated values), which gives the factor g_{grid} of the radiative acceleration which does not depend on the parameters of the stellar model T_{eff} , R , r , and $\bar{\kappa}_{\text{OPAL}}$ for each point of the (T, R_e) grid, or more exactly on the intersection of our grid and that giving the values of $\bar{\kappa}_{\text{OPAL}}$ (Rogers & Iglesias 1992). One then interpolates the values of g_{grid} for the different layers of the model to obtain g_{rad} using:

$$g_{\text{rad}} = T_{\text{eff}}^4 \frac{R^2}{r^2} \bar{\kappa}_{\text{OPAL}} g_{\text{grid}}. \quad (2)$$

We have computed tables containing the values of g_{grid} for each of the elements carbon, nitrogen, and oxygen for the following values of its abundance $[A/H]$: -5.0 , -4.6 , -4.3 , -4.0 , -3.6 , \dots , -0.3 , 0.0 (solar), $+0.3$, $+0.6$, and $+1.0$, all other elements having a solar abundance. A second set of tables has been obtained for mixtures with no helium. The monochromatic opacity has been recalculated in each case from the files containing separately the contribution of each element. In order to take into account the effect of opacity sources not included in

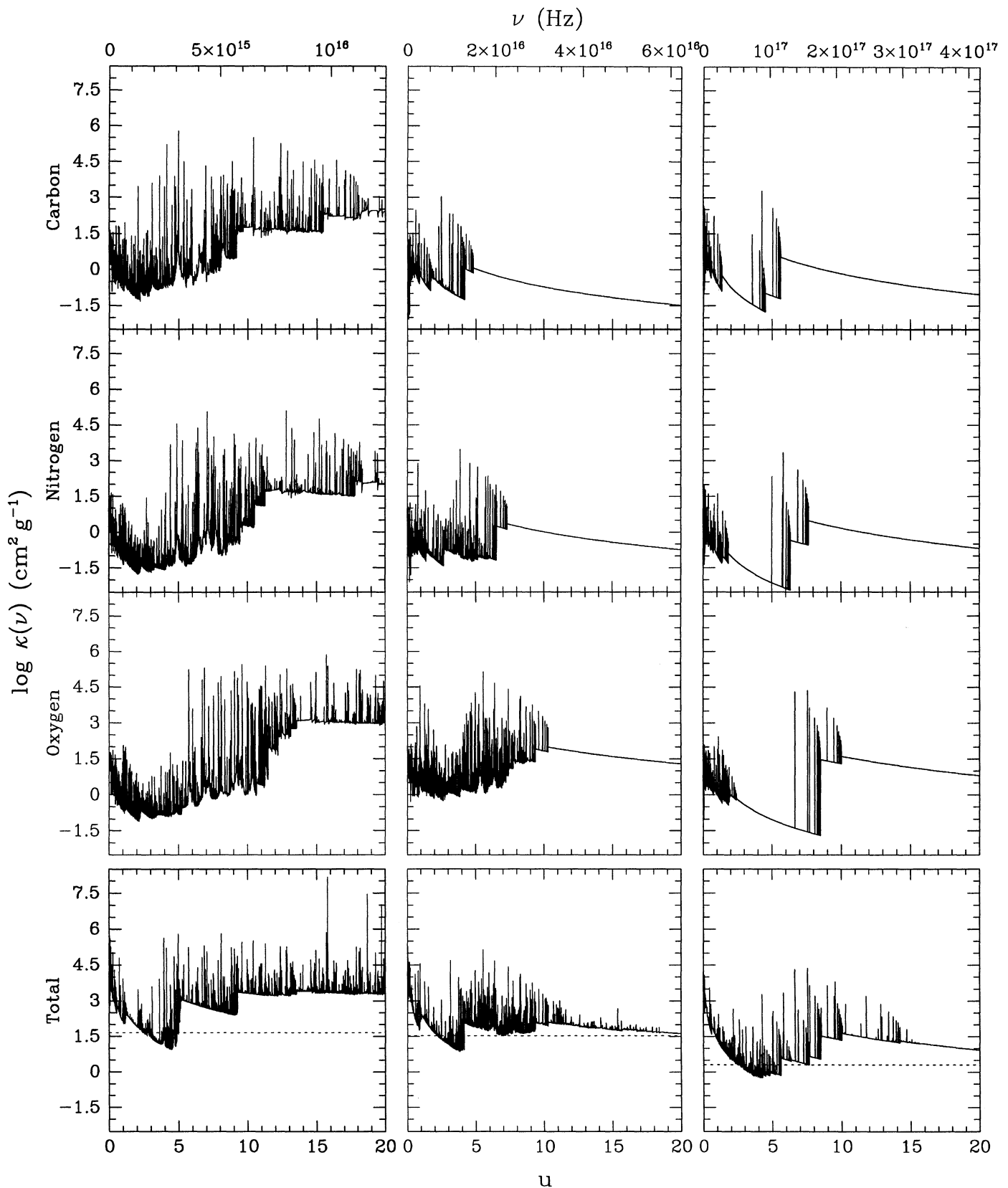


Fig. 1. Contributions of carbon, nitrogen, and oxygen to the opacity spectrum for $\log T = 4.5$ and $\log N_c = 16.4$ (left), $\log T = 5.2$ and $\log N_c = 18.5$ (middle), and $\log T = 6.0$ and $\log N_c = 21.0$ (right). The total opacity spectrum for the mixture (H, He, C, N, O, Fe) with solar abundances is also shown in the lower part of the figure (solid line), together with the Rosseland mean $\bar{\kappa}_R$ (dotted line)

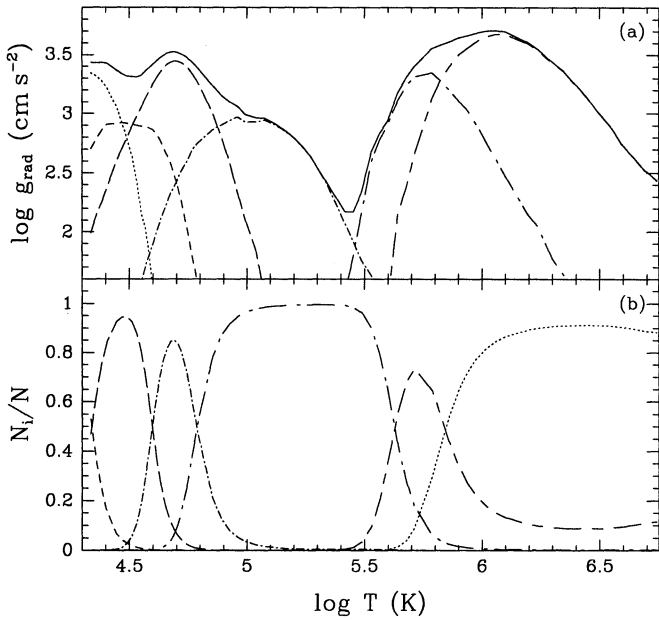


Fig. 2. **a** Radiative acceleration on carbon under the hydrogen convection zone of a model with $T_{\text{eff}} = 8000$ K and $\log g = 4.2$ (solid line) together with the contributions of C I (dots), C II (short dashes), C III (long dashes), C IV (dots-short dashes), C V (dots-long dashes), C VI (short dashes-long dashes). **b** Relative population of each ion and of the nucleus C VII (dots)

