

PART IV

TRANSPORT PROCESSES, WEAK INTERACTION PROCESSES, AND HELIUM-BURNING REACTIONS

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Excerpt

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Particle diffusion and gravitational settling

In constructing models of evolving stars in volume 1 of this monograph, it has been assumed that particle diffusion can be neglected. However, the current abundance of Li at the solar surface is much smaller than predicted by models neglecting diffusion and this suggests that, during the gravitationally contracting phase which precedes the main sequence, diffusion carries Li from the convective envelope into higher temperature regions below the base of the envelope where it can be destroyed. The abundance of Fe observed at the solar surface is smaller than the interior Fe abundance indicated by comparison between neutrino fluxes observed from the Sun and fluxes predicted by solar models, suggesting that Fe has diffused out of the convective envelope during the main sequence phase into regions below the base of the convective envelope. The fact that many low luminosity white dwarfs exhibit mono-elemental surface abundances is a dramatic demonstration that, in regions where the gravitational acceleration is orders of magnitude larger than near the surface of the Sun, gravitationally induced diffusion is a first order effect. Thus, there is ample motivation for studying the physics of diffusion.

A description of the physics of particle diffusion can be given on many levels of sophistication. The description adopted in this chapter is based on an analysis of Boltzmann transport equations constructed on the assumptions that there exists an equilibrium distribution function for every species of particle and that, when a system is not in equilibrium, the time rate of change of each distribution function can be determined as the consequence of binary interactions between all particles.

In a star, three distinct types of particle diffusion occur simultaneously. They are induced, respectively, by the existence of a gravitational field, the existence of a temperature gradient, and the existence of concentration gradients. In regions of nuclear energy generation, concentration gradients are primarily a consequence of nuclear transformations. Elsewhere, they are a consequence of gravitationally and thermally-induced diffusion. All three types of diffusion are familiar in terrestrial contexts. Gravitationally-induced diffusion is responsible for the fact that, in the Earth's atmosphere, the abundance of any given type of molecule decreases exponentially with distance above the Earth's surface over a scale height that is inversely proportional to the mass of the molecule. The second and third forms of diffusion compete: thermal diffusion moves faster-moving lighter particles into regions containing slower-moving heavier particles but concentration gradients set up by this diffusion act in the reverse direction.

In that it demands the existence of an electrical field of strength proportional to the gravitational acceleration, perhaps the most intellectually entertaining process is gravitationally induced diffusion in a region in which ions are at least partially ionized. The discussion of this type of diffusion can be broken into four parts: (1) analysis of the consequences of

the equations when all processes are in equilibrium, (2) establishment of equations which describe how binary interactions affect the time rate of change of each distribution function, (3) estimation of the cross sections which characterize the interactions required to establish and maintain equilibrium, and (4) construction of algorithms for solving the diffusion equations. The discussion in this chapter focuses on parts (1), (2), and (4), with considerations involved in part (3) being described more thoroughly in Chapter 13.

The Boltzmann transport equations and their applications are discussed at length in many textbooks on statistical mechanics. A good example is the discussion by Kerson Huang in *Statistical Mechanics* (1963). Application to diffusion in the stellar context has been treated exhaustively by S. Chapman and T. G. Cowling in *Mathematical Theory of Nonuniform Gases* (1970). The discussion in this chapter leans heavily on the treatment by J. M. Burgers in *Flow Equations for Composite Gases* (1969).

In Section 12.1, it is shown that the lowest order moment of the Boltzmann transport equation for a single element species in an external force field vanishes when number conservation prevails and that the next order (linear momentum) moment vanishes when the pressure-gradient force exerted by the species is in exact balance with the external force on the species. In Section 12.2, it is shown that the distribution in space of an element which can be present in two ionization stages in a constant gravitational field at constant temperature can be found exactly but that a simple solution does not exist when more than two ionization states are present. In Section 12.3, the number conservation and linear momentum moments are found for a multicomponent system in which each species of particle is assumed to move, at any given point, with a well defined diffusion velocity with respect to the center of mass of the entire system; the number conservation moments for each species and for the entire system vanish; the overall linear momentum moment vanishes when overall balance between gravitational forces and pressure-gradient forces is assumed, but, in general, the linear momentum moment of an individual species involves an electrical field strength proportional to the gravitational acceleration and the moment does not vanish unless equilibrium with respect to diffusion has been achieved. The relationship between the electrical and gravitational field strengths when pressure balance prevails is described in Section 12.4.

