THE ASTROPHYSICAL JOURNAL, 360:267–274, 1990 September 1

ELEMENT DIFFUSION IN STELLAR INTERIORS

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Received 1989 May 22; accepted 1990 February 26

ABSTRACT

Simple equations are derived that describe element diffusion in radiative stellar interiors and that may be incorporated in standard stellar evolution codes. For the Sun, diffusion is expected to increase the predicted event rates in the ^{37}Cl solar neutrino experiment and in electron-neutrino scattering experiments by 5%–10%; the expected increase in the predictions for ^{71}Ga solar neutrino experiments is between 1% and 3%.
Subject headings: diffusion — neutrinos — stars: interiors — Sun: interior

I. INTRODUCTION

Precise stellar evolutionary calculations have been carried out by a number of groups in order to compare model results with observations of solar neutrinos and of *p*-mode (helioseismological) oscillation frequencies. The most advanced of these calculations include detailed descriptions of all of the known relevant physical processes, with one exception: element diffusion is usually neglected because of its long time scale. In this paper, we provide a description of element diffusion that is sufficiently simple and sufficiently accurate to be included in precise calculations of solar neutrino fluxes and of *p*-mode oscillation frequencies. The results obtained here are expected to make small changes in the predicted value of the event rate in the ^{37}Cl experiment (increasing the standard theoretical value by ≤ 1 SNU) and slightly ameliorating the small discrepancies between predicted and calculated *p*-mode oscillation frequencies.

The strategy adopted in this paper is different from the strategy used in previous detailed studies (Noerdlinger 1977, 1978; Cox, Guzik, and Kudman 1988) of the expected diffusion of elements in solar models. These two landmark investigations used comprehensive descriptions of the interactions between multiple components of an ionized plasma, requiring in the case of Noerdlinger (1977, 1978) a computer alogrithm to calculate automatically the functions describing the coupled differential equations and in the case of Cox, Guzik, and Kidman (1988) the simultaneous solution at each time step of 23 coupled partial differential equations involving 23 unknown functions.

Our approach is based upon the fact, established in these and in earlier studies (Eddington 1926; Aller and Chapman 1960; Vauclair, Vauclair, and Pamjatnikh 1974; Montmerle and Michaud 1976; Fontaine and Michaud 1979*a*, *b*; Vauclair, Vauclair, and Michaud 1978) that element diffusion is a relatively unimportant process in dwarf stars. We therefore adopt an approximate treatment of the problem. We derive a pair of uncoupled analytic equations that are sufficiently accurate to determine quantitatively the effect of diffusion in a number of applications, including the calculation of helioseismological frequencies and of solar neutrino fluxes. The results may be included, without great complication, in existing stellar evolution codes.

The principal results of this paper can be stated simply. The time evolution of the mass fractions at a given spatial point satisfy (to an acceptable accuracy that is specified below) diffusion equations that can be conveniently included in a stellar evolution code. The hydrogen mass fraction, X, satisfies the equation,

$$\frac{\partial X}{\partial t} = \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left[\frac{r^2 X T^{5/2}\xi_{\rm H}(r)}{(\ln\Lambda/2.2)}\right], \tag{1}$$

where $\ln\Lambda$ is the Coulomb logarithm that has a weak dependence on the plasma characteristics (see, e.g., Braginskii 1965). For the solar interior (and similar plasmas), one can use the approximation: $\ln\Lambda \approx 2.2$ (Noerdlinger 1977). The function $\xi_{\rm H}(r)$ is defined below. The units have been chosen so that the numerical coefficient of the right-hand side of equation (1) is unity (see definition below of the dimensionless variables). The time rate of change of the ^{4}He mass fraction Y is, to the accuracy of the calculations presented in this paper, equal in magnitude and opposite in sign to the rate of change of the hydrogen mass fraction. Hydrogen diffuses slowly upward from the stellar interior while helium diffuses slowly downward. The diffusion of ^{3}He was shown to have a negligible effect on solar models (Loeb, Bahcall and Milgrom 1989), because of the large destruction rate of the diffused ^{3}He ions in the solar core. Accordingly, we shall ignore ^{3}He diffusion in this paper. An equation similar to our equation (1), but with less explicit functional dependences, has been used by Pelletier *et al.* (1986) to discuss the diffusion of carbon in helium-rich white dwarfs.

In equation (1), and in the following equations, the partial time derivatives are evaluated at constant mass shells of the star. In these Lagrangian coordinates, the diffusion equations are solved with zero hydrodynamic velocity of the stellar plasma. The temporal evolution of the radius during the star's lifetime is automatically included via the changes in the spatial positions of the different mass shells.

The mass fraction of very heavy elements, Z, satisfies a similar equation,

$$\frac{\partial Z}{\partial t} = -\frac{1}{\rho r^2}\frac{\partial}{\partial r}\left[\frac{r^2 Z X T^{5/2}\xi_A(r)}{(2-X)\ln\Lambda/2.2)}\right]. \tag{2}$$

The dimensionless functions $\xi(r)$ that appear in equations (1) and (2) are:

$$\xi_{\rm H}(r) = \frac{5(1-X)}{4}\frac{\partial \ln P}{\partial r} + \frac{\partial}{\partial r}\ln\left[\frac{X(1+X)}{(3+5X)^2}\right] + \Phi_{\rm H}(X)\frac{\partial \ln T}{\partial r}, \tag{3}$$

for protons and

$$\xi_A(r) = \xi_H - \frac{0.9}{XZ_A^2}\left\{\left[1 + Z_A - \frac{A(5X+3)}{4}\right]\frac{\partial \ln P}{\partial r} + \frac{\partial}{\partial r}\ln\left[\frac{ZX}{5X+3}\left(\frac{1+X}{5X+3}\right)^{Z_A}\right]\right\} + \Phi_A(X)\frac{\partial \ln T}{\partial r}, \quad (4)$$

for heavy elements. In the last expression, A is the average mass number of the heavy elements of interest (~ 50 for iron group elements that contribute significantly to the opacity) and Z_A is the average charge of the heavy elements. The thermal diffusion coefficients in these expressions $\Phi(X)$ have the following fits, based on previous works (Aller and Chapman 1960; Montmerle and Michaud 1976; Noerdlinger 1978),

$$\Phi(X) \approx \begin{cases} 6(1-X)(X+0.32)/(1.8-0.9X)(3+5X) & \text{for protons} \\ 2.7(2-X)/X^2 & \text{for heavy elements}\,. \end{cases} \quad (5)$$