our mixture, we scaled our monochromatic opacity $\kappa(\nu)$ by the ratio of the Rosseland mean used in the model envelopes ($\bar{\kappa}_{\text{OPAL}}$) to the Rosseland mean of our mixture ($\bar{\kappa}_{\text{R}}$). As only two sets of $\bar{\kappa}_{\text{OPAL}}$ were available to us (for a mixture with and without helium but with solar relative abundances for all metals) we assumed the ratio $\bar{\kappa}_{\text{OPAL}}/\bar{\kappa}_{\text{R}}$ independent of the changes of abundance of either carbon, nitrogen, or oxygen and did not reflect these changes on the structure of the model.

3. Results

Figure 2a shows the radiative acceleration of carbon under the hydrogen convection zone of a model with $T_{\text{eff}} = 8000$ K, together with the contribution of each ion, whose ionization fraction is displayed in Fig. 2b. The maximum of the contribution of a given ion to g_{rad} does not occur where the ion is dominant in population, but somewhat deeper in the envelope. The dip which appears at $\log T \simeq 5.4$ is due to the fact that the He-like ion C V stays longer in its fundamental state, so its contribution to g_{rad} becomes important only after the curve of C IV has significantly dropped. Figure 3 is the same as Fig. 2 for oxygen.

Figure 4 displays the radiative accelerations of carbon, nitrogen, and oxygen under the hydrogen convection zone of models with different effective temperatures, but having the same surface gravity $\log g$. In the 6700 K model (long dashes), the hydrogen and helium convection zones are not separated and g_{rad} is plotted under the bottom of this combined zone. An increase in T_{eff} modifies the envelope structure, increases the radiative flux, and consequently the radiative accelerations.