In Section 12.5, it is shown that, for a system consisting of two species in prescribed stages of ionization, if it is assumed that the ratio of species abundances is independent of position, the linear momentum moment for each species can be found in closed form. The moments are identical in absolute value but opposite in sign, depending on species mass and ionic charge in such a way that the net gravitational force on the species with the larger mass to charge ratio is directed inward and is larger than the pressure-gradient force exerted by the more massive ions *plus the pressure-gradient force exerted by the electrons derived from the ions*. Exactly the opposite is true for the lighter ions plus attendant electrons. The forces are such that ions with the larger mass to charge ratio diffuse inward and those with the smaller mass to charge ratio diffuse outward, with the difference in linear momentum moments being proportional to the difference in diffusion velocities.

In Section 12.6, the concept of a resistance coefficient is introduced in the context of a three component system consisting of two ions and attendant electrons. The coefficient is identified as a consequence of scattering collisions between ions and an estimate of its

dependence on ionic charges, on temperature and density, and on differences between diffusion velocities is obtained heuristically. By equating the resistance coefficient for every ion with its linear momentum moment, one establishes a set of relationships between diffusion velocities and local properties. In Section 12.7, it is shown that the constraints imposed by doing all calculations in the center of mass frame of reference and insisting on no electric current permit one to determine individual diffusion velocities. Resistance coefficients involving scattering interactions between electrons and ions are introduced and shown to be of secondary importance in estimating diffusion velocities. Generalization to a multi-component gas is made in Section 12.8.

In Sections 12.9 and 12.10, gravitational diffusion velocities at the base of the convective envelope in solar models are estimated, indicating that, even when thermal diffusion is neglected, iron and other heavy elements diffuse inward rapidly enough to affect the estimate of the interior heavy element abundances based on observationally based estimates of surface abundances. Including the effects of thermal diffusion increases the rate at which heavy elements are depleted in the convective envelope (by over a factor of two in an early treatment, but perhaps by much less according to more recent estimates of the relative importance of thermal diffusion).

In Section 12.11, equations for the rates of change of abundances due to gravitational and concentration-gradient induced diffusion are presented and algorithms for calculating the changes in abundance due to diffusion in theoretical stellar models are constructed. Evidence that these algorithms lead to a mono-elemental surface abundance in a cooling white dwarf is presented in Section 21.8.

12.1 Moments of the Boltzmann transport equation for a species under conditions of complete equilibrium

Consider a non-relativistic gas composed of particles of type s in thermal equilibrium in an environment where each particle of mass m_s and electrical charge e_s is acted upon by a gravitational field $\mathbf{g}(\mathbf{r}, t)$ and an electrical field $\mathbf{E}(\mathbf{r}, t)$, both of which may be functions of time t and position \mathbf{r} . The force on each particle is given by

$$\mathbf{F}_s(\mathbf{r}_s, t) = m_s \mathbf{g}(\mathbf{r}_s, t) + e_s \mathbf{E}(\mathbf{r}_s, t), \quad (12.1.1)$$

where \mathbf{E} is the strength of an electrostatic field of the sort introduced in Section 3.6 in Volume 1 as the necessary consequence of conditions in ionized matter in a gravitational field of strength \mathbf{g} .

Suppose that, at each point in a seven-dimensional phase space where the coordinates are position \mathbf{x} , velocity \mathbf{v} , and time t , there exists a distribution function

$$f_s = f_s(\mathbf{x}, \mathbf{v}, t) \quad (12.1.2)$$

which has the properties that, at any time t and at any position \mathbf{x} , the number density of particles is given by

$$n_s(\mathbf{x}, t) = \int f_s(\mathbf{x}, \mathbf{v}, t) d^3\mathbf{v} \quad (12.1.3)$$

and the mean, or flow, velocity is given by

$$n_s \mathbf{u}_s(\mathbf{x}, t) = \int f_s(\mathbf{x}, \mathbf{v}, t) \mathbf{v} d^3\mathbf{v}. \quad (12.1.4)$$

In these expressions, $d^3\mathbf{v}$ is a three dimensional volume element in velocity space and the integration is over all three dimensions in velocity space.