These effective coefficients for thermal diffusion can be easily updated after being implemented in a stellar evolution code, such as the standard solar model, according to more precise calculations that may be performed in the future (e.g., following the numerical scheme that was outlined by Paquette *et al.* 1986).

In simplifying the final form of equation (3), we have used the perfect gas equation of state, $p_i = n_i k_B T$, where k_B is the Boltzmann constant. This form for $\xi(r)$ is valid for various applications, including standard solar models in which element diffusion is a small effect and departures from the perfect gas law are also small. The final condition required to complete the implementation of equations (1) and (2) in a stellar evolution code is that the sum of the fractional chemical compositions by mass is equal to unity at each point in space,

$$X + Y + Z = 1\,. \quad (6)$$

This condition can be used in order to enforce the value of the ^{4}He mass fraction, Y, that is consistent with equations (1) and (2) in stellar evolution codes.

Equations (1) and (2) are in a dimensionless form. The unprimed dimensionless variables are defined in terms of primed dimensional variables:

$$r = \frac{r'}{R_\odot}, \quad T = \frac{T'}{T_0}, \quad \rho = \frac{\rho'}{\rho_0}\,. \quad (7)$$

We adopt, for definiteness, $T_0 = 10^7$ K and $\rho_0 = 100$ g cm^{-3}, representative values for the interior region of the standard solar model (Bahcall and Ulrich 1988). The corresponding characteristic diffusion time, τ_0, is

$$t = \frac{t'}{\tau_0}, \quad (8)$$

which for a density, ρ_0, a temperature, T_0, and $\ln \Lambda = 2.2$, is given by

$$\tau_0 = 6 \times 10^{13} \text{ yr}\,. \quad (9)$$

The numerical value given above results when τ_0 is defined such that the coefficients of $1/\rho r^2$ on the right-hand side of equations (1) and (2) are unity. The characteristic time depends simply upon the typical density, radius, and temperature as $\tau_0 \propto \rho_0 R_\odot^2 T_0^{-5/2}$. The fact that τ_0 is larger than 10^{13} yr justifies the usual approximation of neglecting element diffusion in calculations of main-sequence stellar evolution.

The results summarized in equations (1) and (2) are expected to be accurate to of order several tens of percent (about $\pm 30\%$), which should be adequate for exploring the small effects of diffusion in standard solar models and in a number of other applications. The uncertainties in the model predictions associated with diffusion may be evaluated simply by multiplying the value of τ_0 by a constant factor (e.g., 0.7 or 1.3) and recomputing the stellar model. The main uncertainties arise with respect to the exact evaluation of the Coulomb logarithm (see e.g., Ichimaru 1982 and Ichimaru, Iyetomi, and Tanaka 1987 for an overview on strongly coupled plasmas; and Noerdlinger 1978 and Iben and Macdonald 1985 for the calculation of $\ln \Lambda$ at stellar conditions) and the collision integrals needed for the thermal diffusion coefficients (see, e.g., Roussel-Dupre 1981; Paquette *et al.* 1986). In both equations (1) and (2), we have made use of the simplifying approximations

$$\left(\frac{m_e}{m_H}\right)^{1/2} \ll 1\,, \quad Z \ll 1\,, \quad \frac{1}{3} < X \le 1\,, \quad (10)$$

where m_e is the mass of the electron and m_H is the proton mass. The simplified form for heavy element diffusion that is given in equation (2) depends additionally upon the approximations that

$$A\,, \quad Z_A \gg 1\,. \quad (11)$$

The simplified formulae given here only apply in the region of the star in which the composition is dominated by fully ionized hydrogen and ^{4}He and where the radiation pressure is negligible compared with the total thermal pressure.

The basic equations for this problem are summarized in § II, using the same notation as in Loeb, Bahcall, and Milgrom (1989). The diffusion equations for hydrogen and helium are derived in § III, and the equations for heavy elements are derived in § IV. Section V is devoted to thermal diffusion, while the boundary conditions at $r = 0$ are given in § VI. Preliminary estimates of the effects of diffusion on the predicted rates for different solar neutrino detectors are given in § VII.

II. BASIC EQUATIONS

The stellar density, ρ, is a sum of contributions from different components, i, of the stellar plasma,

$$\rho = \sum_i m_i n_i\,, \quad (12)$$

where m_i and n_i are the mass and number density of the ith component.

The rate at which the number density of each component changes with time at a given position is given by balancing the local diffusion of particles against their rate of conversion by nuclear reactions,

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \boldsymbol{v}_i) = \Gamma_i\,, \quad (13)$$

where the quantity Γ_i represents the changes in compositions due to nuclear reactions and will not be treated in this paper. We limit ourselves to the changes in composition caused by diffusion; the effect of nuclear reactions may be added separately in a stellar evolution code. In addition we shall neglect the radiation pressure in the subsequent discussion as is appropriate for solar conditions (see Michaud *et al.* 1976).

