DIFFUSION IN STELLAR ENVELOPES

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In an attempt to make the present summary comprehensible yet sufficiently concise I will risk some over-simplification: further details are given in Seaton (1997, 1998 — Papers I and II).

In a star let $F_\nu \, d\nu$ be the outward flux of radiant and let an atom of element k present an effective area of $\sigma_\nu(k)$ for absorption of radiation. Then the momentum absorbed per atom and per unit area and unit time is $G(k) = (1/c) \int F_\nu \sigma_\nu(k) \, d\nu$ which is just the force acting on the atom. The radiative acceleration is $g_{\rm rad}(k) = G(k)/M(k)$ where $M(k)$ is the atom's mass.

The total opacity cross-section is $\sigma_\nu = \sum_m A(m)\sigma_\nu(m)$ where $A(m)$ is the abundance of element m by number-fraction; and the optical depth at a point with radial co-ordinate r is $\tau_\nu = \int_r^\infty N\sigma_\nu \, dr'$ where $N = \sum_m N(m)$ is the total number of atoms per unit volume. In stellar envelopes, regions with $\tau_\nu \gg 1$, the equation of radiative transfer can be solved in the diffusion approximation to give $F_\nu = (\sigma_{\rm R}/\sigma_\nu) f_\nu F$ where $F = \int F_\nu \, d\nu$, $f_\nu = (dB_\nu/dT)/(dB/dT)$, T is the temperature, B_ν is the Planck function, $B = \int B_\nu \, d\nu$ and $\sigma_{\rm R}$ is the Rosseland-mean cross-section, $(1/\sigma_{\rm R}) = \int (1/\sigma_\nu) f_\nu \, d\nu$. We obtain

$$M(k) g_{\rm rad}(k) = (1/c)\sigma_{\rm R}\gamma(k) F \quad \text{where} \quad \gamma(k) = \int (\sigma_\nu(k)/\sigma_\nu) f_\nu \, d\nu. \tag{1}$$

We may similarly define $\gamma(j,k)$ for production of accelerated ions in ionisation stage j. Absorption of radiation by element k contributes to both $\sigma_\nu(k)$ and to σ_ν in (1): $\gamma(k)$ therefore depends on $A(k)$ and decreases as $A(k)$ increases.

The quantities $\sigma_{\rm R}$ and $\gamma(j,k)$ have been computed using atomic data obtained by the Opacity Project (The Opacity Project Team, 1995). We start with some standard (solar-system) abundances and then vary the abundance of k by a factor χ. Paper I provides tables of $\sigma_{\rm R}$ and $\gamma(j,k)$, for the elements C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, Cr, Mn, Fe and Ni, on a mesh of (T, N_e, χ), where N_e is electron-density, together with codes for making interpolations. The results obtained should give values of $g_{\rm rad}$ of acceptable accuracy for Rosseland-mean optical-depth of $\tau \geq 1$ but not for higher (atmospheric) layers, with $\tau < 1$.

Diffusion processes lead to changes in abundances by factors χ, giving $N(k) = \chi A(k) N$. If atoms k have diffusion velocity v the continuity equation in a plane-parallel geometry is

$$\partial N(k)/\partial t + \partial(vN(k))/\partial r = 0 \tag{2}$$

where t is the time. The flux of atoms k is $vN(k) = vA(k)\chi N$: we put $f \equiv v\chi N$ and we use the total column-density x as depth-variable, $dx = -N \, dr$. Then

$$\partial\chi/\partial t = \partial f/\partial x. \tag{3}$$

The velocity v is determined by radiative and gravitational accelerations and by gradients in concentration and temperature. From Aller and Chapman (1960) and Michaud (1970),

$$f = \mathcal{D}\chi \left\{ [g_{\rm rad} - g_{\rm grav}] - (M(k)/k_{\rm B}T) \left[\partial \ln(\chi)/\partial r + \alpha_T \partial \ln(T)/\partial r \right] \right\} \tag{4}$$

where: $\mathcal{D} = ND(k_{\rm B}T/M(k))$ and D is the diffusion coefficient as usually defined; $g_{\rm grav}$ is the gravitational acceleration; $k_{\rm B}$ is the Boltzmann constant; and α_T the coefficient of thermal diffusion.

Paper II gives results for diffusion of Cr, Mn, Fe and Ni in HgMn stars, assuming no mixing due to convection or meridional circulations. Those elements give large values of $g_{\rm rad}$, which provides the main driving force. As a first approximation, I neglect the derivative terms in (4) to obtain

$$f(x,\chi) = \mathcal{D}(x)\chi \left\{ g_{\rm rad}(x,\chi) - g_{\rm grav}(x) \right\} \tag{5}$$