The rate at which the distribution function changes in phase space may be written as

$$\begin{aligned} \frac{\delta f_s}{\delta t} &= \frac{\partial f_s}{\partial t} + \sum_i \frac{dx_i}{dt} \frac{\partial f_s}{\partial x_i} + \sum_i \frac{dv_i}{dt} \frac{\partial f_s}{\partial v_i} = \frac{\partial f_s}{\partial t} + \sum_i v_i \frac{\partial f_s}{\partial x_i} + \sum_i \frac{dv_i}{dt} \frac{\partial f_s}{\partial v_i}. \\ &= \frac{\partial f_s}{\partial t} + \sum_i v_i \frac{\partial f_s}{\partial x_i} + \sum_i \frac{F_{si}}{m_s} \frac{\partial f_s}{\partial v_i}, \end{aligned} \quad (12.1.5)$$

where the subscript i specifies any of three orthogonal vector directions. The quantity $\delta f_s/\delta t$ at the extreme left in eq. (12.1.5) has been introduced at this point primarily to provide a label for identifying the sums to the right of the equal signs. Under very special circumstances, corresponding to various levels on which equilibrium has been achieved, either $\delta f_s/\delta t$ or the integral over $d^3\mathbf{v}$ of some quantity times $\delta f_s/\delta t$ vanishes.

For example, multiplying the leftmost and rightmost sides of eq. (12.1.5) by $d^3\mathbf{v}$ and integrating produces

$$\int \frac{\delta f_s}{\delta t} d^3\mathbf{v} = \frac{\partial}{\partial t} \int f_s d^3\mathbf{v} + \sum_i \frac{\partial}{\partial x_i} \int v_i f_s d^3\mathbf{v} + \sum_i \frac{F_{si}}{m_s} \int \frac{\partial f_s}{\partial v_i} d^3\mathbf{v} = 0. \quad (12.1.6)$$

The integral has been set equal to zero because, when it is translated into a form involving time and spatial derivatives of the familiar entities, number density and bulk velocity, the term between the equal signs is identical with eq. (8.1.9) in Volume 1, which follows when mass is conserved. Ultimately, $\delta f_s/\delta t$ may be viewed as a device for taking into account interactions between different species of particle, effects of which are absent in the zeroth order distribution functions constructed for isolated species.

Equations (12.1.3)–(12.1.6) are basic in the development of Boltzmann transport equations and the quantity f_s is known as a Boltzmann distribution function. If, in the frame of reference moving with the velocity \mathbf{u}_s , the distribution function is isotropic (depending on the velocity as $|\mathbf{v} - \mathbf{u}_s|$), then $f_s(\mathbf{x}, \mathbf{v}, t)$ is an even function of each $v_i - u_{si}$ and the third integral between equal signs in eq. (12.1.6) vanishes. Making use of eqs. (12.1.3) and (12.1.4), the final result in this case is

$$\frac{\partial n_s}{\partial t} + \sum_i \frac{\partial}{\partial x_i} (n_s u_{si}) = 0, \quad (12.1.7)$$

which can be written in vector notation as

$$\frac{\partial n_s}{\partial t} + \nabla \cdot (n_s \mathbf{u}_s) = \left(\frac{dn_s}{dt} \right)_s + n_s \nabla \cdot \mathbf{u}_s = 0, \quad (12.1.8)$$

where

$$\left(\frac{dn_s}{dt} \right)_s = \frac{\partial n_s}{\partial t} + \mathbf{u}_s \cdot \nabla n_s \quad (12.1.9)$$

is the time derivative in the frame of reference moving with the flow velocity \mathbf{u}_s . Multiplying eqs. (12.1.7) and (12.1.8) by m_s and setting $\rho_s = m_s n_s$, the results are identical in form with the continuity, or mass conservation, equation for the gas as a whole, as expressed by eq. (8.1.9) in Volume 1. In Section 8.1 of Volume 1, the symbol \mathbf{v} is defined as the flow velocity for the gas as a whole, in contrast with the notation in this section where $\mathbf{u}_s = \mathbf{u}_s(\mathbf{x}, t)$ is the flow velocity for a particular species and \mathbf{v} is a variable parameter.