We examine first the effects of gravitational settling, which are associated with the collisional friction between the different plasma components. The effects of thermal diffusion will be added in § V. In between collisions, each plasma component experiences a total force per unit volume, $\boldsymbol{c}_i$,

$$\boldsymbol{c}_i = -\nabla P_i + n_i(q_i \boldsymbol{E} + m_i \boldsymbol{g}) . \quad (14)$$

The net momentum loss per unit volume of the ith fluid can thus be expressed in terms of the frictional force exerted on it by the other plasma components,

$$\boldsymbol{c}_i = \sum_{i \neq j} \boldsymbol{c}_{ij} . \quad (15)$$

The momentum exchange due to collisions between different plasma components is proportional to their number densities, their reduced mass $[m_{ij} = m_i m_j/(m_i + m_j)]$, their velocity difference $\boldsymbol{v}_{ij} = \boldsymbol{v} - \boldsymbol{v}_j$, and a symmetric function, w_{ij}, of the two ion charges:

$$\boldsymbol{c}_{ij} = m_{ij} n_i n_j w_{ij} \boldsymbol{v}_{ij} , \quad (16)$$

where (Braginskii 1965)

$$w_{ij} = w_{ji} = 2.68 \times 10^{-12} Z_i^2 Z_j^2 \left(\frac{m_{ij}}{m_{\mathrm{H}}}\right)^{-1/2} \times \left(\frac{T}{10^7\ \mathrm{K}}\right)^{-3/2} \ln \Lambda\ \mathrm{cm}^3\ \mathrm{s}^{-1} , \quad (17)$$

with $\ln \Lambda$ being the Coulomb logarithm. Below the convective zone in the Sun, the spatial derivative of the Coulomb logarithm can be neglected (Noerdlinger 1977), and $\ln \Lambda \approx 2.2$. The form of w_{ij} can be understood on the basis of dimensional analysis. The only relevant quantity that has the dimensions of a cross section is $(Z_i Z_j e^2/k_{\mathrm{B}} T)^2$ which, when multiplied by the thermal velocity, $(3k_{\mathrm{B}} T/m_{ij})^{1/2}$, yields approximately equation (17).

The electric and gravitational fields satisfy similar equations within the star,

$$\nabla \cdot \boldsymbol{E} = 4\pi \sum_i q_i n_i , \quad (18a)$$

$$\nabla \cdot \boldsymbol{g} = -4\pi G\rho , \quad (18b)$$

and are related similarly to their potentials:

$$\boldsymbol{E} = \nabla \phi = \frac{Q(r)\hat{e}_r}{r^2} , \quad (19a)$$

$$\boldsymbol{g} = -\nabla \Psi = -\frac{GM(r)}{r^2} \hat{e}_r . \quad (19b)$$

Here $\hat{e}_r$ is a unit vector in the radial direction; the enclosed charge is

$$Q(r) = 4\pi \int_0^r \left(\sum_i q_i n_i\right) r'^2\, dr' ; \quad (20a)$$

and the enclosed mass is

$$M(r) = 4\pi \int_0^r \rho r'^2\, dr' . \quad (20b)$$

The sum of all of the momentum exchanges between the plasma particles equals zero and can also be expressed in terms of the sum of the forces on individual particles, i.e.,

$$\sum_i \boldsymbol{c}_i = -\nabla P + \left(\sum_i n_i q_i\right)\boldsymbol{E} + \left(\sum_i n_i m_i\right)\boldsymbol{g} = 0 , \quad (21)$$

where the total pressure $P = \sum_i P_i$ is the sum of the partial pressures. We now give a simple argument which shows that the momentum conservation equation (21) is equivalent to high accuracy to the familiar equation of hydrostatic equilibrium. For electrons, the electric field is the dominant force that pulls the particles down while gravity plays the same role for the positively charged ions. Since the stellar plasma is by assumption in quasi-static equilibrium, the electric force on electrons must be comparable to the gravitational force on positive ions (Eddington 1926; Loeb 1988). Moreover, the ratio of the electric and gravitational forces is the same as the ratio of their source strengths, which is given in equation (18). Hence,

$$\frac{g}{E} \sim \frac{e}{m_{\mathrm{H}}} \sim \frac{G\rho}{\sum q_i n_i} . \quad (22)$$

By rearranging factors between the two right-hand parts of equation (22), one finds that the fractional departure from local charge neutrality is tiny. The local charge density divided by the total number density multiplied by a unit charge is of the order of (Pannekoeck 1922; Eddington 1926)

$$\therefore \frac{\sum_i q_i n_i}{e \sum_i n_i} \sim \frac{G m_{\mathrm{H}}^2}{e^2} \sim 10^{-37} . \quad (23)$$

Inserting the result of equation (23) in equation (21), one finds that the usual equation of hydrostatic equilibrium

$$\nabla P = \rho \boldsymbol{g} , \quad (24)$$

is satisfied to about a part in 10^{37}.

III. HYDROGEN AND HELIUM DIFFUSION

We consider in this section the diffusion of hydrogen and ^{4}He, the assumed dominant elements of the chemical mixture, by collisions among themselves and with ambient electrons. We denote the different species by subscripts with the labels,

$$i = e , \quad \mathrm{H} , \quad \mathrm{He} . \quad (25)$$

Local charge neutrality implies that the average diffusion velocity of electrons, v_e, is comparable to that of the hydrogen and helium ions, i.e., $v_e \sim O(v_{\mathrm{H}}, v_{\mathrm{He}})$. Therefore, the net momentum that the electrons transport is small compared to that of the heavy ions, i.e., $m_e v_e \ll m_{\mathrm{H}} v_{\mathrm{H}}$. The net velocity of the stellar plasma, $\boldsymbol{u}$, is by definition assumed to be zero. Since the momentum carried by electrons is small, the equation for the net velocity of the plasma only involves ionic variables,

$$\boldsymbol{u} \propto (m_{\mathrm{H}} n_{\mathrm{H}} \boldsymbol{v}_{\mathrm{H}} + m_{\mathrm{He}} n_{\mathrm{He}} \boldsymbol{v}_{\mathrm{He}}) \approx 0 . \quad (26)$$