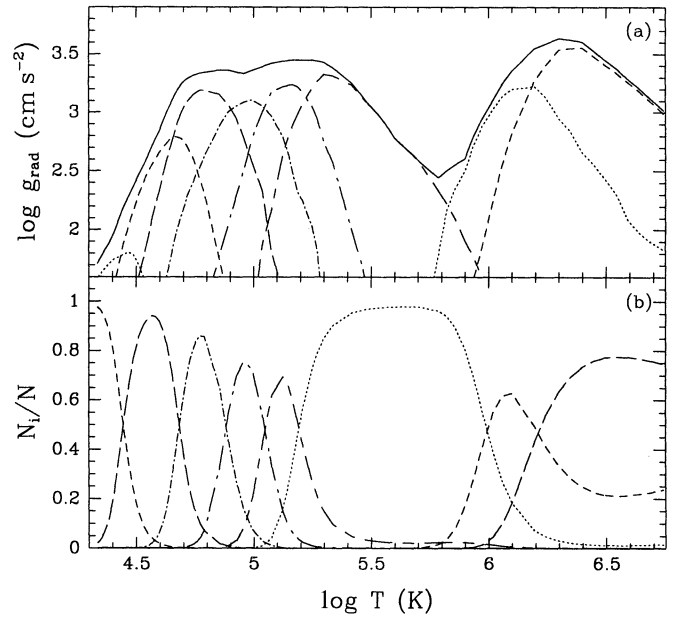


Fig. 3a and b. Same as Fig. 2 for oxygen, O VIII is shown with short dashes and O IX with long dashes

The curves for the three elements have similar shapes, with a shift towards higher temperatures from carbon to oxygen, which illustrates the increase of the ionization potential with atomic number within an iso-electronic sequence.

Also shown in Fig. 4 is our result for a 6700 K model with no helium (short dashes). The absence of this element lowers the background opacity and the Rosseland mean opacity, and acts on the stellar structure as well as on the radiative accelerations of other elements. The radiative acceleration is larger by up to 0.2 dex when no helium is included in the model. The diffusion of helium and of other important contributors to the opacity such as carbon, nitrogen, oxygen, or iron, when it leads to a reduction of their abundance, would have similar effects on g_{rad} .

Figure 5 displays the radiative accelerations of C, N, and O in models with $T_{\text{eff}} = 8000$ K and different values of $\log g$. The significant variations of g_{rad} with the surface gravity (a change in $\log g$ of 0.4 dex translates into a change in g_{rad} of 0.2 dex at the bottom of the convection zone) show that this parameter is important in the derivation of equilibrium abundances (see Sect. 5).

In Fig. 6 are displayed the values of g_{rad} for carbon, nitrogen, and oxygen in a model with $T_{\text{eff}} = 8000$ K and $\log g = 4.2$, computed for all the abundances considered in this study (see Sect. 2), together with the local gravity (heavy solid line). This figure illustrates the effect of abundance changes on the radiative acceleration: the decrease of g_{rad} with increasing abundance is caused by the saturation effect; it shows that the three elements are not supported by their radiative acceleration for solar abundances. Deep in the envelope, the radiative acceleration reaches its non-saturated limit for the lowest abundances in our range. This limit is already nearly reached for a solar abundance in the cases of C and N.

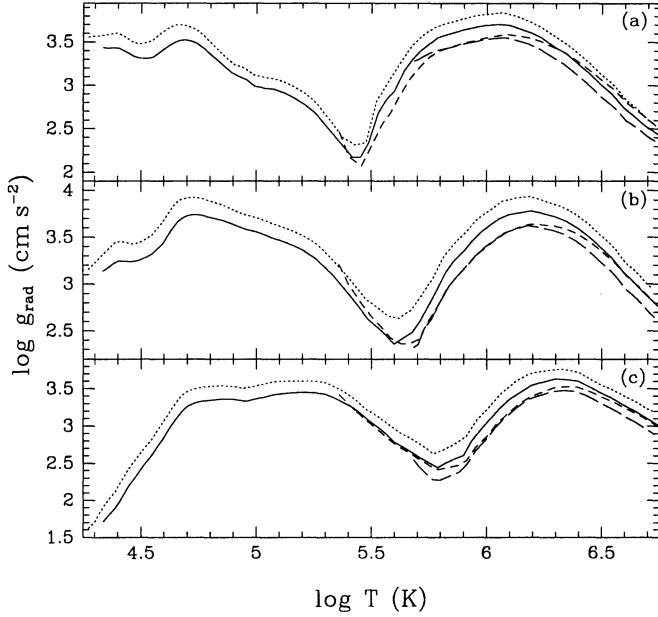


Fig. 4a–c. Radiative accelerations under the hydrogen convection zone of models with $T_{\text{eff}} = 10\,000$ K (dots), $T_{\text{eff}} = 8\,000$ K (solid line), $T_{\text{eff}} = 6\,700$ K (long dashes), and $T_{\text{eff}} = 6\,700$ K without helium (short dashes). For all these models, $\log g = 4.2$. **a** Carbon **b** Nitrogen **c** Oxygen

