1 High atmosphere equations

1.1 Boltzmann equation (Week 8)

We now proceed to derive the equations of motion from the Boltzmann equation that describes the evolution of the 7-dimensional phase space distribution function. The derivation of the Boltzmann equation can be found, for example, in Chapter 5 of Gom- bosi (1994). The number of particles in the $d^3r d^3v$ phase space volume element around $(r, v)$ at time $t$ is

$$d^6N = F(t, r, v) d^3r d^3v$$  \hspace{1cm} (1)

where $F(t, r, v)$ is the phase space distribution function (m$^{-6}$ s$^3$). It is important to note that $t$, $r$ and $v$ are assumed to be independent variables. Then the Boltzmann equation is

$$\frac{\partial F}{\partial t} + v_i \frac{\partial F}{\partial x_i} + \frac{\partial}{\partial v_i} (a_i F) = \frac{\delta F}{\delta t}$$  \hspace{1cm} (2)

where repeated indices imply a sum and $\delta F/\delta t$ is the rate of change of the distribution function due to collisions. In most applications, the acceleration is such that $\partial a_i/\partial v_i = 0$, which applies to gravity and the Lorentz force. Therefore, we have

$$\frac{\partial F}{\partial t} + v_i \frac{\partial F}{\partial x_i} + a_i \frac{\partial F}{\partial v_i} = \frac{\delta F}{\delta t},$$ \hspace{1cm} (3)

where the left hand side is the material derivative in six-dimensional phase space.

It is convenient to write the random thermal velocity as

$$\mathbf{c}(t, r) = v - \mathbf{u}(t, r)$$ \hspace{1cm} (4)

where $\mathbf{u}$ is the bulk flow velocity:

$$\mathbf{u}(t, r) = \frac{\int d^3v v F(t, r, v)}{\int d^3v F(t, r, v)}$$ \hspace{1cm} (5)
Repeating the derivation of the Boltzmann equation in Gombosi (1994) with \( \mathbf{c}(t, \mathbf{r}) \) yields the transformations

\[
\frac{\partial F(t, \mathbf{r}, \mathbf{v})}{\partial t} \rightarrow \frac{\partial F(t, \mathbf{r}, \mathbf{c})}{\partial t} - \frac{\partial u_i(t, \mathbf{r})}{\partial t} \frac{\partial F(t, \mathbf{r}, \mathbf{c})}{\partial c_i} \tag{6}
\]
\[
\frac{\partial F(t, \mathbf{r}, \mathbf{v})}{\partial x_j} \rightarrow \frac{\partial F(t, \mathbf{r}, \mathbf{c})}{\partial x_j} - \frac{\partial x_j(t, \mathbf{r})}{\partial x_j} \frac{\partial F(t, \mathbf{r}, \mathbf{c})}{\partial c_i} \tag{7}
\]
\[
\frac{\partial F(t, \mathbf{r}, \mathbf{v})}{\partial v_j} \rightarrow \frac{\partial F(t, \mathbf{r}, \mathbf{c})}{\partial c_j} \tag{8}
\]

With these transformations, the Boltzmann equation for \( F(t, \mathbf{r}, \mathbf{c}) \) is

\[
\frac{\partial F}{\partial t} + (u_i + c_i) \frac{\partial F}{\partial x_i} - \left[ \frac{\partial u_i}{\partial t} + (u_j + c_j) \frac{\partial u_i}{\partial x_j} - a_i \right] \frac{\partial F}{\partial c_i} = \frac{\delta F}{\partial t}. \tag{9}
\]

### 1.2 Collisions (Week 10)

An extensive treatment of the collision problem is out of scope for this course. Below, we simply sketch some basic principles. Please refer to, for example, Chapters 3 and 5 in Gombosi (1994) for a more thorough treatment. The number of particles with velocities between \( \mathbf{v}_1 \) and \( \mathbf{v}_1 + d\mathbf{v}_1 \) (group 1) scattered by collisions with a single particle that has a velocity between \( \mathbf{v}_2 \) and \( \mathbf{v}_2 + d\mathbf{v}_2 \) (group 2) into a solid angle element \( d\Omega \) in direction \( \mathbf{g}' \) per unit time is

\[
dN_1 = I_1 S(\mathbf{g}, \mathbf{g}') d\Omega \tag{10}
\]

where \( \mathbf{g} = \mathbf{v}_1 - \mathbf{v}_2 \) is the relative velocity vector of the particles, \( I_1 \) is the flux of group 1 particles \( (m^{-2} s^{-1}) \) at relative velocity between \( \mathbf{g} \) and \( \mathbf{g} + d^3\mathbf{g} \) impinging on the group 2 particle, and \( S(\mathbf{g}, \mathbf{g}') \) is the differential collision cross section. Note that the particles in groups 1 and 2 can be like or unlike particles.

We assume spherically symmetric central force fields and simplify the collision cross section accordingly. We define \( \chi \) as the deflection angle away from the original direction of \( \mathbf{g} \) and note that for central force fields, the interaction between particles is a planar motion specified by a constant azimuth angle \( \epsilon \) around the direction of \( \mathbf{g} \). Therefore, the differential cross section is \( S(\mathbf{g}, \mathbf{g}') = S(\mathbf{g}, \chi) \) and the solid angle element is \( d\Omega = \sin \chi d\chi d\epsilon \). Then, the flux of group 1 particles impinging on the group 2 particle is \( I_1 = gF(t, \mathbf{r}, \mathbf{v}_1) d^3\mathbf{v}_1 \) and we have

\[
dN_1 = gS(\mathbf{g}, \chi) \sin \chi d\chi d\epsilon F(t, \mathbf{r}, \mathbf{v}_1) d^3\mathbf{v}_1. \tag{11}
\]

Thus, the total number of interactions per unit time and unit volume for particles with velocity between \( \mathbf{v}_1 \) and \( \mathbf{v}_1 + d\mathbf{v}_1 \) and particles with velocity between \( \mathbf{v}_2 \) and \( \mathbf{v}_2 + d\mathbf{v}_2 \) is

\[
dN_{12} = gS(\mathbf{g}, \chi) \sin \chi d\chi d\epsilon F(t, \mathbf{r}, \mathbf{v}_1) F(t, \mathbf{r}, \mathbf{v}_2) d^3\mathbf{v}_1 d^3\mathbf{v}_2 \tag{12}
\]

where we used the phase space distribution function to express the number density of group 2 particles.
1.2.1 Boltzmann collision integral

We will make the following assumptions: (i) only binary collisions are taken into account and the gas is presumed to be sufficiently dilute to justify this assumption, (ii) velocities are assumed to be statistically independent and correlations between the position and velocity of the individual particles are ignored (molecular chaos), (iii) particles and associated force fields are spherically symmetric, (iv) the scale length of the distribution function is much larger than the range of intermolecular forces, (v) the effect of external forces on collision cross sections are ignored, and (vi) the phase space distribution function does not change significantly during the time interval of molecular collisions.