The basic equation describing the time evolution of the number density of hydrogen due to diffusion can be written, specializing equation (13) to a spherical geometry,

$$\frac{\partial n_{\mathrm{H}}}{\partial t} = -\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 n_{\mathrm{H}} v_{\mathrm{H}}) . \quad (27)$$

The diffusion of ^{4}He is described by a similar equation. Hence, we must solve for the diffusion velocities of hydrogen and helium. The results are most easily presented in terms of the fractional abundances by mass, X and Y, of hydrogen and helium, respectively. Here

$$X \equiv \frac{m_{\mathrm{H}} n_{\mathrm{H}}}{\rho} , \quad Y \equiv \frac{m_{\mathrm{He}} n_{\mathrm{He}}}{\rho} . \quad (28)$$

The net velocities of the hydrogen and helium fluids satisfy simple relations among themselves because electrons can be neglected in the overall momentum balance. Equations (26) and (28) imply that

$$\frac{v_{\rm H}}{v_{\rm He}} = -\frac{Y}{X}\,, \tag{29a}$$

and, consequently,

$$Y = v_{\rm H}/(v_{\rm H} - v_{\rm He})\,. \tag{29b}$$

The momentum exchange due to collisions between positive ions and electrons is small compared to the momentum exchanged in collisions between positive ions. Quantitatively, the ratio of the momentum exchange due to electron collisions to the exchange in ion-ion collisions is of order the square root of the electron to proton mass ratio, i.e.,

$$\frac{c_{e,\rm H}}{c_{\rm H,He}} \sim \frac{c_{e,\rm He}}{c_{\rm H,He}} \sim \left(\frac{m_e}{m_{\rm H}}\right)^{1/2} \ll 1\,. \tag{30}$$

The inequality stated in the last equation follows from the form of the symmetric collision function, w_{ij}, given in equation (17), that implies $w_{e,\rm H}/w_{\rm H,He} \sim (m_{\rm H}/m_e)^{1/2}$.

The flux of hydrogen ions can be written in terms of the relative velocity of the hydrogen and helium fluids,

$$n_{\rm H} v_{\rm H} = \frac{(m_{\rm He}\, n_{\rm H}\, n_{\rm He}) v_{\rm H,He}}{\rho}\,. \tag{31}$$

The momentum conservation equation for hydrogen ions is (see eq. [14])

$$c_{\rm H} \cong c_{\rm H,He} = -\frac{\partial P_{\rm H}}{\partial r} + n_{\rm H}(eE + m_{\rm H}\, g)\,, \tag{32}$$

where collisions with electrons have been neglected. The corresponding conservation equation for helium ions is

$$c_{\rm He} \cong -c_{\rm H,He} = -\frac{\partial P_{\rm He}}{\partial r} + n_{\rm He}(2eE + 4m_{\rm H}\, g)\,. \tag{33}$$

The conservation of total momentum, $c_{\rm H,He} = -c_{\rm He,H}$, determines the strength of the electric field:

$$E = -\frac{1}{en_e}\left(\frac{\partial P_e}{\partial r}\right). \tag{34}$$

The above result states that the gradient of the electron pressure is balanced by the electric force density on the electron fluid. This is physically obvious because the negligible electron mass cannot provide significant gravitational or frictional forces that will support the electron pressure gradient (unlike the situation for the ions, which are gravitationally bound). The electric potential over the star is about $k_{\rm B}T/e$, since it is formed by particles with thermal energies of order $k_{\rm B}T$. Therefore, the magnitude of the electric field for the Sun is about, $E \sim k_{\rm B}T/eR_\odot \sim {\rm kV}/10^{11}$ cm $\sim 10^{-8}$ V cm^{-1}, or more precisely: for a star with a mass $M(r)$ (containing mainly protons and electrons), $E = (2.8 \times 10^{-8}\ {\rm V\ cm^{-1}})(P_e/P)[M(r)/M_\odot](R_\odot/r)^2$ (see Loeb 1988 for a general relativistic consideration of these fields at arbitrary hydrodynamical conditions). in deriving equation (34), we have used the local charge neutrality of the plasma and the fact that the total pressure is the sum of the pressures due to electrons and to hydrogen and ^{4}He ions. Substituting for $c_{\rm H,He}$ in equation (32) and using equation (16), one finds

$$v_{\rm H,He} = -\frac{m_{\rm He}\, T}{m_{\rm H,He}\, Y \rho w_{\rm H,He}}\left[\frac{\partial \ln}{\partial r}(P_e P_{\rm H}) - m_{\rm H}\, g\right]. \tag{35}$$

It is convenient to define a dimensionless function $\xi_{\rm H}(r)$ by the relation

$$\xi_{\rm H}(r) \equiv \frac{\partial}{\partial r}\ln(P_e P_{\rm H}) + \frac{GM(r)m_{\rm H}}{r^2 k_{\rm B}\, T}\,, \tag{36}$$

where $g(r) = -GM(r)/r^2$ and the stellar mass is expressed in units of the solar mass,

$$M(r) = M(r')/M_\odot\,. \tag{37}$$

The expression given in equation (36) makes use of the assumed perfect gas equation of state:

$$\frac{1}{n_i k_{\rm B}\, T}\frac{\partial P_i}{\partial r} \approx \frac{\partial \ln P_i}{\partial r}\,, \tag{38}$$

where $k_{\rm B}$ is the Boltzmann constant. The form of $\xi_{\rm H}$ can be further simplified by expressing all the variables in terms of the total pressure, P, and the hydrogen mass fraction, X. We find

$$P_{\rm H} = \frac{4X}{(5X+3)}\,P\,, \quad P_e = \frac{2(1+X)}{(5X+3)}\,P\,, \tag{39}$$

and

$$\frac{GM(r)m_{\rm H}}{r^2 T} = -\frac{(5X+3)}{4}\frac{\partial \ln P}{\partial r}\,. \tag{40}$$

Inserting the expressions given in equations (39) and (40) in equation (36), we arrive at the convenient formula given in the introduction, namely,

$$\xi_{\rm H}(r) = \frac{5(1-X)}{4}\frac{\partial \ln P}{\partial r} + \frac{\partial}{\partial r}\ln\left[\frac{X(1+X)}{(3+5X)^2}\right], \tag{41}$$

apart from the effects of thermal diffusion.