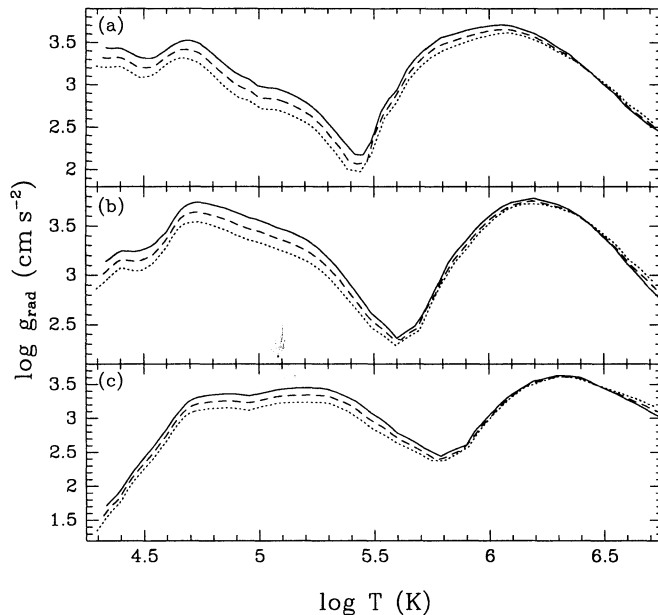


Fig. 5a–c. Radiative accelerations under the hydrogen convection zone of models with $\log g = 4.2$ (solid line), $\log g = 4.0$ (dashes), and $\log g = 3.8$ (dots). For all these models, $T_{\text{eff}} = 8\,000$ K. **a** Carbon **b** Nitrogen **c** Oxygen

4. Parameterization

Some astrophysical applications, in particular stellar evolution calculations, require calculating the radiative acceleration of several elements for numerous envelope conditions. Calculations as detailed as those presented here would then be computationally prohibitive. In order to obtain a good evaluation of g_{rad} rapidly, Alecian & Artru (1990) proposed an approximate expression for the contribution of bound-bound transitions making the assumption that the line profiles are mainly Lorentzian, and that within a line profile $\kappa_{\nu}(\nu) \simeq \text{constant} \simeq \bar{\kappa}_{\text{R}}$ and $P(u) \simeq \text{constant} = P_{ij}$ (for transition j of ion A^i). They obtained the following formula for the radiative acceleration on ion A^i due to all b-b transitions:

$$g_{\text{rad},b-b}^i \simeq \frac{\pi^2 k^3 e^2}{2c^4 h^2 m_e m_A} \frac{T_{\text{eff}}^4 R^2}{T r^2} \Phi_i \left(1 + \frac{C_i}{C_{i,0}}\right)^{-1/2}, \quad (3)$$

where m_e and m_A are the electronic mass and the mass of element A , R is the stellar radius, r the distance from the center of the star, $C_i = N_i/N_{\text{H}}$ the concentration of ion A^i , and

$$C_{i,0} = \frac{c m_e m_{\text{H}} \bar{\kappa}_{\text{R}} N_e}{2e^2 X \sqrt{T}} \Psi_i^2 \quad (4)$$

(m_{H} is the atomic mass of hydrogen and X its mass fraction), with

$$\Phi_i = \sum_{j,b-b} \frac{N_{ij}}{N_i} f_{ij} P_{ij} = \sum_{j,b-b} \Phi_{ij}, \quad (5)$$

and

$$\Psi_i = \frac{\sum_{j,b-b} \left(\frac{\gamma_{ij}}{N_{ij} f_{ij}} \right)^{1/2} \Phi_{ij}}{\sum_{j,b-b} \Phi_{ij}} = \frac{\sum_{j,b-b} \Psi_{ij} \Phi_{ij}}{\sum_{j,b-b} \Phi_{ij}}. \quad (6)$$

In Eqs. (5) and (6), N_{ij} is the population of the lower level of transition j , N_i the number density of ion A^i , and f_{ij} the oscillator strength of the line. The coefficient γ_{ij} represents the part of the line width which depends only on atomic data; the collisional width (FWHM) is then written $\Delta\nu_c = \gamma_{ij} N_e / \sqrt{T}$. The parameter Ψ_i allows one to take into account saturation effects. Φ_i and Ψ_i depend on the plasma conditions through the population ratio N_{ij}/N_i ; they have been evaluated for each layer of the model envelope.