The collision integral is the sum of collisions that deplete (-) and replenish (+) the particles with velocities between \(v_1\) and \(v_1 + dv_1\) inside the phase space volume element at a given location i.e.,

\[
\frac{\delta F}{\delta t} = \left( \frac{\delta F}{\delta t} \right)^+ - \left( \frac{\delta F}{\delta t} \right)^-.
\]  

(13)

We divide equation (12) by \(d^3v_1\) and integrate to obtain the rate of change in \(F\) due to collisions that deplete particles with velocities between \(v_1\) and \(v_1 + dv_1\):

\[
\left( \frac{\delta F}{\delta t} \right)^+ = \int d^3v_2 \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi)gF(t, r, v_1)F(t, r, v_2)
\]  

(14)

where the total collision cross section is defined as

\[
\sigma(g) = \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi).
\]  

(15)

The rate of change in \(F\) due to collisions that replenish particles with velocities between \(v_1\) and \(v_1 + dv_1\) can be written as

\[
\left( \frac{\delta F}{\delta t} \right)^+ = \int d^3v_2 \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi)gF(t, r, v'_1)F(t, r, v'_2)
\]  

(16)

where the superscript \(\prime\) denotes initial velocities (while the lack of superscript denotes final velocity). Deducting the depleting collisions from the replenishing collisions gives

\[
\frac{\delta F}{\delta t} = \int d^3v_2 \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi)g \left(F'F'_2 - FF_2\right),
\]  

(17)

which is the total collision integral.

We will generally work with the Boltzmann equation in the thermal velocity space. Following the steps above, we could have just as easily argued that

\[
\frac{\delta F}{\delta t} = \int d^3c_2 \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi)g \left(F'F'_2 - FF_2\right),
\]  

(18)
where the phase space distribution functions are $F = F(t, r, c_1)$ and $F_2 = F(t, r, c_2)$. Also, for a single species $s$ in a multi-species gas, the collision integral is

$$\frac{\delta F_s}{\delta t} = \sum_t \int d^3c \int_0^{2\pi} d\chi \sin \chi S(g, \chi) g \left( F'_s F'_t - F_s F_t \right)$$

(19)

where the sum is over all species $t$, including $s$.

1.2.2 The equilibrium distribution

In equilibrium, the collision integral vanishes and the Boltzmann equation becomes

$$\frac{\partial F}{\partial t} + (u_i + c_i) \frac{\partial F}{\partial x_i} - \left[ \frac{\partial u_i}{\partial t} + (u_j + c_j) \frac{\partial u_i}{\partial x_j} - a_i \right] \frac{\partial F}{\partial c_i} = 0,$$

(20)

which means that $F'_t F'_s = F F_s$ i.e., that $\ln F_s$ is a summation invariant (conserved quantity) of the collisions. Noting that the conserved quantities in collisions of particles without internal degrees of freedom are the momentum vector and kinetic energy, it can be shown that the equilibrium distribution is the Maxwell-Boltzmann (M-B) distribution (Gombosi, 1994):

$$F(t, r, c) = n(r) \left( \frac{m}{2\pi kT} \right)^{3/2} \exp \left( -\frac{mc^2}{2kT} \right)$$

(21)

where $n$ is the number density.

1.2.3 Collision term with the normalized distribution function

We can write the collision term (12) by using normalized distribution functions as:

$$dN_{12} = gS(g, \chi) \sin \chi d\chi c_n n_1 f(v_1) f(v_2) d^3v_1 d^3v_2$$

(22)

where $n_1$ and $n_2$ are number densities. In general, the normalized distribution function is defined as

$$f(r, v) = \frac{F(r, v)}{n(r)},$$

(23)

which normalizes to

$$\int d^3v f(r, v) = \frac{1}{n(r)} \int d^3v F(r, v) = 1$$

(24)

to comply with the definition of the phase space distribution function. In equilibrium, the normalized M-B distribution function does not depend on position. Now, the total number of encounters per unit volume per unit time is

$$N_{12} = \kappa_{12} n_1 n_2 \int d^3v_1 \int d^3v_2 gS(g) f(v_1) f(v_2)$$

(25)
where $\kappa_{12} = 1/2$ for like particles and $\kappa_{12} = 1$ for unlike particles to prevent double counting of like particle collisions in this integral. We can use the M-B distribution to write this as

$$N_{12} = 4\pi\kappa_{12}n_1n_2 \left(\frac{m_{12}}{2\pi kT}\right)^{3/2} \int_0^\infty g^3 \sigma(g) \exp \left(-\frac{m_{12}g^2}{2kT}\right) \, dg$$  \hspace{1cm} (26)

where $m_{12}$ is the reduced mass.

### 1.2.4 Binary chemical reaction rates

The rate coefficient for chemical reactions is an application of kinetic theory. Consider a reaction of two particles. The intermolecular potential $U$ of these particles is faintly attractive at relatively large intermolecular distances but becomes strongly repulsive at close approach. If the particles have sufficient energy to overcome the potential barrier (activation energy $U_0$) to be brought within the reaction distance $d_0$ of each other, they will form a short-lived compound molecule that decays into the reaction products. The interaction cross section is

$$\sigma(g) = \sigma_0 H(g-g_0)$$  \hspace{1cm} (27)

where $H$ is the Heaviside step function and

$$g_0 = \sqrt{\frac{2U_0}{m_{12}}}.$$  \hspace{1cm} (28)

Thus, we can integrate equation (26) to obtain

$$Z_{12} = \kappa_{12}\sigma_0 n_1n_2 \sqrt{\frac{8kT}{\pi m_{12}}} \exp \left(-\frac{U_0}{kT}\right) \left(1 + \frac{U_0}{kT}\right).$$  \hspace{1cm} (29)

If we assume that $U_0 >> kT$, we can write the binary reaction rate coefficient as

$$k_{12} = \frac{Z_{12}}{\kappa_{12}n_1n_2} = \sigma_0 \sqrt{\frac{8kT}{\pi m_{12}}} \alpha \exp(-\alpha)$$  \hspace{1cm} (30)

where $\alpha = U_0/(kT)$. This expression motivates one of the standard expressions for the reaction rate coefficient in photochemical models:

$$k_{12} = a \left(\frac{T}{300}\right)^b \exp \left(-\frac{c}{T}\right)$$  \hspace{1cm} (31)

where $a, b, c$ are fit coefficients. An upper limit can be obtained by crudely writing

$$k_{12} \approx Q\langle v_T \rangle$$  \hspace{1cm} (32)

where $Q$ is an estimate of the cross section based on the rough molecular diameter ($Q \sim 5 \times 10^{-19} \text{ m}^2$) and $\langle v_T \rangle$ is the mean thermal velocity.
1.3 Maxwell’s equation of change (Week 11)

Consider a molecular quantity \(W(c)\) that is independent of time and spatial location (i.e., given a value of \(c\), the quantity always has the same value). The average value of this quantity is simply given by

\[
\langle W \rangle = \frac{1}{n} \int d^3 c W(c) F(t, r, c).
\]

(33)

Setting \(W = 1\) then gives the obvious result that

\[
n = \int F d^3 c
\]

(34)

and setting \(W = c\) is

\[
\int c_i F d^3 c = 0
\]

(35)

because \(c_i\) is the random thermal velocity that must average to zero.