The flux of hydrogen atoms may therefore be written compactly,

$$n_{\rm H} v_{\rm H} = -\frac{X m_{\rm He}\, T \xi_{\rm H}(r)}{m_{\rm H}\, m_{\rm H,He}\, w_{\rm H,He}}\,. \tag{42}$$

Note that, as expected, the diffusive flux (42) is inversely proportional to the square of the charges on each of the ions. The actual diffusive velocity is small,

$$v_{\rm H} = -8 \times 10^{-11}\left[\frac{T^{5/2}}{\rho \ln \Lambda}\,\xi_{\rm H}(r)\right] {\rm cm\ s^{-1}}\,, \tag{43}$$

where for convenience all variables in equation (43) have been expressed in terms of the dimensionless variables indicated in equation (7). The numerical values for the diffusion velocities that are calculated from equation (43) are similar to those obtained by Noerdlinger (1977), who used a much more complicated formalism, but they are more than an order of magnitude smaller than the values obtained by Wambsganss (1988), who also used Noerdlinger's method.

Substituting equation (42) in equation (27) and making use of equation (17), one finds:

$$\frac{\partial X}{\partial t} = \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left[r^2\,\frac{X T^{5/2}}{\ln \Lambda}\,\xi_{\rm H}(r)\right], \tag{44}$$

which is equation (1) of the introduction, neglecting thermal diffusion. The units are defined by equations (7), (8), and (9). To the accuracy of the present computations, the hydrogen and ^{4}He diffusion rates are equal in magnitude and opposite in sign:

$$\frac{\partial Y}{\partial t} = -\frac{\partial X}{\partial t} . \quad (45)$$

IV. HEAVY ELEMENT DIFFUSION

The diffusion of heavy elements can be calculated in a similar way as for hydrogen and helium, with a surprisingly simple answer. We consider the diffusion of a representative ion of mass number A and nuclear charge Z_A.

The equation for momentum balance is

$$\boldsymbol{c}_A \cong \boldsymbol{c}_{A,\mathrm{H}} + \boldsymbol{c}_{A,\mathrm{He}} \equiv \eta(A, r) , \quad (46)$$

where from equations (19b) and (34),

$$\eta(A, r) = -\frac{\partial \boldsymbol{P}_A}{\partial r} + n_A(Z_A e\boldsymbol{E} + Am_{\mathrm{H}}\boldsymbol{g})$$
$$= -n_A k_{\mathrm{B}} T\left(\frac{\partial \ln P_A}{\partial r} + Z_A \frac{\partial \ln P_e}{\partial r} + \frac{AGm_{\mathrm{H}} M}{r^2 k_{\mathrm{B}} T}\right) . \quad (47)$$

The diffusion equation for n_A is

$$\frac{\partial n_A}{\partial t} = -\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 n_A v_A) . \quad (48)$$

The flux of heavy elements, $n_A v_A$, is determined primarily by the collision of heavy ions with hydrogen and ^{4}He ions. The rate of momentum exchange due to collisions of heavy ions with hydrogen can be written

$$\boldsymbol{c}_{A,\mathrm{H}} = m_{A,\mathrm{H}} n_A n_{\mathrm{H}} w_{A,\mathrm{H}}(\boldsymbol{v}_A - \boldsymbol{v}_{\mathrm{H}}) ; \quad (49)$$

a similar equation can be written for collisions with He ions. Inserting the expression (49) for collisions with hydrogen ions and the similar expression for scattering by He ions in equations (46) and (47), one finds

$$n_A v_A(m_{A,\mathrm{H}} n_{\mathrm{H}} w_{A,\mathrm{H}})\left(1 + 2\frac{Y}{X}\right)$$
$$= -n_A v_{\mathrm{H}}(m_{A,\mathrm{H}} n_{\mathrm{H}} w_{A,\mathrm{H}}) + \eta(A, r) , \quad (50)$$

where we have moved all terms involving the velocities of hydrogen and helium ions to the right-hand side of equation (50) and have made use of the relations between velocities given in equation (29). Therefore, the diffusion equation of heavy elements becomes

$$\frac{\partial Z}{\partial t} = \frac{1}{r^2 \rho}\frac{\partial}{\partial r}\left\{\frac{r^2 Z m_{\mathrm{H}} n_{\mathrm{H}} v_{\mathrm{H}}}{(2 - X)}\left[1 - \frac{m_A X \eta_A(A, r)}{m_{\mathrm{H}} Z(m_{A\mathrm{H}} n_{\mathrm{H}} w_{A\mathrm{H}}) n_A v_{\mathrm{H}}}\right]\right\} . \quad (51)$$

Using the result given in equation (42) for the flux of hydrogen ions, one obtains the following diffusion equation for heavy elements with $A \gg 1$,

$$\frac{\partial Z}{\partial t} = -\frac{1}{\rho r^2}\frac{\partial}{\partial r}\left[r^2 \frac{XZT^{5/2}}{(2 - X)\ln \Lambda}\xi_A(r)\right] , \quad (52)$$

where

$$\xi_A(r) = \xi_{\mathrm{H}} - \frac{0.9}{XZ_A^2}\left\{\left[1 + Z_A - \frac{A(5X + 3)}{4}\right]\frac{\partial \ln P}{\partial r} + \frac{\partial}{\partial r}\ln\left[\frac{ZX}{5X + 3}\left(\frac{1 + X}{X + 3}\right)^{Z_A}\right]\right\} . \quad (53)$$

This result is the same, apart from the thermal diffusion term, as equation (2) that was presented in the introduction. The units are defined by equations (7), (8), and (9). Note that the ratio of the two terms on the right-hand side of equation (53) (or eq. [50]) is

$$\frac{\eta(A, r)}{n_A v_{\mathrm{H}}(m_{A,\mathrm{H}} n_{\mathrm{H}} w_{A,\mathrm{H}})} \sim \frac{1}{XZ_A} , \quad (54)$$

and therefore for reasonably large abundances of hydrogen and helium, such as exist in the solar interior, one may neglect $\eta(A, r)$ in equation (50) and approximate $\xi_A \approx \xi_{\mathrm{H}}$.