Such a parameterization of the radiative accelerations includes the contribution of lines only (b-b transitions). An approximate formula was developed by Alecian (1994) to add the effect of photoionization (b-f transitions), but it cannot be applied in the case of abundant elements such as carbon, nitrogen, and oxygen.

We have modified the approach described above slightly in order to take into account the distribution of the radiative acceleration between ions A^i and A^{i+1} in proportions r_{ij} and

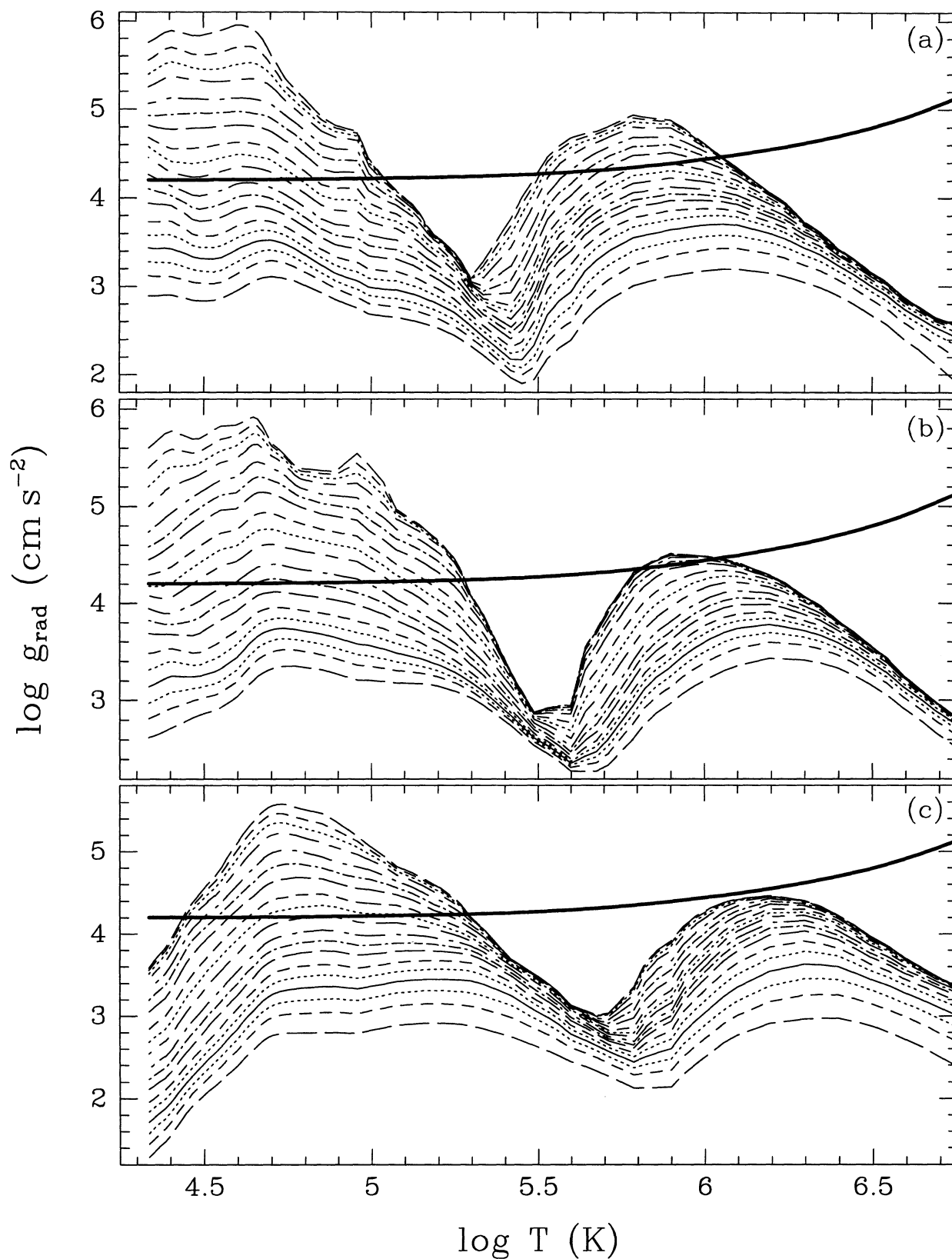


Fig. 6a–c. Radiative accelerations under the hydrogen convection zone in a model with $T_{\text{eff}} = 8000 \text{ K}$ and $\log g = 4.2$, for $[A/H] = -5.0, -4.6, -4.3, -4.0, -3.6, \dots, -0.3, 0.0, +0.3, +0.6, \text{ and } +1.0$ (in order of decreasing g_{rad}) together with the local gravity (heavy solid line). **a** Carbon **b** Nitrogen **c** Oxygen