We can now use the Boltzmann equation to track the evolution of the quantity \(W(c)\) by writing:

\[
\int d^3 c W(c) \left\{ \frac{\partial F}{\partial t} + (u_i + c_i) \frac{\partial F}{\partial x_i} - \left[ \frac{\partial u_i}{\partial t} + (u_j + c_j) \frac{\partial u_i}{\partial x_j} - a_i \right] \frac{\partial F}{\partial c_i} \right\} = \int d^3 c W(c) \frac{\delta F}{\delta t}.
\]

(36)

Here, we write

\[
\int d^3 c W(c) \frac{\partial F}{\partial t} = \frac{\partial}{\partial t} \int d^3 c W(c) F = \frac{\partial}{\partial t} \left( n \langle W \rangle \right)
\]

(37)

\[
\int d^3 c W(c) u_i \frac{\partial F}{\partial x_i} = u_i \frac{\partial}{\partial x_i} \left( n \langle W \rangle \right)
\]

(38)

\[
\int d^3 c W(c) c_i \frac{\partial F}{\partial x_i} = \frac{\partial}{\partial x_i} \left( n \langle c_i W \rangle \right)
\]

(39)

because \(c_i\) and \(t\) are independent and \(u_i\) does not depend on \(c_i\). Also, we can write

\[
\int d^3 c W(c) \frac{\partial F}{\partial c_i} = \int d^3 c \frac{\partial}{\partial c_i} \langle WF \rangle - \int d^3 c F \frac{\partial W}{\partial c_i} = -n \langle \frac{\partial W}{\partial c_i} \rangle
\]

(40)

because the first term in the middle is a perfect differential and \(F \to 0\) at \(c_i = \pm \infty\).

Employing the same logic, we also obtain

\[
\int d^3 c W(c) a_i \frac{\partial F}{\partial c_i} = -n \langle a_i \frac{\partial W}{\partial c_i} \rangle
\]

(41)

\[
\int d^3 c W(c) c_j \frac{\partial F}{\partial c_i} = -n \langle c_j \frac{\partial W}{\partial c_i} \rangle - n \delta_{ij} \langle W \rangle.
\]

(42)
Thus, we have derived new expressions for all of the terms on the r.h.s of equation (36).

Lengthy algebra can be employed to demonstrate that, in the absence of chemical reactions (e.g., Gombosi, 1994),

\[
\int d^3c \frac{\delta F}{\delta t} = \frac{\delta W}{\delta t} = \Delta [W]
\]

\[
= 1/2 \int d^3c \int d^3c_2 \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi) g (W' + W_1^2 - W - W_2) FF_2.
\]

(43)

For species \( s \) in a multi-species gas, the collision integral is

\[
\frac{\delta W_s}{\delta t} = \sum_t \int d^3c_s \int d^3c_t \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi) g (W_s' - W_s) F_s F_t.
\]

(44)

where the sum is over all species \( t \). Using the collision integral and the other terms in equation (36) gives the result

\[
\frac{\partial}{\partial t} (n_s \langle W \rangle) + \frac{\partial}{\partial x_i} (n_s \langle W u_i \rangle) + n_s \langle c_i W \rangle \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) + n_s \langle c_i W \rangle \frac{\partial u_i}{\partial c_i} + n_s \langle c_j W \rangle \frac{\partial u_i}{\partial x_j} - n_s \langle u_i \frac{\partial W}{\partial c_i} \rangle = \Delta [W],
\]

which is Maxwell’s equation of change.

1.4 Equations of motion (Week 11)

Maxwell’s equation of change can be used to obtain equations of motion at different levels of approximation. As we will see, the level of approximation depends on the closure of the transport equations. In order to retain generality, we consider species \( s \) in a multi-species gas, noting that all of our derivations carry over to this case and interactions between different particles are captured by the collision integral.

1.4.1 Equation of mass continuity

We begin by deriving the equation of mass continuity by using Maxwell’s equation of change with \( W_s = m_s \). This gives

\[
\frac{\partial}{\partial t} (\rho_s) + \frac{\partial}{\partial x_i} (\rho_s u_i) = P_s - L_s
\]

(46)

because \( \langle c_s \rangle = 0 \), the derivatives of \( m_s \) with respect to \( c_s \) are zero, \( P_s \) is the chemical production rate and \( L_s \) is the chemical loss rate. The number density \( n_s \) is a zeroth order moment of the distribution function. In the absence of chemical reactions, the right hand side is zero since kinetic collisions do not alter species mass.
1.4.2 Momentum equation

The momentum equation is extracted from equation (45) by setting \( W_s = m_s c_{sk} \), keeping in mind that \( \langle c_{sk} \rangle = 0 \) and noting that

\[
\frac{\partial c_{sk}}{\partial c_{si}} = \delta_{ki}.
\]

(47)

Thus, it is easy to show that the momentum equation is

\[
\rho_s \left( \frac{\partial u_{si}}{\partial t} + u_{sj} \frac{\partial u_{si}}{\partial x_j} \right) + \frac{\partial P_{sik}}{\partial x_i} - \rho_s \langle a_{si} \rangle = \frac{\delta M_{si}}{\delta t}
\]

(48)

where

\[
P_{sik} = \rho_s \langle c_{si} c_{sk} \rangle
\]

(49)

is the pressure tensor, the acceleration is

\[
\langle a_s \rangle = g + \frac{e_s}{m_s} \left( E + u_s \times B + c_s \times B \right) = g + \frac{e_s}{m_s} \left( E + (u_s + \mathbf{c}_s) \times B \right),
\]

(50)

where \( e_s \) is particle charge, and \( \delta M_s / \delta t \) is the momentum transfer collision integral. Thus, the general momentum equation in inertial space is

\[
\rho_s \left( \frac{\partial u_{si}}{\partial t} + u_{sj} \frac{\partial u_{si}}{\partial x_j} \right) + \frac{\partial P_{sik}}{\partial x_i} - \rho_s g_i - n_s e_s (E_i + \epsilon_{ijl} u_{sj} B_l) = \frac{\partial M_{si}}{\partial t}
\]

(51)

where \( \epsilon_{ijl} \) is the Levi-Civita symbol. The components of the bulk velocity vector constitute three first order moments of the distribution function.