V. THERMAL DIFFUSION

We discuss the effects of thermal diffusion in this section. Thermal diffusion occurs because of the energy dependence of the Coulomb collision frequencies. As a result of Coulomb interactions with heavier particles, each element is pushed by a thermal force toward cooler regions. From momentum conservation, the thermal force density acting on two interacting components is equal in magnitude and opposite in sign in their corresponding equations of motion. Burgers (1969) considered thermal diffusion by introducing another variable for the description of each fluid, namely the residual heat flow vector. His approach was applied by several authors (see, e.g., Noerdlinger 1977, 1978; Muchmore 1984; Wambsganss 1988) to element diffusion in stars. However, other techniques have suggested (Paquette *et al.* 1986; Fontaine and Michaud 1979*a*, *b*) that the original discussions of Burgers's method overestimate the effects of thermal diffusion in dense plasmas, such as in the solar core.

Accordingly, we adopt in this paper a parametric description of thermal diffusion that does not involve doubling the total number of variables. The formulae given here can be improved easily as progress is made in evaluating more accurately the collision integrals for the thermal diffusion coefficients in dense plasmas.

Consider first the thermal force on the electron fluid. This force results from the different probabilities of transferring the electron momentum to the ions in opposite directions along a temperature gradient. The essential aspects of thermal diffusion in this case can be easily understood by the following physical argument. Let us consider, for simplicity, an electron-proton plasma. For a constant plasma temperature, the electrons are pushed by equal frictional forces in all directions (and therefore experience no net drift), as a result of their collisions with the protons. This frictional force density is of the order of $m_e n_e n_{\mathrm{H}} w_{e\mathrm{H}} v_{e_{\mathrm{th}}}$, where $v_{e_{\mathrm{th}}} \sim (k_{\mathrm{B}} T/m_e)^{1/2}$ is the electron thermal velocity. However, when a temperature gradient is introduced, the frictional forces in the opposite directions along this gradient no longer balance each other. The effective temperature of the electrons coming from one direction is different by about $\lambda \nabla T$ from that of the electrons coming from the opposite direction, where $\lambda \sim v_{e_{\mathrm{th}}}/n_{\mathrm{H}} w_{e\mathrm{H}}$ is the electron Coulomb mean free path. Thus, because of the temperature dependence of $w_{e\mathrm{H}}$, there is an unbalanced thermal force density along the temperature gradient with a magnitude,

$$c_{e_{\rm th}} \sim (\lambda \nabla T/T) m_e n_e n_{\rm H} w_{e\rm H} v_{e\rm H} \sim n_e k_{\rm B} \nabla T \,, \tag{55}$$

The above thermal force density was evaluated accurately for a plasma consisting of electrons and protons by Braginskii (1965), who considered the different velocity moments of the Boltzmann equation. His final result was:

$$c_{e_{\rm th}} = \alpha_e n_e k_{\rm B} \nabla T \,, \tag{56}$$

with $\alpha_e = 0.71$. The numerical coefficient α_e depends weakly on the ion composition of the plasma (e.g., it turns to 0.9 for a pure helium-electron plasma). To the accuracy with which we are working, the presence of helium ions in the stellar plasma can be ignored when evaluating α_e. The thermal force in equation (56) adds an extra term to the expression for the electric field given in equation (34). Including the effect of thermal diffusion, the field can be written as

$$eE = -\frac{1}{n_e}\left(\frac{\partial P_e}{\partial r}\right) - \alpha_e k_{\rm B} \frac{\partial T}{\partial r} \,, \tag{57}$$

From momentum conservation, the electron-hydrogen thermal force term appears in the electron and proton equations of motion with opposite signs. Consequently, the two thermal terms that should be added to the proton equation of motion (35) according to equations (56) and (57) tend to cancel each other. Nevertheless, the presence of ^{4}He ions adds to equation (35) a net thermal force density. Within our accuracy of several tens of percent, this force density can be written symmetrically in the helium and hydrogen densities (Chapman and Cowling 1970) as,

$$c_{\rm H,He_{th}} = \alpha_{\rm H,He} n_{\rm He} n_{\rm H} \left(\frac{T}{P}\right) \nabla T \,, \tag{58}$$

where $\alpha_{\rm H,He} \approx 6(X + 0.32)/(1.8 - 0.9X)$. (The numerical expression for $\alpha_{\rm H,He}$ was obtained by fitting a simple functional form to the calculation of Montmerle and Michaud 1976; see also Noerdlinger 1978, Fontaine and Michaud 1979*a*, *b*, Michaud 1985, Wambsganss 1988, and the detailed computations by Paquette *et al.* 1986). Thus, for hydrogen the additional thermal contribution to the function $\xi(r)$ that was defined previously in equations (41) and (53) is

$$\xi_{\rm th}(r) \approx \left(\frac{\alpha_{\rm H,He} P_{\rm He}}{P}\right) \frac{\partial \ln T}{\partial r} \,. \tag{59}$$

For heavy elements, one can add an effective thermal term (Aller and Chapman 1960; Noerdlinger 1978) to the diffusion velocity in equation (50):

$$v_{A_{\rm th}} = \alpha_{A,\rm H} Z_A^2 \left(\frac{T}{m_{\rm H} n_{\rm H} w_{A,\rm H}}\right) \frac{\partial \ln T}{\partial r} \,, \tag{60}$$

where $\alpha_{A,\rm H} \approx 3$, independent of the atomic number of the elements (Montmerle and Michaud 1976; Noerdlinger 1978). The uncertainty in the exact value of $\alpha_{A,\rm H}$ is smaller than the required accuracy in this paper and therefore will be ignored. The contribution to the diffusion velocity from equation (60) exceeds the thermal part of the electric force density ($\sim Z_A n_A k_{\rm B} \partial T/\partial r$) by about a factor of Z_A. This additional factor results from the fact that the thermal diffusion velocity in equation (60) does not depend on Z_A.