$1 - r_{ij}$: in the same manner as in Sect. 5 of Paper I, we define an effective value of the parameter Φ_{ij} by

$$\begin{cases} \Phi_{ij}^{\text{eff}} = r_{ij} \Phi_{ij} \\ \Phi_{i+1,j}^{\text{eff}} = (1 - r_{ij}) \Phi_{ij}. \end{cases} \quad (7)$$

One then obtains Φ_i^{eff} as the sum of Φ_{ij}^{eff} over all b-b transitions of both ions A^{i-1} and A^i . The parameter Ψ_i^{eff} is also obtained by averaging Ψ_{ij} over the same transitions and weighted by the corresponding values of Φ_{ij}^{eff} . The total radiative acceleration on element A is obtained by

$$g_{\text{rad}} = \frac{\sum_i N_i D_i g_{\text{rad}}^i}{N \bar{D}}, \quad (8)$$

where D_i is the diffusion coefficient of ion A^i in protons and $\bar{D} = \sum_i N_i D_i / N$.

The approximate expression, when compared to the detailed calculation, yields values of the radiative accelerations systematically too high by factors of 2 to 5, and does not reproduce the variations of the radiative acceleration with respect to depth very well. Following the procedure used by Alecian et al. (1993), who computed radiative accelerations for iron including ions Fe IX through Fe XVII, we decided to adjust each parameter Φ_i^{eff} or Ψ_i^{eff} separately for each ion by a factor independent of plasma conditions, so that the radiative accelerations obtained from the approximation fit the detailed calculation in the model with $T_{\text{eff}} = 8000$ K and $\log g = 4.2$ for abundances going from $[A/H] = -3.0$ to $+1.0$. It was necessary to lower Φ_i^{eff} and Ψ_i^{eff} by a factor as high as 10 in some cases, and even higher in the case of the He-like ion, essentially because the approximate g_{rad} poorly reproduces the dip at $\log T \simeq 5.4$. Figure 7 compares the detailed radiative accelerations to those obtained by the adjusted approximation for carbon in models with $\log g = 4.2$ and $T_{\text{eff}} = 6700$ K (a), 8000 K (b), and 10000 K (c), and for $[C/H] = -3.0, -1.0, 0.0$, and $+1.0$. The adjusted approximation gives good results over a large part of the envelope with an error smaller than 0.2 dex, but departs from the detailed calculation in the region where g_{rad} is minimum as well as in the deepest layers, where the difference can reach 0.5 dex. This deviation will also be larger for abundances outside the range used for the fit.

Alecian et al. (1993) obtained good fits with the same method applied to the detailed radiative acceleration of iron, their approximations being basically those described in Paper I for the reference calculation. The present fits of CNO, based on improved detailed calculations (see Paper I), do not agree so well. The main reason is the variation of the background opacity with frequency. In Alecian et al. (1993), $\kappa_b(\nu)$ was obtained from the approximate formula of Borsenberger et al. (1979), which is calibrated on the Rosseland mean. The hypothesis $\kappa_b(\nu) \simeq \text{constant} \simeq \bar{\kappa}_R$, made for the derivation of the approximate expression of Alecian & Artru (1990), is then a good approximation. In our detailed calculations, the monochromatic opacity is introduced with a high resolution in frequency, as can be seen in Fig. 1, and can be smaller or greater than $\bar{\kappa}_R$, depending on the frequency or plasma conditions. This alters the