It is useful to recognize that the diagonal elements of the pressure tensor are equivalent to kinetic pressure and the trace of the tensor is \( P_{sii} = 3p_s \). Thus, we can write the pressure tensor as

\[
P_{sik} = p_s \delta_{ik} + \tau_{sik}
\]

(52)

where the trace of the deviatoric stress tensor \( \tau_{sik} \) is zero. Note that the vector component of gravity is positive, the direction to be specified later i.e., for vertical gravity \( g_r = -g \).

1.4.3 Pressure tensor

In order to derive an equation for the pressure tensor, we set \( W_s = m_s c_{sk} c_{sl} \) in equation (45). This yields

\[
\frac{\partial P_{sik}}{\partial t} + P_{sik} \frac{\partial u_{si}}{\partial t} + u_{sj} \frac{\partial P_{sik}}{\partial x_j} + \frac{\partial P_{sik}}{\partial x_i} + P_{sij} \frac{\partial u_{sk}}{\partial t} + P_{skj} \frac{\partial u_{sl}}{\partial t} - \rho_s \langle a_{sk} c_{si} + a_{si} c_{sk} \rangle = \frac{\delta P_{sik}}{\delta t}
\]

(53)
where
\[ Q_{sikl} = \rho_s \langle c_{si} c_{sk} c_{sl} \rangle \] (54)
is the heat flow tensor, \( \delta P_{skl}/\delta t \) is the pressure tensor collision integral and we used
\[ \langle \frac{\partial (c_{sk} c_{sl})}{\partial c_{si}} \rangle = \langle \delta_k c_{si} + \delta_l c_{sk} \rangle = 0 \] (55)
\[ \rho_s \langle c_s j \frac{\partial (c_{sk} c_{sl})}{\partial c_{si}} \rangle \frac{\partial u_{si}}{\partial x_j} = \rho_s \langle \delta_k c_{sk} c_{sj} + \delta_l c_{sk} c_{sj} \rangle \frac{\partial u_{si}}{\partial x_j} = P_{slj} \frac{\partial u_{sk}}{\partial x_j} + P_{skj} \frac{\partial u_{sl}}{\partial x_j} \] (56)

Let us now evaluate the acceleration terms. We have
\[ \langle a_{sk} c_{sl} \rangle = \langle g_k c_{sl} + \epsilon_s m_s \epsilon_{kab} c_{sa} B_b + \epsilon_s m_s (\epsilon_{kab} c_{sb} B_b + \epsilon_{kab} u_{sb} B_b) c_{sl} \rangle \]
\[ = \langle \epsilon_s m_s \epsilon_{kab} c_{sa} B_b \rangle = \epsilon_s \frac{m_s}{m_s} \epsilon_{kab} P_{sla} B_b = \epsilon_s \frac{m_s}{m_s} P_s \times B \] (57)
\[ \langle a_{sl} c_{sk} \rangle = -\epsilon_s \frac{m_s}{m_s} \epsilon_{lab} B_a P_{sbk} = -\epsilon_s \frac{m_s}{m_s} B \times P_s. \] (58)
because \( \langle c_{sl} \rangle = 0 \). Thus, the pressure tensor equation is
\[ \frac{\partial P_{skl}}{\partial t} + P_{skl} \frac{\partial u_{si}}{\partial x_j} + u_{si} \frac{\partial P_{skl}}{\partial x_j} + \frac{\partial Q_{sikl}}{\partial x_j} + P_{slj} \frac{\partial u_{sk}}{\partial x_j} + P_{skj} \frac{\partial u_{sl}}{\partial x_j} - \epsilon_s \frac{m_s}{m_s} (\epsilon_{kab} P_{sla} B_b - \epsilon_{kab} B_a P_{sbk}) = \frac{\delta P_{skl}}{\delta t}. \] (59)
The pressure tensor contains 9 elements but only 6 are independent because the devia-
toric stress tensor is symmetric. The independent elements constitute six second order
moments of the distribution function.

1.4.4 Energy equation

We may now note that
\[ P_{iii} = \rho_s \langle \epsilon_s^2 \rangle = 3 p_s = 3 n_s k T_s, \]
which means that temperature can be obtained from
\[ \frac{3}{2} k T_s = \frac{1}{2} m_s \langle \epsilon_s^2 \rangle. \] (61)
We now recognize that the energy equation can simply be extracted as the trace of the
pressure tensor equation i.e., setting \( k = l \):
\[ 3 \frac{\partial p_s}{\partial t} + 3 p_s \frac{\partial u_{si}}{\partial x_i} + 3 u_{si} \frac{\partial p_s}{\partial x_i} + 2 \frac{\partial q_{sij}}{\partial x_i} + 2 P_{sij} \frac{\partial u_{si}}{\partial x_j} = 3 \frac{\delta p_s}{\delta t}. \] (62)

9
where the heat flow vector $q_{si}$ is defined as

$$q_{si} = \frac{1}{2} \rho_s (c_i c_s^2) = \frac{1}{2} Q_{sij}.$$  

(63)

Thus, we obtain the energy equation

$$\frac{\partial}{\partial t} \left( \frac{3}{2} p_s \right) + u_{si} \frac{\partial}{\partial x_i} \left( \frac{3}{2} p_s \right) + \frac{5}{2} p_s \frac{\partial u_{si}}{\partial x_i} + \frac{\partial q_{si}}{\partial x_j} + \tau_{sij} \frac{\partial u_{sj}}{\partial x_j} = \frac{3}{2} \frac{\delta p_s}{\delta t}.$$  

(64)

where $T_s$ represents a second order moment of the distribution function. Here it is useful to recognize that for a monatomic or ideal gas

$$\frac{3}{2} p_s = \frac{3}{2} k m_s \rho_s T_s = c_v \rho_s T_s.$$  

(65)

where $c_v$ is the specific heat capacity at constant volume.

### 1.5 13-moment equations (Week 11)

In deriving the equations of motion above, the reader will have noticed that one can continue building higher order moments indefinitely. We could obtain the heat flow tensor equation from Maxwell’s equation of change but the equation depends on higher order moments and so on. Different levels of closure are discussed in the literature, ranging from 5 to 20 moments. We truncate the system at 13-moment level.