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For a given depth x, f as defined by (5) has the following behaviour as a function of χ: (i) $f = 0$ for $\chi = 0$ due to the factor of χ in (5); (ii) for χ small we have $g_{\rm rad} > g_{\rm grav}$ (for iron-group elements) and hence $f > 0$; (iii) $g_{\rm rad}$ decreases as χ increases and eventually one obtains a maximum value of f, $f = f_{\rm mx}$ at a value of $\chi = \chi_{\rm mf}$; (iv) for a sufficiently large value of χ, $\chi = \chi_{\rm stat}$, one can obtain $g_{\rm rad} = g_{\rm grav}$ and $f = 0$. Since f depends on t only because χ depends on t we have

$$\partial f/\partial t = w\partial\chi/\partial t \quad \text{with} \quad w = \partial f/\partial\chi \tag{6}$$

and hence, from (3),

$$\partial f(x,\chi)/\partial t = w(x,\chi)\partial f(x,t)/\partial x. \tag{7}$$

We solve (7) using a linearisation method. For the step from $t = t_0$ to $t = t_0 + \delta t$ we replace $w(x,\chi)$ by $w(x,\chi_0)$ where $\chi_0 = \chi(x,t_0)$: (7) then reduces to a simple wave equation, $\partial f(x,t)/\partial t = w(x)\partial f(x,t)/\partial t$ with general solution $f = \Phi(t + y(x))$ where $\Phi(\zeta)$ is any differentiable function of ζ and where $y = \int(1/w)\,{\rm d}x$. Given $f(x,t_0)$ one can therefore obtain $f(x,t_0+\delta t)$. At each time-step one can then allow for the derivative terms in (4) as perturbations.

Features in f move with velocity w. We obtain 3 regions:

regions A have $\chi < \chi_{\rm mf}$, $w > 0$ and features move outwards;
regions B have $\chi > \chi_{\rm mf}$, $w < 0$ and features move inwards;
regions C have $\chi \simeq \chi_{\rm mf}$, w is small and features move slowly.

At a time $t = t_0$, consider a value x_0 of x in a region A. All information required to continue the solutions for $x \geq x_0$ is provided by $\chi(x)$ for $x \gtrsim x_0$. It is therefore possible to continue the solutions for $x \geq x_0$ without having any information about solutions for $x < x_0$.

We construct models of HgMn stars ($T_{\rm eff}$ in the range 10000 K to 15000 K), take $\chi = 1$ at time $t = 0$, and follow the diffusion of iron-group elements for times of order 10^8 years and for depths of $\tau \geq \tau_0$ such that at τ_0 we are always in a region A. Initially, with $\chi = 1$, we obtain large maxima in f in the vicinity of $\log(T) \simeq 5.3$, the region of the "Z-bump" in opacities (see Rogers and Iglesias, 1992 and Seaton *et al.*, 1994). That feature moves outwards but is slowed down in the vicinity of $\log(T) \simeq 5.1$, a region in which the dominant ionisation stages are near Ar-like and which is referred to as the "Ar-barrier". For Mn and Ni we are able to obtain solutions with $\tau_0 = 1$ and to attempt some comparisons between observed atmospheric abundances and those computed for $\tau = 1$. At $\tau = 1$ we obtain maximum values of χ at times when the maximum in f has passed through the Ar-barrier (those times are of order 4×10^6 years for the case of the 13000 K model). At later times $\chi(\tau = 1)$ decreases. For Ni and Fe we encounter regions B at the tops of the envelopes, and are then only able to study the envelope diffusion at depths $\tau_0 > 1$.

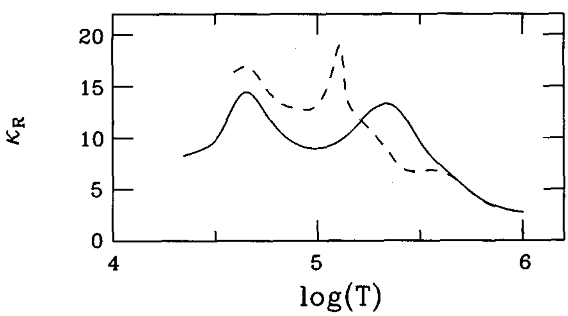

Figure 1. Rosseland-mean opacity for the 13000 K model. Full line, unmodified abundances; dashed line, after diffusion of iron-group elements for a time of 10^8 years

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Diffusion of iron-group elements can lead to substantial changes in Rosseland-mean opacities. Figure 1 shows results for the 13000 K model. The Z-bump shifts from its normal position at $\log(T) \simeq 5.3$ to a position closer to $\log(T) = 5.1$ and becomes more sharply peaked. It can be expected that the modified opacities, after diffusion of iron-group elements, will lead to the introduction of new convection zones.

In later work it will be desirable to study time-dependent diffusion in the stellar atmospheres (regions $\tau < \tau_0$), allowing for selective outflow of iron-group elements, using methods such as those discussed by Babel (1995, 1996). In such work it should be possible to use the methods described in the present paper to impose lower boundary conditions, at $\tau = \tau_0$. The present calculations make no allowance for evolution of the star, neither normal main-sequence evolution nor the modifications which will result from changes in opacities. When solutions for both envelopes and atmospheres are available it will be possible to follow the evolution allowing for opacity modifications.

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