In conclusion, the function $\xi(r)$ in equations (41) and (53) is increased by an amount

$$\xi_{\rm th}(r) = \Phi(X) \frac{\partial \ln T}{\partial r} \,, \tag{61}$$

which has the following effective dependence on X,

$$\Phi(X) \approx \begin{cases} 6(X + 0.32)(1 - X)/(1.8 - 0.9X)(3 + 5X) & \\ \qquad\qquad\qquad \text{for protons ;} & \\ 2.7(2 - X)/X^2 \qquad \text{for heavy elements .} & \end{cases} \tag{62}$$

These results are summarized in equations (3) and (5) of the introduction.

VI. BOUNDARY CONDITIONS AT $r = 0$

In order to implement the differential equations (1) and (2) in a computer code developed to describe stellar evolution, one must have an expression for the diffusion rate near the origin, i.e., at infinitesimal r. The limiting form of the equations near the stellar center must be evaluated separately because of the presence of the r^2 term in the denominator of the right-hand side in

$$\left.\frac{\partial X}{\partial t}\right|_{r\to 0} = \frac{1}{\rho r^2} \frac{\partial}{\partial r} \left.[r^2 X T^{5/2} \xi_{\rm H}(r)]\right|_{r\to 0} \,. \tag{63}$$

One can rewrite equation (63) in terms of a function $f(r)$ that must vanish at $r = 0$ in order to satisfy the physical condition that the rate of increase of X with time is finite at the center of the star. The diffusion equation then takes the form

$$\left.\frac{\partial X}{\partial t}\right|_{r\to 0} \equiv \frac{1}{\rho r^2} \frac{\partial}{\partial r} \left.[r^2 f(r)]\right|_{r\to 0} \,, \tag{64}$$

or, using the fact that $f(r)$ goes to zero at the center,

$$\left.\frac{\partial X}{\partial t}\right|_{r\to 0} = \frac{3}{\rho_0} \left(\frac{\partial f}{\partial r}\right)_{r\to 0} \,. \tag{65}$$

The boundary conditions on the physical variables at $r = 0$ are

$$\frac{\partial T}{\partial r} = 0 \,, \quad \frac{\partial P}{\partial r} = 0 \,, \quad \frac{\partial \rho}{\partial r} = 0 \,, \quad \frac{\partial X_i}{\partial r} = 0 \,. \tag{66}$$

The derivative of the temperature must vanish at the origin because there is no infinite heat source at $r = 0$ (this fact can be seen easily by examining the diffusion equation for heat near the origin). The vanishing of the pressure derivative follows from the equation of hydrostatic equilibrium. The derivatives of the mass fractions, X_i, must vanish at the origin because there is no infinite source or sink for the compositions. Finally, the density derivative must vanish because the pressure can be written as a function of the density, temperature, and composition.

The boundary conditions for the physical variables given in equation (66) can be used to derive an explicit expression for the derivative of ξ at $r = 0$. Using equation (41) and assuming that: $\xi_A \approx \xi_{\rm H} \equiv \xi$ according to equation (54), we find

$$\xi'(0) = \left.\frac{\partial \xi_{\rm H}}{\partial r}\right|_{r\to 0} = -\frac{5\pi G \rho_0^2 (1 - X_0)}{3P_0} + \frac{(3 + X_0)}{X_0(1 + X_0)(3 + 5X_0)} \times \left[\frac{\partial^2 X(0)}{\partial r^2}\right] + \frac{\Phi(X_0)}{T_0} \frac{\partial^2 T(0)}{\partial r^2} \,, \tag{67}$$

where we have denoted by a subscript zero the values of quantities that are evaluated at $r = 0$ and, $\Phi(X)$ is given in equation (62). This simplified form of the boundary condition does not apply for evolved stars that have a very small hydrogen abundance in their cores. In a stellar evolution code, the values of all of the quantities entering the right-hand side of equation (67) will normally be stored in memory with the exception of the second derivatives of X and T at $r = 0$. In order to solve the diffusion problem near $r = 0$, one must store enough values of $X(r)$ and $T(r)$, for small r, in order that one can calculate the second derivatives required in equation (67).