#### 1.5.1 The 13-moment distribution function

The 13-moment distribution function is derived by using the Chapman-Enskog method. In reasonable dense gases, deviations from thermal equilibrium can be treated as perturbations to the M-B distribution function:

$$F(t, r, c) = F_0(t, r, c) \left[ 1 + A_i(t, r)c_i + B_{ij}(t, r)c_ic_j + D_{ijkl}(t, r)c_ic_jc_k \right]$$  

(66)

where $F_0$ is the M-B distribution function and $A, B, D$ are coefficient matrices. Note that the 13-moment version of this expansion terminates at third order. Symmetry arguments and normalization can be used to show that (Gombosi, 1994):

$$B_{ii} = 0$$  

(67)

$$A_i + \left( \frac{3kT}{m} \right) D_{ijj} = 0.$$  

(68)

Further developments along similar lines (e.g., Chapter 6 in Gombosi, 1994) yield

$$F_s = F_{s0} \left[ 1 + \frac{\rho_s}{2p_s^2} \tau_{sij} c_{si} c_{sj} + \frac{\rho_s^2}{p_s^3} \left( \frac{c_s^2}{5} - \frac{p_s}{\rho_s} \right) q_{si} c_{si} \right],$$  

(69)
which is the 13-moment phase space distribution function.

The heat flow tensor is extracted from this distribution function by taking the moment

\[ Q_{stij} = \rho_s \langle c_{st} c_{sk} c_{sl} \rangle, \]

which is

\[ Q_{sikl} = \frac{2}{5} \left( \delta_{il} q_{sl} + \delta_{il} q_{sk} + \delta_{ik} q_{sl} \right), \]  

meaning that the heat flow tensor is now fully defined by the heat flow vector. Another important moment that we will make use of later is the higher order stress tensor

\[ \mu_{stik} = \frac{1}{2} \rho_s \langle c_s^2 c_{st} c_{sk} \rangle = \frac{5}{2} k T_s \frac{m_s}{m_s} \left( p_s \delta_{ik} + \frac{7}{5} \tau_{sik} \right). \]  

1.5.2 Equation of mass continuity

The general equation of mass continuity (46) holds without additional developments:

\[ \frac{\partial}{\partial t} \rho_s + \frac{\partial}{\partial x_i} (\rho_s u_{si}) = P_s - L_s, \]

where \( P_s \) and \( L_s \) are chemical production and loss rates, respectively.

1.5.3 Momentum equation

The momentum equation is

\[ \rho_s \left( \frac{\partial u_{si}}{\partial t} + u_{sj} \frac{\partial u_{si}}{\partial x_j} \right) + \frac{\partial p_s}{\partial x_i} + \frac{\partial \tau_{sji}}{\partial x_j} - \rho_s g_i - n_s e_s (E_i + \epsilon_{ijl} u_{sj} B_l) = \frac{\partial M_{si}}{\partial t}, \]  

where the 13-moment collision integral is (Schunk and Nagy, 2000)

\[ \frac{\delta M_{si}}{\delta t} = \sum_i \rho_s v_{si} (u_{ti} - u_{si}) - \sum_i u_{si} v_{si} m_{st} \left( \frac{\rho_t}{\rho_i} q_{ti} - q_{si} \right). \]  

Here \( m_{st} \) is the reduced mass,

\[ T_{st} = \frac{1}{2} (T_s + T_t) \]

is the average temperature of species \( s \) and \( t \), and \( z_{st} \) is a species-specific pure number (see Chapter 4 in Schunk and Nagy, 2000, and other tabulations).
1.5.4 Energy equation

The energy equation is given by:

\[
\frac{\partial}{\partial t} \left( \frac{3}{2} p_s \right) + u_{si} \frac{\partial}{\partial x_i} \left( \frac{3}{2} p_s \right) + \frac{5}{2} p_s \frac{\partial u_{si}}{\partial x_i} + \frac{\partial q_{si}}{\partial x_i} + \tau_{ijkl} \frac{\partial u_{si}}{\partial x_j} = \frac{3}{2} \frac{\delta p_s}{\delta t}
\]

where the 13-moment collision integral is (Schunk and Nagy, 2000)

\[
\frac{3}{2} \frac{\delta p_s}{\delta t} = \sum_t \rho_s \nu_{st} \left[ 3k(T_s - T) + m_s (u_s - u_t)^2 \right].
\]

(74)

1.5.5 Stress tensor equation

We start with the 13-moment pressure tensor equation

\[
\frac{\partial p_s}{\partial t} \delta_{kl} + \frac{\partial \tau_{skl}}{\partial t} + (p_s \delta_{kl} + \tau_{skl}) \frac{\partial u_{si}}{\partial x_i} + u_{si} \frac{\partial \tau_{skl}}{\partial x_i} + \frac{2}{5} \left( \frac{\partial q_{sk}}{\partial x_l} \delta_{kl} + \frac{\partial q_{sl}}{\partial x_k} + \frac{\partial q_{kl}}{\partial x_s} \right) + \frac{2}{3} (p_s \delta_{kl} + \tau_{skl})
\]

where we used the fact that

\[
\frac{\partial Q_{skl}}{\partial x_i} = \frac{2}{5} \left( \frac{\partial q_{sk}}{\partial x_l} + \frac{\partial q_{sl}}{\partial x_k} + \frac{\partial q_{kl}}{\partial x_s} \right).
\]

(75)

We multiply the energy equation by \((2\delta_{kl}/3)\) and subtract it from the above equation:

\[
\frac{\partial \tau_{skl}}{\partial t} + (p_s \delta_{kl} + \tau_{skl}) \frac{\partial u_{si}}{\partial x_i} + u_{si} \frac{\partial \tau_{skl}}{\partial x_i} - \frac{10}{6} p_s \delta_{kl} \frac{\partial u_{si}}{\partial x_i} + \frac{2}{5} \left( \frac{\partial q_{sk}}{\partial x_l} + \frac{\partial q_{sl}}{\partial x_k} + \frac{\partial q_{kl}}{\partial x_s} \right) + \frac{2}{3} (p_s \delta_{kl} + \tau_{skl})
\]

which gives the result:

\[
\frac{\partial \tau_{skl}}{\partial t} + u_{si} \frac{\partial \tau_{skl}}{\partial x_i} + \tau_{skl} \frac{\partial u_{si}}{\partial x_i} - \frac{e_s}{m_s} (\epsilon_{skl} \tau_{skl} B_{b} - \epsilon_{b} B_{a} \tau_{skl}) + \frac{2}{5} \left( \frac{\partial q_{sk}}{\partial x_l} + \frac{\partial q_{sl}}{\partial x_k} + \frac{2}{3} \frac{\partial q_{kl}}{\partial x_s} \right) + p_s \left( \frac{\partial u_{sk}}{\partial x_l} + \frac{\partial u_{sl}}{\partial x_k} - \frac{2}{3} \frac{\partial u_{kl}}{\partial x_s} \right)
\]

\[
+ \tau_{skl} \frac{\partial u_{si}}{\partial x_i} + \tau_{skl} \frac{\partial u_{si}}{\partial x_i} + \frac{2}{3} \tau_{skl} \frac{\partial u_{si}}{\partial x_j} \delta_{kl} = \frac{\delta \tau_{skl}}{\delta t}.
\]

