Atomic Diffusion Theory

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The following is re-written derivation from Francis Leblanc in Ch. 7 from "An Introduction to Stellar Physics"

1 The Mean Free Path of Species

We want to quantify the number density gradient of species related to physical principles. Lets first say that we have a bulk of hydrogen gas (x) with a small amount of a single metal (z), such that $n_x >> n_z$. Imagine we have a box of that gas in equilibrium, but we want to measure how the metal diffuses within the gas.

$$\frac{dn_x}{dr} = -\frac{dn_z}{dr} \tag{1}$$

n = number density for species x
r = radius of a 1D star

The rate at which particles enter a box is equal to the rate of particles which leave that same box in order for the pressure to be equal to a constant.

The flux (F) of said particles can be defined as...

$$F = nV \tag{2}$$

where V is the velocity of the particles out-of or in-to an imaginary box.

Particles traveling outward...

$$n_z^+ = \frac{1}{6}\left(n_z - \ell_z \frac{dn_z}{dr}\right) \tag{3}$$

Particles traveling inward...

$$n_z^- = \frac{1}{6}\left(n_z + \ell_z \frac{dn_z}{dr}\right) \tag{4}$$

ℓ_z = mean free path

Assuming velocity of diffusion is isotropic and in three dimensional space (a box; $1/6 sides$). From a "three stream" approximation you have 1/(n-dimensions) of the particles travel in the radial direction outward as well as inward in equal amounts (divide by 2). Regions neighbouring the box in azimuth will also freely exchange particles.

The diffusion of species under consideration is in the radial direction of our 1D star. So the flux of particles can be written as...

$$F_z = n_z V_z = (n_z^+ - n_z^-)V_z = -\frac{1}{3} V_z \ell_z \frac{dn_z}{dr} \tag{5}$$

What we really want to know is the difference between the average diffusion in equilibrium versus the metals diffusion. We can estimate the average velocity through the following...

$$\bar{V} = \frac{n_z V_z + n_x V_x}{n_z + n_x} \tag{6}$$

Remember: We defined the diffusion of the number density of particles to be equal and opposite in order to keep the gas pressure constant, so $F_z = -F_x$ by only knowing the diffusion velocity of one of those species.

$$\frac{1}{3} \bar{V}_z \ell_z \frac{dn_z}{dr} = -\frac{1}{3} \bar{V}_z \ell_z \frac{dn_x}{dr} \tag{7}$$

$$\bar{V} = \frac{1}{n_z + n_x} (F_z - F_x) \frac{dn_z}{dr} \tag{8}$$

$$\bar{V} = -\frac{1}{n_z + n_x} \left(\frac{1}{3} \bar{V}_z \ell_z - \frac{1}{3} \bar{V}_x \ell_x \right) \frac{dn_z}{dr} \tag{9}$$

Subtract the diffusion of the metal species from the bulk motion to get the following...

$$F_z - \bar{F} = n_z V_z - n_z \bar{V} = n_z V_{z,diff} \tag{10}$$

About to do a massive amount of algebra so writing it out gives...

$$= \left(-\frac{1}{3} V_z \ell_z \frac{dn_z}{dr} \right) - n_z \bar{V}_z = \tag{11}$$

$$= -\frac{1}{3} V_z \ell_z \frac{dn_z}{dr} - n_z \left(\frac{n_z V_z + n_x V_x}{n_z + n_x} \right) \tag{12}$$

Remember: $nV \sim \bar{V}\ell/3 \; dn/dr$ from mean free path.

$$= -\frac{1}{3} V_z \ell_z \frac{dn_z}{dr} + n_z \frac{1}{3} \frac{dn_z}{dr} \left(\frac{V_z \ell_z + V_x \ell_x}{n_z + n_x} \right) \tag{13}$$

$$= -\frac{1}{3} \frac{dn_z}{dr} \left(\bar{V}_z \ell_z + n_z \left(\frac{V_z \ell_z + V_x \ell_x}{n_z + n_x} \right) \right) \tag{14}$$

$$= -\frac{1}{3}\frac{dn_z}{dr}\frac{1}{n_z + n_x}\left((n_z + n_x)\bar{V}_z\ell_z + n_z\left(V_z\ell_z + V_x\ell_x\right)\right) \tag{15}$$

$$= -\frac{1}{3}\frac{dn_z}{dr}\frac{1}{n_z + n_x}\left(n_z\bar{V}_z\ell_z + n_x\bar{V}_z\ell_z - n_z\bar{V}_z\ell_z + n_z\bar{V}_x\ell_x\right) \tag{16}$$

Finally...

$$n_z V_{z,diff} = -\frac{1}{3}\frac{dn_z}{dr}\frac{1}{n_z + n_x}\left(n_x\bar{V}_z\ell_z + n_z\bar{V}_x\ell_x\right) \tag{17}$$

Since that massive amount of junk are all constants, we can throw them into a new constant (D_{zx}) and call it the "diffusion coefficient"

$$D_{zx} = \frac{1}{3(n_z + n_x)}\left(n_x V_z\ell_z + n_z V_x\ell_x\right) \tag{18}$$

$$V_{z,diff} = -\frac{D_{zx}}{n_z}\frac{dn_z}{dr} \tag{19}$$

The solution for the other species is symmetric (just replace z with x and see for yourself), so we can calculate the diffusion velocity of the previous in one line.

$$V_{x,diff} = -\frac{D_{zx}}{n_x}\frac{dn_x}{dr} \tag{20}$$

Remember: That z is the metal a minuscule mass and x is hydrogen or the bulk of the mass. So we take the limit, as n_x goes to one and n_z goes to zero.

$$D_{zx} = \frac{\bar{V}_2\ell_2}{3} \tag{21}$$

That was a long and comprehensive way of illustrating that we don't care as much about the diffusion of hydrogen in a star, given equilibrium, as much as the metals relative diffusion within the bulk gas. All we need to do is look at the mean free path of the metal and we can determine the rate of diffusion.