Using the values of $\xi'(0)$ given above, the limiting forms of the diffusion equations become

$$\left.\frac{\partial X}{\partial t}\right|_{r\to 0} = \left(\frac{3X_0 T_0^{5/2}}{\rho_0}\right)\xi'(0)\,, \qquad (68)$$

and

$$\left.\frac{\partial Z}{\partial t}\right|_{r\to 0} \approx \left[\frac{3X_0 Z_0 T_0^{5/2}}{\rho_0(2-X_0)}\right]\xi'(0)\,. \qquad (69)$$

VII. EFFECT OF DIFFUSION ON PREDICTED SOLAR NEUTRINO FLUXES

We discuss in this section the expected effects of diffusion on the predicted neutrino fluxes for the Sun. The assumptions used in deriving the equations given in § I are valid for the solar interior. In particular, the radiative forces can be neglected (the radiation pressure $P_{\rm rad}$ satisfies, $P_{\rm rad} \lesssim 10^{-3} P_e$ in the solar core) in the diffusion equations (see, e.g., Michaud *et al.* 1976). In order to determine accurately the effects of element diffusion on solar models, the expression given in equations (1)–(6) should be incorporated self-consistently in a precise model calculation. This has not yet been accomplished, because of the complications involved in including in the same part of the code the spatial and temporal derivatives that are associated with the diffusion equations. Work is underway to include diffusion in the approximations described in this paper within the standard solar models of Bahcall and Ulrich (1988) and the Paczyński stellar evolution program (see Sienkiewicz, Bahcall, and Paczyński 1990). These in-progress studies should yield slightly improved values for the solar neutrino fluxes expected from the standard solar model. Bahcall and Ulrich (1988) made a preliminary estimate of the effect of diffusion by considering models with inhomogeneous primordial compositions in which the initial helium abundance was about 10% larger in the core of the Sun than in the outer region. For these models (see the discussion in their § IX and in their Table XVIII), the predicted solar neutrino capture rate for the ^{37}Cl experiment (Davis 1986) increased by about 1 SNU (from 8 SNU to 9 SNU) for the models that showed the most marked improvement with respect to the splitting of the p-mode oscillations (see their Table XX for p-mode oscillation frequencies calculated with and without the simulated effects of diffusion). The total range of increase in the predicted rate for the ^{37}Cl experiment was, for the different inhomegeneous models that were considered, 0.4–1.3 SNU. The predicted rate for the ^{71}Ga experiment (Kirsten 1986; Barabanov *et al.* 1985) was increased from about 132 SNU to about 140 SNU by the simulated effects of diffusion.

Wambsganss (1988) calculated the effect of hydrogen and helium diffusion on the central temperature and the primordial helium abundance in some illustrative solar models. His results were obtained using the computer algorithm provided by Noerdlinger (1977) for evaluating the various diffusion velocities (although the numerical values he obtained for the velocities are larger than calculated by Noerdlinger and by us, see discussion following eq. [43]) and the residual heat flow vectors that enter the different coupled diffusion equations in Burgers's method. The nuclear reaction rates that were employed in the calculations of Wambsganss were not specified in his paper, and an older version of the Los Alamos opacity tables was used; therefore, the results cannot be interpreted easily in terms of an absolute effect of diffusion on neutrino fluxes. However, the effect of diffusion can be estimated using Wambsganss's results by making use of the approximate dependence of calculated neutrino fluxes on central temperature. The ratio of the central temperature in Wambsganss's best-estimate diffusion model to the temperature of the model without diffusion is about 1.0062. For standard solar models, the ^{8}B neutrino flux depends upon central temperature, T, approximately as (Bahcall and Ulrich 1988)

$$\phi(^8\mathrm{B}) \propto T^{18}\,, \qquad (70)$$

and the ^{7}Be neutrino flux depends upon temperature as (Bahcall 1989)

$$\phi(^7\mathrm{Be}) \propto T^{8}\,. \qquad (71)$$

The scaling relations given in equations (70) and (71) yield an estimated correction in the predicted capture rate for the ^{37}Cl experiment of

$$\Delta(\phi\sigma)_{^8\mathrm{B}} \cong 0.72 \text{ SNU}\,, \quad \Delta(\phi\sigma)_{^7\mathrm{Be}} \cong 0.06 \text{ SNU}\,, \qquad (72)$$

where σ is the cross section for the corresponding neutrino detection. The equivalent increase in the predicted rate for the ^{71}Ga experiment is 4 SNU. The ^{8}B flux is increased by about 12%. Since the diffusion velocities used by Wambsganss appear to be too large, the estimates given in equation (72) may be an upper limit.

Cox, Guzik, and Kidman (1989) have evaluated the effect of diffusion on the helioseismological frequencies of a standard solar model by solving numerically a set of 23 coupled partial differential equations. They have used an older set of nuclear reaction rates (taken from the review by Fowler, Caughlin, and Zimmerman 1975), an equation of state that yielded pressures that may be slightly too large, and an opacity at the base of the convective zone that was adjusted to give improved agreement between calculated and observed solar p-mode frequencies. Most of the other input parameters and physical quantities that were adopted were state-of-the-art values. The results of Cox, Guzik, and Kidman can be used to estimate the effect of diffusion on neutrino fluxes with the aid of the scaling relations given in equations (70) and (71). For the Cox, Guzik, and Kidman (1989) calculations, the ratio of the central temperature calculated with and without including diffusion is 1.0032, indicating approximately one-half the change found by Wambsganss (1988). With the aid of the Cox, Guzik, and Kidman result, we find:

$$\Delta(\phi\sigma)_{^8\mathrm{B}} \cong 0.36 \text{ SNU}\,, \quad \Delta(\phi\sigma)_{^7\mathrm{Be}} \cong 0.03 \text{ SNU}\,. \qquad (73)$$

The corresponding increase in the predicted rate for the ^{71}Ga experiment is 1.5 SNU, and the ^{8}B flux is increased by about 6%.

We conclude from the above considerations that the capture rate predicted by the standard solar model for the ^{37}Cl neutrino experiment will probably be increased by about 5%–10% due to element diffusion and that the rate predicted for the ^{71}Ga experiment will probably be increased by about 1%. The standard flux of ^{8}B neutrinos, the quantity that is measured in neutrino electron scattering experiments (Beier 1986; Totsuka 1987; Bahcall 1989) and in the SNO (Ewan *et al.* 1987) and ^{98}Mo (Cowan and Haxton 1982; Wolfsberg *et al.* 1985) experiments, will most likely be increased by between 1% and 3%.

This work was supported in part by NSF grant no. PHY-86-20266. It is a pleasure to thank A. Cox and R. K. Ulrich for valuable private communications.

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