(76)
1.5.6 Heat flow equation

In order to close the system of equations, we need an equation that describes the evolution of the heat flow vector, which is obtained by setting $W = (1/2) m_s c_s^2 c_{sk}$ in equation (45). It is straightforward but tedious to show that

$$
\frac{\partial q_{sk}}{\partial t} + u_{sl} \frac{\partial q_{sk}}{\partial x_i} + q_{si} \frac{\partial q_{sk}}{\partial x_i} + q_{sl} \frac{\partial u_{sk}}{\partial x_i} + q_{sk} \frac{\partial u_{sl}}{\partial x_i} + Q_{skij} \frac{\partial u_{sj}}{\partial x_i} + \frac{\partial \mu_{sk}}{\partial x_i}
\left[ \frac{\partial u_{sl}}{\partial t} + u_{sl} \frac{\partial u_{sl}}{\partial x_i} - g_{il} - \frac{e_s}{m_s} (E_l + \epsilon_{lij} u_{si} B_j) \right]
\left( \tau_{sk} + \frac{5}{2} P_s \delta_{lk} \right)
- \frac{e_s}{m_s} \epsilon_{kij} q_{si} B_j = \frac{\delta q_{sk}}{\delta t}
$$

where $\mu_{sk}$ is the higher order stress tensor given by equation (71). Noting that

$$
\frac{\partial \mu_{sk}}{\partial x_i} = \frac{5}{2} \frac{k}{m_s} \left[ \frac{\partial (T_s p_s)}{\partial x_k} + \frac{7}{5} \frac{\partial (T_s \tau_{sk})}{\partial x_i} \right],
$$

we obtain

$$
\frac{\partial q_{sk}}{\partial t} + u_{sl} \frac{\partial q_{sk}}{\partial x_i} + q_{si} \frac{\partial q_{sk}}{\partial x_i} + q_{sl} \frac{\partial u_{sk}}{\partial x_i} + q_{sk} \frac{\partial u_{sl}}{\partial x_i} + Q_{skij} \frac{\partial u_{sj}}{\partial x_i} + \frac{5}{2} \frac{k}{m_s} \left[ \frac{\partial (T_s p_s)}{\partial x_k} + \frac{7}{5} \frac{\partial (T_s \tau_{sk})}{\partial x_i} \right]
\left[ \frac{\partial u_{sl}}{\partial t} + u_{sl} \frac{\partial u_{sl}}{\partial x_i} - g_{il} - \frac{e_s}{m_s} (E_l + \epsilon_{lij} u_{si} B_j) \right]
\left( \tau_{sk} + \frac{5}{2} P_s \delta_{lk} \right)
- \frac{e_s}{m_s} \epsilon_{kij} q_{si} B_j = \frac{\delta q_{sk}}{\delta t},
$$

Next, we write

$$
Q_{skij} \frac{\partial u_{sj}}{\partial x_i} = \frac{2}{5} \left( \delta_{kq} q_{sj} + \delta_{kj} q_{si} + \delta_{ij} q_{sk} \right) \frac{\partial u_{sj}}{\partial x_i} = \frac{2}{5} \left( \frac{\partial u_{sj}}{\partial x_k} q_{sj} + \frac{\partial u_{sk}}{\partial x_i} q_{si} + \frac{\partial u_{sl}}{\partial x_i} q_{sk} \right),
$$

and note that the momentum equation gives us

$$
\frac{\partial u_{sl}}{\partial t} + u_{sl} \frac{\partial u_{sl}}{\partial x_j} - g_{sl} - \frac{e_s}{m_s} (E_l + \epsilon_{lij} u_{si} B_j) = \frac{1}{\rho_s} \left( \frac{\partial M_{sl}}{\partial t} - \frac{\partial p_s}{\partial x_l} - \frac{\partial \tau_{sil}}{\partial x_i} \right).
$$

Based on these, the heat flow equation is

$$
\frac{\partial q_{sk}}{\partial t} + u_{sl} \frac{\partial q_{sk}}{\partial x_i} + q_{si} \frac{\partial q_{sk}}{\partial x_i} + q_{sl} \frac{\partial u_{sk}}{\partial x_i} + q_{sk} \frac{\partial u_{sl}}{\partial x_i} + Q_{skij} \frac{\partial u_{sj}}{\partial x_i} + \frac{5}{2} \frac{k p_s}{m_s} \frac{\partial T_s}{\partial x_k} + \frac{5}{2} \frac{k p_s}{m_s} \frac{\partial T_s}{\partial x_i}
\left[ \frac{\partial u_{sl}}{\partial t} + u_{sl} \frac{\partial u_{sl}}{\partial x_i} - g_{il} - \frac{e_s}{m_s} (E_l + \epsilon_{lij} u_{si} B_j) \right]
\left( \tau_{sk} + \frac{5}{2} P_s \delta_{lk} \right)
- \frac{e_s}{m_s} \epsilon_{kij} q_{si} B_j = \frac{\delta q_{sk}}{\delta t} \frac{\partial M_{sl}}{\partial t} - \frac{\partial p_s}{\partial x_l} - \frac{\partial \tau_{sil}}{\partial x_i},
$$

13
which, after some manipulation, gives us the result

\[
\frac{\partial q_{sk}}{\partial t} + u_{sl} \frac{\partial q_{sk}}{\partial x_i} + 7 \frac{7}{5} q_{sl} \frac{\partial u_{si}}{\partial x_i} + \frac{7}{5} q_{sk} \frac{\partial u_{sj}}{\partial x_j} + \frac{2}{5} \frac{\partial u_{sj}}{\partial x_j} q_{sj} + \frac{5}{2} p_{is} \frac{\partial T_i}{\partial x_k} + \frac{1}{\rho_s} \frac{\partial \tau_{sil}}{\partial x_i} (p_s \delta_{kl} - \tau_{slk}) + \left( \frac{7}{2} m_s \frac{\partial T_i}{\partial x_j} - \frac{1}{\rho_s} \frac{\partial p_s}{\partial x_l} \right) \tau_{slk} \\
- \frac{e_i}{m_s} \epsilon_{kl} q_{si} B_j = \frac{\delta q_{sk}}{\delta t} - \frac{1}{\rho_s} \frac{\partial M_{sl}}{\partial t} \left( \tau_{lk} + \frac{5}{2} p_{is} \delta_{lk} \right). \tag{82}
\]

This completes the development of the 13-moment equations.