In the absence of nuclear transformations, individual particle species are conserved. When nuclear reactions occur, because the number of nucleons is conserved, mass is, to a good approximation, also conserved. Thus, the identity between eq. (8.1.9) and eqs. (12.1.7) and (12.1.8) means that the latter two equations are essentially rigorously true, even if full equilibrium has not been achieved. The fact that the integral of $\delta f_s / \delta t$ over $d^3\mathbf{v}$ must vanish also places a constraint on the manner in which interactions between particles of different species enter into the construction of $\delta f_s / \delta t$.

Multiplying the integrands in eq. (12.1.6) by any quantity Q and integrating over all velocity space produces what may be called the moment of Q . When $Q = m_s$, the resultant moment M_{s0} may be called the continuity moment, in recognition of the fact that the assumption that M_{s0} vanishes under equilibrium conditions leads to the same continuity equation which is obtained when particle or mass conservation is assumed.

Choosing $Q = m_s \mathbf{v}$ produces what may be called a linear momentum moment. In a reference frame moving with velocity $\mathbf{u}_s(\mathbf{x}, t)$, the velocity parameter \mathbf{c} is related to the velocity parameter \mathbf{v} in the fixed frame by

$$\mathbf{c} = \mathbf{v} - \mathbf{u}_s(\mathbf{x}, t). \quad (12.1.10)$$

If in the moving frame the distribution function has the Maxwell–Boltzmann form

$$f_s(\mathbf{x}, \mathbf{c}, t) = A_s(\mathbf{x}, t) e^{-m_s c^2 / 2kT}, \quad (12.1.11)$$

where

$$A_s(\mathbf{x}, t) = n_s(\mathbf{x}, t) \left(\frac{m_s}{2\pi kT} \right)^{3/2}, \quad (12.1.12)$$

in the stationary frame it has the form

$$f'_s(\mathbf{x}, \mathbf{v}, t) = A_s(\mathbf{x}, t) e^{-m_s |\mathbf{v} - \mathbf{u}_s|^2 / 2kT}. \quad (12.1.13)$$

It is evident that $f_s(\mathbf{x}, \mathbf{c}, t) = f'_s(\mathbf{x}, \mathbf{v}, t)$ and that $\partial f_s(\mathbf{x}, \mathbf{c}, t)/\partial c_i = \partial f'_s(\mathbf{x}, \mathbf{v}, t)/\partial v_i$. In both frames,

$$n_s = \int f_s(\mathbf{x}, \mathbf{c}, t) d^3\mathbf{c} = \int f'_s(\mathbf{x}, \mathbf{v}, t) d^3\mathbf{v}, \quad (12.1.14)$$

but

$$\bar{\mathbf{c}} = \int \mathbf{c} f_s(\mathbf{x}, \mathbf{c}, t) d^3\mathbf{c} = 0 \quad (12.1.15)$$

and

$$\bar{\mathbf{v}} = \int \mathbf{v} f'_s(\mathbf{x}, \mathbf{v}, t) d^3\mathbf{v} = \mathbf{u}_s. \quad (12.1.16)$$

Derivatives in the two frames are related by

$$\begin{aligned} \frac{\partial f'_s(\mathbf{x}, \mathbf{v}, t)}{\partial t} &= \frac{\partial f_s(\mathbf{x}, \mathbf{c}, t)}{\partial t} + \sum_i \frac{\partial f_s(\mathbf{x}, \mathbf{c}, t)}{\partial c_i} \frac{\partial c_i}{\partial t} \\ &= \frac{\partial f_s(\mathbf{x}, \mathbf{c}, t)}{\partial t} - \sum_i \frac{\partial f_s(\mathbf{x}, \mathbf{c}, t)}{\partial c_i} \frac{\partial u_{si}(\mathbf{x}, t)}{\partial t} \end{aligned} \quad (12.1.17)$$