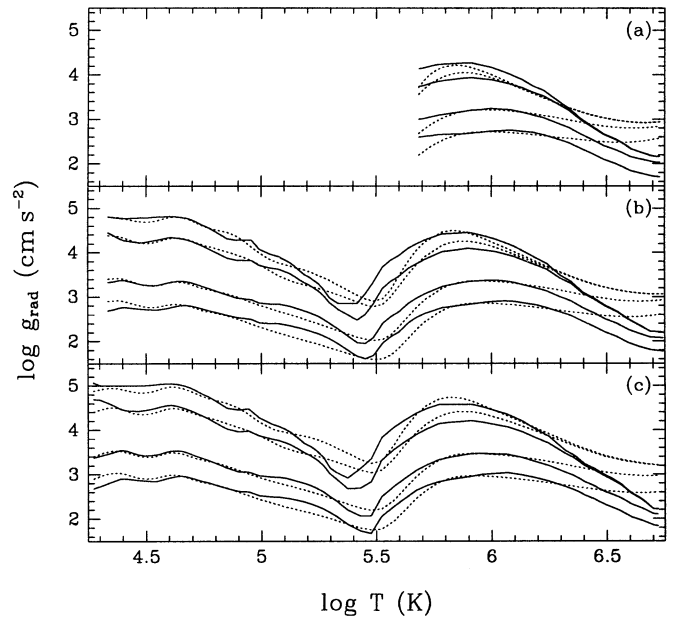


Fig. 7a–c. Radiative acceleration on carbon (b-b transitions): comparison of the detailed calculation (solid line) and the adjusted approximation (dots) for $[C/H] = -3.0, -1.0, 0.0$, et $+1.0$ (in order of decreasing g_{rad}) under the hydrogen convection zone of models with $\log g = 4.2$ and **a** $T_{\text{eff}} = 6700$ K **b** $T_{\text{eff}} = 8000$ K **c** $T_{\text{eff}} = 10000$ K

shape of the variations of g_{rad} with depth in a complicated way. Moreover, for an abundant element like C, N, O, or Fe, the opacity $\kappa_{ij}(\nu)$ of its own transitions may dominate the background opacity, which then depends on the abundance of the element; this lowers the radiative acceleration. This effect is not taken into account in the approximate expression (both parameters Φ_i and Ψ_i should be a function of the ratio $\bar{\kappa}_R / \kappa_b(\nu)$) and explains why one obtains systematically larger values. Calculations of the non-adjusted approximate radiative acceleration with very small abundances (not shown) have indeed yielded values closer to the detailed ones. Finally, blends with lines of other elements, which are taken into account in an average way (see Paper I) lead to an increase of the background opacity of a given line. This is also not reproduced by the approximate expression.

The breakdown of the assumption $\kappa_b(\nu) \simeq \text{constant} \simeq \bar{\kappa}_R$, which was implicit in Eqs. (3) and (4), then explains most of the discrepancies appearing on Fig. 7. The strong dependency of the opacities on CNO concentrations prevents us from adjusting the functions Φ_i and Ψ_i as easily as for un abundant elements. This leads us to adjust them simultaneously in order to reproduce as well as possible the total acceleration, regardless of the physical meaning of Φ_i and Ψ_i as defined in Alecian & Artru (1990). Nevertheless, the approximate formulae given by Eqs. (3) and (4), fitted empirically to the detailed results, allow one to quickly estimate radiative accelerations with a precision better than 0.5 dex, except in the deepest layers of the envelope.

5. Discussion

This paper applies the improvements developed in Paper I to the computation of radiative accelerations on carbon, nitrogen, and oxygen, for different values of their abundances, in several model envelopes of A and F stars. In particular, the background opacity was significantly improved compared to the fitting formula of Borsenberger et al. (1979) used in previous studies, by calculating its values for 4 000 frequency points, on a grid of 21 densities and 50 temperatures, for each element of a mixture composed of H, He, C, N, O, and Fe. The pressure broadening is now evaluated using the MSE method developed by Dimitrijević & Konjević (1980,1986,1987) and the OP data, and a simple model is proposed to take into account the distribution of radiative acceleration between adjacent ions after photoabsorption. Finally, we have included the contribution of photoionization to the radiative acceleration, which has often been neglected in past studies.

In order to allow fast computations of radiative accelerations, we have adjusted the approximate expression proposed by Alecian & Artru (1990) to fit our values of g_{rad} . However, the agreement of this approximation is not satisfactory over the whole envelope and this rapid method is only useful for a first estimate. For improved accuracy, we propose instead tables of g_{rad} for carbon, nitrogen, and oxygen, computed on a grid containing numerous plasma conditions. These tables are available from the authors for models with or without helium and for several values of the abundance of the considered element. The radiative acceleration can then be quickly obtained in any stellar envelope by interpolation. Such tables are also available for iron from LeBlanc & Michaud (1995). The monochromatic opacity tables used in this study (see Paper I) can likewise be obtained from the authors.

The radiative accelerations calculated in this work (Sect. 3 and Fig. 6) for the three elements C, N, and O, are smaller than gravity for a large abundance range. It is consistent with their general deficiency observed in chemically peculiar stars. Our results allow a derivation of a first approximation of the equilibrium abundances of C, N, and O, in stable stellar atmospheres. When neglecting the effects of abundance gradients, thermal diffusion and electric fields, the observed abundance can be estimated from the value for which $g_{\text{rad}} \simeq g$ at the bottom of the convection zone. Figure 8 gives the equilibrium abundances derived in this way for model envelopes with T_{eff} between 6 700 K and 10 000 K, and with $\log g = 3.8$ or 4.2.