### 1.6 Navier-Stokes equations (Week 12)

The 13-moment formulation can be simplified further to obtain the Navier-Stokes (N-S) equations. The N-S equations rely on simplified versions of the 13-moment stress tensor and heat flow equations. For convenience, we assume a single neutral species and ignore external forces. The general equation of mass continuity remains as it is. The momentum transfer and energy collision integrals vanish for a single species and thus the momentum and energy equations are:

\[
\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) + \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ji}}{\partial x_j} = 0 \tag{83}
\]

\[
\frac{\partial}{\partial t} \left( \frac{3}{2} p \right) + u_i \frac{\partial}{\partial x_i} \left( \frac{3}{2} \frac{\partial p}{\partial x_i} \right) + \frac{5}{2} p \frac{\partial u_i}{\partial x_i} + \frac{\partial q_i}{\partial x_i} + \frac{\tau_{ij}}{\partial x_j} = 0. \tag{84}
\]

The stress and heat flow collision integrals can be estimated by replacing the collision integral for the distribution function in Maxwell’s equation of change with

\[
\frac{\delta F}{\delta t} = -\frac{F - F_0}{\tau_0} = \frac{F_0}{\tau_0} \left[ \rho \tau_{ij} c_i c_j + \rho \frac{p^2}{2} \left( \frac{c^2}{5} - \frac{p}{\rho} \right) q_i c_i \right], \tag{85}
\]

which allows for the integration of the collision moments. The results are

\[
\frac{\delta \tau_{ij}}{\delta t} \approx -\frac{\tau_{ij}}{\tau_0} \tag{86}
\]

\[
\frac{\delta q_i}{\delta t} \approx -\frac{q_i}{\tau_0} \tag{87}
\]

where \( \tau_0 \) is the collisional relaxation time i.e., the time it takes for the system to relax to the M-B distribution and LTE.

The additional approximation necessary to reach the N-S equations is to assume that all terms in the stress tensor and heat flow equations that include the stress tensor and
heat flow vector vanish, with the exception of the collision terms that are divided by a presumed small number $\tau_0$. Inspecting equations (76) and (82) then yields:

$$\tau_{ij} = -\tau_0 p \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right)$$ (88)

$$q_i = -\frac{5}{2} k \frac{m}{\tau_0} \frac{\partial T}{\partial x_i},$$ (89)

The reader should note that the pressure tensor for the Newtonian fluid is written as

$$P_{ij} = p \delta_{ij} - \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right)$$ (90)

where the coefficient of dynamic viscosity (kg m$^{-1}$ s$^{-1}$) is

$$\mu = \alpha T^\beta.$$ (91)

We have shown that the dynamic viscosity is $\mu \approx p \tau_0$ i.e., proportional to the collisional relaxation time and pressure. We expect the effect of viscosity to become more significant as the collision time increases. Also, we have found that the stress tensor vanishes under equilibrium conditions where the M-B distribution holds.

We recognize the heat flux vector as conductive flux and note that the coefficient of heat conduction is

$$\kappa \approx \frac{5}{2} k \frac{m}{\tau_0} p$$ (92)

i.e., the coefficient is also proportional to $p \tau_0$. We are now ready to rewrite the N-S momentum and energy equations as

$$\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) + \frac{\partial p}{\partial x_i} = \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \right]$$ (93)

$$\frac{\partial}{\partial t} \left( \frac{3}{2} p \right) + u_i \frac{\partial}{\partial x_i} \left( \frac{3}{2} p \right) + 5 \frac{\partial u_i}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \kappa \frac{\partial T}{\partial x_i} \right)$$

$$+ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \frac{\partial u_i}{\partial x_j}.$$ (94)

These equations agree with the classical equations of motion for a Newtonian fluid. It should be noted that the equations are only valid when $\tau_0$ is a small number i.e., small deviations from the M-B distribution.

In terms of global-scale simulations, we can evaluate the importance of the viscosity and heat conduction by using the Reynolds and Péclet numbers. The Reynolds number is given by

$$Re = \frac{LU}{\nu}.$$ (95)
where $L$ is the length scale of interest, $U$ is the typical flow speed and

$$\nu = \frac{\mu}{\rho}$$  \hspace{1cm} (96)

is the coefficient of kinematic viscosity, which has the same unit as the coefficient of diffusion ($\text{m}^2 \text{s}^{-1}$). The Péclet number is

$$Pe = \frac{LU}{\alpha}$$  \hspace{1cm} (97)

where the thermal diffusivity is

$$\alpha = \frac{\kappa}{\rho c_p}$$  \hspace{1cm} (98)

and $c_p$ is the specific heat capacity at constant pressure.

### 1.7 Neutral momentum equation (Week 12)

As an application of the momentum equation, we consider the neutral bulk flow equation. This is obtained by summing the individual momentum equations

$$\sum_n \frac{D_n \mathbf{u}_n}{Dt} + \sum_n \nabla \cdot P_n \mathbf{u}_n - \rho \mathbf{g} = \sum_n \sum_t \rho_n \nu_{nt} (\mathbf{u}_t - \mathbf{u}_n)$$  \hspace{1cm} (99)

where $t = i, e$ refer to ions and electrons while collisions with other neutrals cancel out and $\rho = \sum_n \rho_n$. Here

$$\sum_n \frac{D_n \mathbf{u}_n}{Dt} = \sum_n \rho_n \frac{\partial \mathbf{u}_n}{\partial t} + \sum_n \rho_n (\mathbf{u}_n \cdot \nabla) \mathbf{u}_n$$

$$= \sum_n \left[ \frac{\partial}{\partial t} (\rho_n \mathbf{u}_n) - \mathbf{u}_n \frac{\partial \rho_n}{\partial t} \right] + \sum_n \rho_n (\mathbf{u}_n \cdot \nabla) \mathbf{u}_n$$

$$= \frac{\partial}{\partial t} (\rho \mathbf{u}) + \sum_n \mathbf{u}_n \nabla \cdot (\rho_n \mathbf{u}_n) + \sum_n \rho_n (\mathbf{u}_n \cdot \nabla) \mathbf{u}_n$$

$$= \frac{\partial}{\partial t} (\rho \mathbf{u}) + \sum_n \nabla \cdot (\rho_n \mathbf{u}_n \mathbf{u}_n)$$  \hspace{1cm} (100)

where we used the center of mass velocity

$$\mathbf{u} = \frac{1}{\rho} \sum_n \rho_n \mathbf{u}_n$$  \hspace{1cm} (101)

and the continuity equation

$$\frac{\partial \rho_n}{\partial t} + \nabla \cdot (\rho_n \mathbf{u}_n) = 0.$$  \hspace{1cm} (102)
In order to write the sum over the pressure tensor term, we write the pressure tensor as

$$P_s = P_s^* - \rho_s w_s w_s$$  \hspace{1cm} (103)$$

where we used subscript $s$ instead of $n$ to retain generality at this point. Here $w_s = u_s - u$ is the diffusion velocity of species $s$ and the thermal velocity with respect to center of mass flow is $c_s^* = v_s - u_s$ so that $c_s = v_s - u_s = c_s^* - w_s$. Therefore,

$$\sum_n \nabla \cdot P_n = \nabla \cdot \left[ \sum_n P_n^* - \sum_n \rho_n (u_n - u) (u_n - u) \right]$$

$$= \nabla \cdot P - \sum_n \nabla \cdot (\rho_n u_n u_n) + \nabla \cdot (\rho u u).$$  \hspace{1cm} (104)$$