and

$$\begin{aligned} \frac{\partial f'_s(\mathbf{x}, \mathbf{v}, t)}{\partial x_j} &= \frac{\partial f_s(\mathbf{x}, \mathbf{c}, t)}{\partial x_j} + \sum_i \frac{\partial f_s(\mathbf{x}, \mathbf{c}, t)}{\partial c_i} \frac{\partial c_i}{\partial x_j} \\ &= \frac{\partial f_s(\mathbf{x}, \mathbf{c}, t)}{\partial x_i} - \sum_i \frac{\partial f_s(\mathbf{x}, \mathbf{c}, t)}{\partial c_i} \frac{\partial u_{si}(\mathbf{x}, t)}{\partial x_j}, \end{aligned} \quad (12.1.18)$$

where, again, the index i specifies one of three orthogonal directions. The second line in each of the last two equations follows from the first line by differentiating c_i in eq. (12.1.10) with respect to x_j , recognizing that \mathbf{v} in this equation is independent of \mathbf{x} .

Using eqs. (12.1.15)–(12.1.17) in the last form of eq. (12.1.5) gives

$$\begin{aligned} \frac{\delta f'_s}{\delta t} &= \frac{\partial f_s}{\partial t} + \sum_i (u_{si} + c_i) \frac{\partial f_s}{\partial x_i} \\ &\quad - \sum_i \frac{\partial f_s}{\partial c_i} \left[\frac{\partial u_{si}}{\partial t} + \sum_i (u_{sj} + c_j) \frac{\partial u_{si}}{\partial x_j} \right] + \sum_i \frac{F_{si}}{m_s} \frac{\partial f_s}{\partial c_i}, \end{aligned} \quad (12.1.19)$$

or

$$\frac{\delta f'_s}{\delta t} = \frac{df_s}{dt} + \sum_i c_i \frac{\partial f_s}{\partial x_i} - \sum_i \frac{\partial f_s}{\partial c_i} \left[\frac{du_{si}}{dt} + \sum_j c_j \frac{\partial u_{si}}{\partial x_j} \right] + \sum_i \frac{F_{si}}{m_s} \frac{\partial f_s}{\partial c_i}. \quad (12.1.20)$$

Multiplying by $Q d^3c$ and integrating gives

$$\begin{aligned} \int \frac{\delta f_s}{\delta t} Q d^3c &= \frac{d}{dt} \int f_s Q d^3c + \sum_i \frac{\partial}{\partial x_i} \int c_i f_s Q d^3c \\ &\quad - \sum_i \frac{du_{si}}{dt} \int \frac{\partial f_s}{\partial c_i} Q d^3c - \sum_i \sum_j \frac{\partial u_{si}}{\partial x_j} \int \frac{\partial f_s}{\partial c_i} c_j Q d^3c \\ &\quad + \sum_i \frac{F_{si}}{m_s} \int \frac{\partial f_s}{\partial c_i} Q d^3c. \end{aligned} \quad (12.1.21)$$

The three terms containing $\partial f_s/\partial c_i$ can be integrated by parts and, since f_s must vanish at the limits, one has that

$$\begin{aligned} \int \frac{\delta f_s}{\delta t} Q d^3c &= \frac{d}{dt} \int f_s Q d^3c + \sum_i \frac{\partial}{\partial x_i} \int c_i f_s Q d^3c \\ &\quad + \sum_i \frac{du_{si}}{dt} \int f_s \frac{\partial Q}{\partial c_i} d^3c + \sum_i \sum_j \frac{\partial u_{si}}{\partial x_j} \int f_s \frac{\partial(c_j Q)}{\partial c_i} d^3c \\ &\quad - \sum_i \frac{F_{si}}{m_s} \int f_s \frac{\partial Q}{\partial c_i} d^3c. \end{aligned} \quad (12.1.22)$$

It follows from eq. (12.1.15) that, if $Q = m_s c_k$, the first and fourth terms on the right hand side of eq. (12.1.22) vanish. The integrals in the third and fifth terms are just $m_s n_s \delta_{ki}$, where δ_{ki} is a delta function, and the i th integral in the second term is $m_s n_s \bar{c}_i^2 \delta_{ki}$, where the bar over c_i^2 denotes an average over the distribution function. Summing over i then gives for the k th component of the linear momentum moment:

$$M_{sk} = \frac{\partial}{\partial x_k} \left(\bar{c}_k^2 m_s n_s \right) + \frac{du_{sk}}{dt} m_s n_s - F_{sk} n_s. \quad (12.1.23)$$