A value equal to -5 represents an upper limit: even with an abundance $[A/H] = -5.0$, the radiative acceleration is still weaker than the local gravity at the bottom of the convection zone. We have also displayed on this figure the observed abundances determined in LTE by Roby & Lambert (1990) for non-magnetic and magnetic stars, and those obtained in NLTE by García López et al. (1993) for oxygen.

The comparison is mainly relevant for non-magnetic stars: the predicted equilibrium abundances as well as the upper limits are much smaller, sometimes by several orders of magnitude, than the observed ones. The results for carbon are the closest

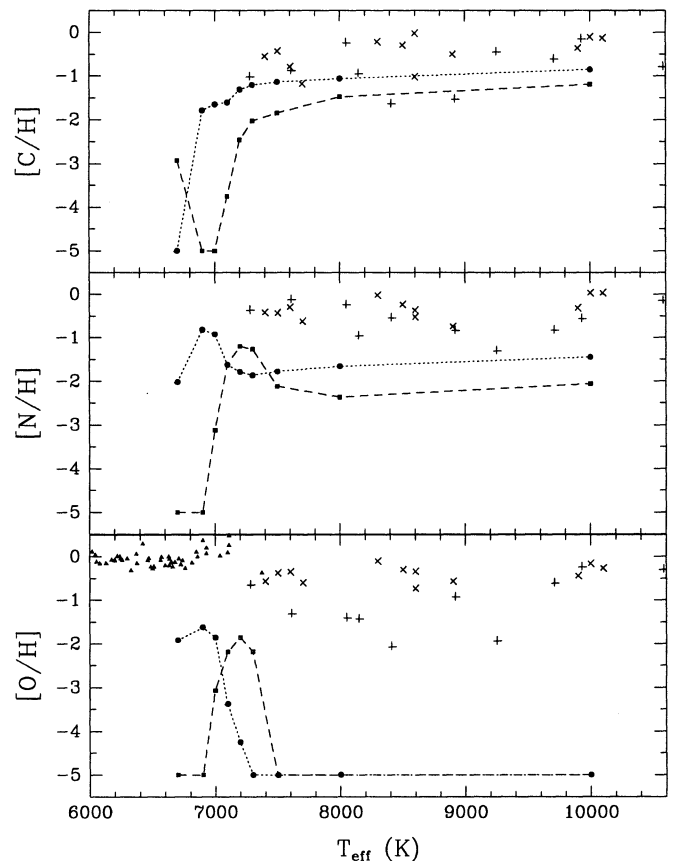


Fig. 8. Equilibrium abundances of carbon, nitrogen, and oxygen in models with $\log g = 3.8$ (dots) and $\log g = 4.2$ (dashes), together with the observed abundances of Roby & Lambert (1990, LTE) for non-magnetic (crosses) and magnetic (pluses) stars, and the ones of García López et al. (1993, NLTE) for oxygen (triangles)

to the observed values, with differences not exceeding 1 dex. However, some observed trends are reproduced by the theoretical estimate, at least for effective temperatures higher than 7 500 K: for example the underabundances of carbon are smaller than those of nitrogen, which are smaller than those of oxygen. Our equilibrium abundances are also correlated to the effective temperature: they are larger for the hottest stars. Moreover, as mentioned in Sect. 3, the surface gravity is a critical parameter in the derivation of our abundances; it would be interesting to know the dependence of observed abundances with respect to $\log g$.

The prediction of equilibrium abundances shown in Fig. 8 is very sensitive to the position of the convection zones since their bottom is located in regions where the radiative acceleration varies rapidly with depth, especially for the coldest models (see Fig. 4). Then it would become worthwhile to perform detailed calculations of time-dependent diffusion, accounting for abundance gradients, thermal diffusion, and electric fields. This would constrain the positions of convection zones thanks to the accuracy that can be achieved in the calculation of radiative accelerations.

However, we recall that the results are presented here for uninhibited diffusion which, in real cases, competes with hydrodynamical mixing processes such as meridional circulation, turbulence, or mass loss. Mass loss in particular has been suggested to play an important role (Michaud & Charland 1986; Babel 1992).

Part of the discrepancy appearing between predicted and observed abundances in Fig. 8 can be also due to an underestimate of the calculated values of g_{rad} . In particular, our approach does not take into account the possible desaturation due to fine-structure splitting. On the other hand, our partial treatment of blends may not reproduce accurately enough the reduction of the radiative acceleration they cause.

Acknowledgements. This research benefitted from the financial support of the Centre Jacques Cartier and of NSERC. The authors would like to thank J. Richer for calculating the stellar envelope models used and for helpful discussions, as well as G. Alecian for useful comments on improving the manuscript.

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