2 Force Diagram

Now we want to know what forces are acting on the metal to give rise to a diffusion velocity. Again assuming equilibrium, one can derive the following:

$$(P(r + dr) - P(r))dA = -NF \tag{22}$$

Where **P** is pressure, **r** is radius of the star, **A** is area. **N** is number of particles and **F** is the force acting on those particles. Remember that force is equal to pressure times area, so we are balancing an inward force (**F**) against outward force from pressure (**P**). We assumed previously that the pressure *gradient* was constant but not zero.

With the ideal gas law and a basic definition of number density we can rewrite the equilibrium equation as...

$$P = nkT \; ; \; N = n \, dA \, dr \tag{23}$$

$$dn \, kT \, dA = -n \, dA \, dr \, F \tag{24}$$

Pressure gradient becomes a gradient of the number density assuming local thermal equilibrium.

$$\frac{1}{n}\frac{dn}{dr} = -\frac{F}{kT} \tag{25}$$

If we now combine this equilibrium argument, we can now see how the diffusion coefficient and dispersion velocity can be related to the forces acting on individual particles.

$$V_{z,diff} = -D_{zx}\left(\frac{1}{n}\frac{dn}{dr} + \frac{F_z}{kT}\right) \tag{26}$$

2.1 Gravity

The relative gravity between the metal and the bulk gas of hydrogen can be written as...

$$F_z = m_z g - m_p g \tag{27}$$

where m_z is the mass of the metal nucleus and m_p is the mass of the proton (i.e hydrogen nucleus). g is the acceleration due to gravity.

2.2 Radiation Pressure

Since a metal will have more transition states then a hydrogen atom it can effectively absorb more photons. This imparts a pressure force do to photons. We can approximate this as an acceleration like gravity, mostly just because we can. But we also know the number of transitions states is proportional to the number of atomic particles in the nucleus. *waves hands vigorously* So basically its an acceleration per atomic mass unit. It is also operating in the opposite direction as to gravity, hence the minus.

$$F_z = m_z(g - g^z_{rad}) - m_p g = Am_p(g - g^z_{rad}) - m_p g \tag{28}$$

$$F_z = ((A-1)g - Ag^z_{rad})m_p \tag{29}$$

A = atomic number.

2.3 Electric Fields

The free electrons in a fully ionized plasma have partial pressures for protons (p) and electrons (e) represented by the following equations...

$$\frac{lnP_p}{dr} = -\frac{m_p g}{kT} + \frac{eE}{kT} \tag{30}$$

$$\frac{lnP_e}{dr} = -\frac{m_e g}{kT} - \frac{eE}{kT} \tag{31}$$

E is the electric Field, e is atomic charge unit (charge of electron).

To converse electric neutrality in the plasma the the pressure gradients between electrons and protons must be equal.

$$\frac{lnP_e}{dr} = \frac{lnP_p}{dr} \tag{32}$$

Lets assume that the plasma is pure hydrogen, because why not. We already went down that rabbit hole once.

$$-\frac{m_p g}{kT} + \frac{eE}{kT} = -\frac{m_e g}{kT} + \frac{eE}{kT} \tag{33}$$

$$-m_p g + eE = -m_e g - eE \tag{34}$$

$$-m_p g + m_e g = -2eE \tag{35}$$

$$\frac{(m_p + m_e)g}{2e} = E \tag{36}$$

Electrons have no mass so they will "float" relative to the protons which have mass. So in other words lets throw out the mass of an electron while we are at it. The difference in charge can derive the force acting on the metal. The electric field is negative towards the core (metal nucleus is positively charged, surface is negatively charged)

$$F_z = -\Delta qE \tag{37}$$

$$F_z = -(Z-1)\frac{m_p g}{2e} \tag{38}$$

(Z-1) is the charge difference between a metal and a hydrogen nucleus number of protons relative to the bulk gas.

3 Sum of All Forces

Bringing this all together now...

$$V_{z,diff} = -D_{zx} \left(\frac{1}{n} \frac{dn}{dr} + \frac{1}{kT} \left(((A-1)g - Ag^{z}_{rad})m_p - (Z-1)\frac{m_p g}{2e} \right) \right) \quad (39)$$

This can be cleaned up a bit...

$$V_{z,diff} = -D_{zx} \left(\frac{1}{n} \frac{dn}{dr} + \frac{m_p}{kT} \left((g - g^{z}_{rad})A - (Z-1)\frac{g}{2e} \right) \right) \quad (40)$$

Whats neat about this equation is that you can clearly see that the atomic mass and charge are the fundemental things which determine the relative diffusion of atoms, so naturally a metalicity grdient should develop in the absence of large scale motion.