If the particles obey Maxwell–Boltzmann statistics, the appropriate distribution function is given by eqs. (12.1.11) and (12.1.12), and, using eq. (12.1.3), one has that

$$\bar{c}_k^2 m_s n_s = n_s \left(\frac{m_s}{2\pi kT} \right)^{3/2} \int c_k^2 e^{-m_s c^2/2kT} d^3c = n_s kT = P_s, \quad (12.1.24)$$

where it has been recognized that the product $n_s kT$ is the isotropic pressure P_s exerted by the s -type particles in the frame of reference moving with the flow velocity \mathbf{u}_s . As long as particles do not move with relativistic velocities, the relationship between the isotropic pressure and the quantity $\bar{c}_k^2 m_s n_s$ is independent of the statistics adopted in deriving the distribution function, as may be seen by setting $p_x = p_{sk} = m_s c_{sk}$ and $n = n_s$ in eq. (4.3.1) in Chapter 4 of Volume 1, which follows from the definition of pressure as the rate at which momentum is transferred to a specularly reflecting wall. On the other hand, the pressure calculated in this way is a function of the frame of reference in which

the calculation is performed. For example, adopting the distribution function given by eq. (12.1.13), and choosing the k direction so that $\hat{\mathbf{k}} \cdot \mathbf{u}_s = u_s$, one has that

$$\begin{aligned} (P_s)'_k &= \int f_s v_k^2 d^3\mathbf{v} = \int \left[(v_k - u_k)^2 + 2(v_k - u_k) + u_k^2 \right] f_s d^3\mathbf{v} \\ &= n_s kT + n_s m_s u_s^2, \end{aligned} \quad (12.1.25)$$

which may be written as

$$(P_s)'_k = P_s + P_{s,\text{ram}} \hat{\mathbf{k}} \cdot \hat{\mathbf{u}}_s, \quad (12.1.26)$$

where

$$P_{s,\text{ram}} = n_s m_s u_s^2 \quad (12.1.27)$$

is called a ram pressure. Thus, in the stationary frame, the pressure is composed of a component which is identical with the isotropic gas pressure in the moving frame and of a vector component which, being the product of the bulk linear momentum density and the bulk velocity, is the flux of bulk linear momentum.

In any case, in the frame of reference moving with the flow velocity \mathbf{u}_s , the linear momentum moment, eq. (12.1.23), can be written as

$$M_{sk} = \frac{\partial P_s}{\partial x_k} + \frac{du_{sk}}{dt} m_s n_s - F_{sk} n_s, \quad (12.1.28)$$

or, setting $\rho_s = m_s n_s$,

$$M_{sk} = \frac{\partial P_s}{\partial x_k} + \rho_s \left(\frac{du_{sk}}{dt} - \frac{F_{sk}}{m_s} \right). \quad (12.1.29)$$

Setting $M_{sk} = 0$ is tantamount to stating that particles of type s are in exact pressure balance with themselves, whether or not other types of particle are present. If other types of particle are present, the assumption that $M_{sk} = 0$ places constraints on the nature of the interactions between particles of different types which will permit this condition to be achieved. In vector notation, the condition $M_{sk} = 0$ may be written as

$$\rho_s \frac{d\mathbf{u}_s}{dt} = -\nabla P_s + \frac{\mathbf{F}_s}{m_s}, \quad (12.1.30)$$

or, adopting \mathbf{F}_s given by eq. (12.1.1),

$$\rho_s \frac{d\mathbf{u}_s}{dt} = -\nabla P_s + \left(\mathbf{g} + \frac{e_s}{m_s} \mathbf{E} \right) \rho_s. \quad (12.1.31)$$

If the particles of species s are not ionized, eq. (12.1.31) is identical with the overall linear momentum balance equation, eq. (8.1.14) in Volume 1, an identity which motivates the choice of the name linear momentum moment for M_{sk} .