DIFFUSION COEFFICIENTS IN DENSE PLASMAS

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It has been known for some time (Schatzman 1958) that diffusion
could play an important role in the spectral evolution of white dwarfs.
However, it is only recently that quantitative estimates have become
available, making use of detailed envelope models (Fontaine and Michaud
1979, hereafter referred to as FM; Vauclair, Vauclair, and Greenstein
1979; Alcock and Illarionov 1979). These studies suggest that the
observed monoelemental character of white dwarf spectra can qualita-
tively be explained in terms of the diffusion model. Moreover, it
appears that the diffusion time scales are so short compared to evolu-
tionary times that competing mechanisms, such as accretion, must be
invoked to explain the small but measurable abundances of heavy ele-
ments in the spectra of cooler white dwarfs.

Unfortunately, estimates of diffusion time scales under white
dwarf conditions suffer from large uncertainties. First, if thermal
diffusion dominates, the characteristic time scales strongly depend on
the average charge of the diffusing ion. However, in cooler white
dwarf envelopes, the ionization equilibrium is dominated by non-ideal
effects, and it becomes very difficult to estimate the degree of ioni-
zation of a given element. Detailed numerical computations of the
kind described by Fontaine, Graboske, and Van Horn (1977) must then
be employed. Otherwise, as estimated by FM, the diffusion time scales
of metals may be uncertain by factors 3-4.

More importantly, however, is the fact that all estimates have so
far been obtained from formulae derived by Chapman and Cowling (1970)
which strictly apply in one limiting case: the plasma must be suffi-
ciently dilute so that charged particles interact via a pure Coulomb
potential. Using such a potential leads to a well-known divergence
of the interaction cross-section which is removed with the introduction

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of an arbitrary long-range cutoff distance (usually taken as the Debye length). Such an approach has the main advantage that the cross-sections are expressable analytically; they have a logarithmic form such as equations (4) and (A4) of FM. A better approach is the use of screened Coulomb potentials. They permit, in principle, a better description of the collective effects of all the surrounding charges. They also remove the need for an ad hoc cutoff distance as the cross-section integrals converge naturally, but the computations must be done numerically.

A second, non-essential, approximation used by Chapman and Cowling is to take the logarithmic term of the Coulomb cross-section outside of the integral over the velocity distribution on the assumption that the energy dependence of this logarithmic term would be weak. Again, this was done in order to obtain analytic expressions for the transport coefficients. The diffusion coefficient given, for exemple, by equation (3) of FM is the result of such an approximation. Numerical computations indicate, however, that systematic effects are introduced by such an approximation and that these effects may be large, even in main-sequence stars.

We have developed a computer code that numerically evaluates the Chapman-Cowling collision integrals for spherically symmetric potentials. The details of these calculations will be given elsewhere. We wish here to report on some preliminary calculations with special emphasis on white dwarfs. Table 1 gives both the diffusion coefficient D_{12} and the thermal diffusion coefficient α_{12} of carbon diffusing in helium for a typical isotherm. Four cases are considered: CC is the result of applying directly the Chapman and Cowling equations; PC is for a pure Coulomb potential with Debye cutoff without taking the logarithmic term outside of the velocity distribution integral; DH stands for the Debye-Hückel potential; TF is for the Thomas-Fermi potential which is a better representation of electron screening than the DH model at higher densities.

Comparing CC and PC gives the effects of taking the logarithmic term of the Coulomb cross-section outside of the velocity distribution integral. Comparing PC and DH leads to an estimate of the consequences of having to choose an arbitrary cutoff distance. The most obvious feature is that the thermal diffusion coefficient, as estimated by CC, strongly diverges to large positive values with increasing densities. By contrast, PC gives results for α_{12} which are quite close to those of DH up to log $\rho \sim -2$, beyond which there is a divergence to large negative values. On the other hand, the screened potentials lead to small absolute values of α_{12} at high densities. It thus would appear that the thermal diffusion coefficient can be substantially overestimated if the Chapman-Cowling formulae are used.

TABLE 1

Transport coefficients for log T = 5.0 (C/He)

log ρ	D_{12}				α_{12}			
	CC	PC	DH	TF	CC	PC	DH	TF
-10	9.76+4	1.13+5	1.20+5	--	1.49+1	1.08+1	1.06+1	--
- 8	1.34+3	1.66+3	1.82+3	--	1.52+1	9.58+0	9.14+0	--
- 6	2.15+1	3.09+1	3.77+1	--	1.60+1	7.12+0	6.10+0	--
- 4	5.33-1	1.10+0	1.49+0	--	2.00+1	2.52+0	2.42+0	--
- 2	8.64-2	1.92-1	1.55-1	2.36-1	1.48+2	-3.28-1	5.32-1	2.64-1
0	7.85-2	1.57-1	3.71-2	2.53-2	1.26+4	-4.15+0	-7.77-3	-1.79-1
2	7.85-2	1.57-1	1.43-2	3.46-3	1.25+6	-3.44+2	-1.81-1	-3.55-1

We also find that the diffusion coefficient D_{12} tends toward a constant value with increasing densities in the CC and PC formalisms. By contrast, D_{12} keeps decreasing if the screened potentials are used. This means that in the denser, cooler white dwarfs, D_{12} is also over-estimated if the Chapman-Cowling formulae are employed.

It is striking to note how α_{12} is much more affected than D_{12} by the various approximations. It is easy to understand. While D_{12} comes in a rather simple way from the collision probability, α_{12}, the thermal diffusion coefficient, comes from a delicate cancellation of large and small velocity terms. Thermal diffusion is related to the energy flux when a temperature gradient is present (Cowling 1970). Because energy is flowing upwards, the upgoing protons, in the thermal distribution, will have more energy than the downgoing protons in a hydrogen-rich star. If the element of interest has a larger cross-section for interacting with the upgoing protons it will be pushed upwards, downwards in the other case. This implies a very delicate cancellation which can be strongly affected by any approximation on an energy dependent term such as taking A_{12} (see equation (4) of FM) out of the integral.

We have applied these considerations to reestimate the diffusion time scales of carbon and calcium in the helium-rich white dwarf envelopes discussed by FM. In figure 1, we compare the diffusion time scales computed by FM using the Chapman and Cowling formulae with the numerically-evaluated time scales obtained from the DH screened potential. The helium-rich envelope models used here are parametrized by $M/M_\odot = 0.612$ and log q = -5.0, where q is the fractional mass in the envelope.

It is most important to have reliable estimates of the diffusion time scales for cooler white dwarfs since metals are seen only in the spectra of these stars. Figure 1, however, indicates that for $T_e < 20000$ K, the CC formulae lead to substantial underestimates of the characteristic time scales. Detailed calculations are therefore needed at the low-temperature end of the white dwarf cooling sequence.
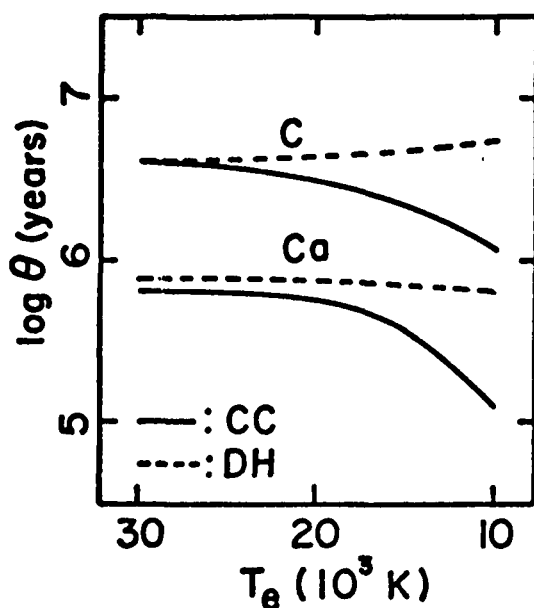
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Fig. 1. Diffusion Time Scale
vs Effective Temperature

The diffusion time scales estimated here are still much smaller
than the evolutionary times so that the central conclusion of FM is
left unchanged: if allowed to proceed freely without competition,
diffusion leads to completely pure hydrogen or helium white dwarf at-
mospheres. We note, however, that before quantitative comparisons can
be made with the observed abundances of heavy elements in the spectra
of cooler white dwarfs, calculations such as those reported here will
be needed. In particular, estimates of equilibrium abundances of
heavy elements based on a balance between accretion and diffusion have
to take into account the large uncertainties in both the accretion rate
and the diffusion time scale.

It should be noted that the preliminary results presented here yet
suffer from another uncertainty. Indeed, thermal diffusion not only
depends on α_{12} but also on α_{1e}, the thermal diffusion coefficient of
electrons relative to the main ionic species. We have not yet solved
all the numerical problems in obtaining α_{1e} for screened potentials.
In calculating the time scales of figure 1, we used in all cases the
α_{1e} of CC as given by equation (A3) of FM. It is not clear at the mo-
ment whether α_{1e} will be positive or negative! The changes indicated
on figure 1 could actually be larger. In particular, the slight elec-
tron degeneracy that is beginning to appear at the bottom of the con-
vection zone may play an important role. Indeed, at this stage, it
is not completely excluded that it could stop diffusion and eliminate
the need for accretion.

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As a final remark, we wish to stress that while our approach takes into account screening effects in a more correct way, it is based on the Chapman-Enskog solution of the Boltzmann equation and does not apply at very large densities. Rigorous statistical mechanical results based on molecular dynamics simulation are becoming available (DeWitt 1976, 1977; Vieillefosse and Hansen 1975; Hansen 1977). Unfortunately, these estimates of transport coefficients are valid only at relatively high densities where the one-component plasma model applies. Thus the electrons must be strongly degenerate so as to provide a uniform neutralizing background, and the ions must be strongly correlated. Except for the coolest white dwarfs these conditions are encountered only much deeper than the base of the convection zone so that these results cannot be directly applied to the problem of the spectral evolution of white dwarfs. However, it is not clear at the moment exactly where one should shift from one regime to the other.

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