With these expressions, the neutral momentum equation is

$$\frac{\partial}{\partial t} (\rho u) + \nabla \cdot P - \rho g = \sum_t \sum_n \rho_t \nu_t (u_n - u_t)$$  \hspace{1cm} (105)$$

Using the equation of mass continuity yields

$$\frac{\rho D u}{D t} + \nabla \cdot P - \rho g = \sum_t \sum_n \rho_t \nu_t (u_n - u_t) = - \sum_t \sum_n \rho_t \nu_t (u_n - u_t)$$  \hspace{1cm} (106)$$

where $P = \sum_n P_n^*$ and $\rho_t \nu_t = \rho_t \nu_t$. We approximate the collision term by assuming that the charged particle momentum equation is given by

$$-\frac{e_t}{m_t} (E + u_t \times B) = \sum_n \rho_t \nu_t (u_n - u_t)$$  \hspace{1cm} (107)$$

where $e_t$ is particle charge. This means that charged particle motion is controlled by the Lorentz force only and only collisions with neutrals are taken into account. In other words, charged particle motion consists of the electric drift

$$u_E = \frac{E \times B}{B^2}$$  \hspace{1cm} (108)$$

disturbed by collisions with the neutral atmosphere. We sum the charged particle momentum equations (107) over $t$ and replace the collision term in equation (106):

$$\frac{\rho D u}{D t} + \nabla \cdot P - \rho g = \sum_t n_t e_t (E + u_t \times B) = \left( \sum_t n_t e_t u_t - \sum_i e_i u_i \right) \times B.$$

(109)$$

Thus, the neutral bulk flow momentum equation is

$$\frac{\rho D u}{D t} + \nabla \cdot P - \rho g - j \times B = 0$$  \hspace{1cm} (110)$$
where the current density is
\[ j = \sum_i n_i e_i u_i - n_e e u_e \]  
(111)
and \( j \times B \) is the ion drag term. It is interesting that this equation is identical in form to the momentum equation for fully ionized MHD, despite the fact that the neutral atmosphere does not react to the Lorentz force directly. The influence of the Lorentz force is nevertheless felt through momentum transfer collisions.

2 Ionospheres

2.1 Chapman layer (Week 3)

Consider the continuity equation for a single ion \( i \), given by
\[ \frac{dn_i}{dt} = q_i - \alpha n_i n_e \]  
(112)
where \( n_i \) is the number density of ion \( i \), \( q_i \) is the production rate, \( \alpha \) is the recombination rate coefficient and \( n_e \) is the electron density. In photochemical equilibrium for a major ion \( (n_i = n_e) \), this gives
\[ n_e = \sqrt{\frac{q_i}{\alpha}}. \]  
(113)
For example, on Venus \( q_i \) is the photoionization rate of \( \text{CO}_2 \) and \( \alpha \) is the rate coefficient for dissociative recombination of \( \text{O}^+ \).

We shall assume plane parallel geometry and obtain the production rate \( q_{\nu} \) at altitude \( z \) and cosine of the solar zenith angle \( \mu = \cos \chi \) as
\[ q_{\nu}(z, \mu) dz = \mu \frac{dI_{\nu}}{h_{\nu}} = \sum_s \sigma_{\nu s} n_s(z) \frac{I_{\nu}}{h_{\nu}} dz \]  
(114)
where \( h_{\nu} \) is the photon energy, higher than the ionization potential of the parent species \( s \), \( n_s \) is the number density of the parent species and \( I_{\nu} \) is the intensity of radiation at \((z, \mu)\). For a single parent species, the production rate is
\[ q_{\nu}(z, \mu) = \sigma_{\nu s} n(z) F_{\infty,\nu} \exp \left[ - \int_z^{\infty} \frac{n(z') \sigma_{\nu s} dz'}{\mu'} \right] \]  
(115)
where \( F_{\infty,\nu} \) is the solar photon flux \((m^{-2} s^{-1}) \) above the atmosphere. Note that \( \mu \) depends on \( z \) along the line of sight according to (e.g., Rees, 1989):
\[ \mu' = \sqrt{1 - \left( \frac{R+z'}{R+2z'} \right)^2 \sin^2 \chi} \]  
(116)
where $\mu$ applies at $z$. This means that $\mu' \approx \mu$ when $\chi \lesssim 75^\circ$, which we shall assume hereafter.

We assume an isothermal atmosphere:

$$n(z) = n(z_0) \exp \left( -\frac{z-z_0}{H} \right)$$  \hspace{1cm} (117)

and write

$$q_\nu(z, \mu) = \sigma_\nu n(z) F_{\infty \nu} \exp \left[ -\int_z^\infty \frac{\sigma_\nu' dz'}{\mu} n(z_0) \exp \left( -\frac{z'-z_0}{H} \right) \right]$$  \hspace{1cm} (118)

or

$$q_\nu(z, \mu) = \sigma_\nu n(z_0) F_{\infty \nu} \exp \left[ -\frac{z-z_0}{H} - \frac{\sigma_\nu n(z_0)H}{\mu} \exp \left( -\frac{z-z_0}{H} \right) \right].$$  \hspace{1cm} (119)

If we write

$$A(z) = \exp \left( -\frac{z-z_0}{H} \right),$$  \hspace{1cm} (120)

the derivative of the production rate is

$$\frac{\partial q_\nu}{\partial z} = \sigma_\nu n(z_0) F_{\infty \nu} \frac{\partial A}{\partial z} \left\{ \exp \left[ -\frac{\sigma_\nu n(z_0)H}{\mu} A(z) \right] \right.$$

$$- A(z) \frac{\sigma_\nu n(z_0)H}{\mu} \exp \left[ -\frac{\sigma_\nu n(z_0)H}{\mu} A(z) \right] \right\}. $$  \hspace{1cm} (121)

Setting this to zero gives us an expression for the altitude of maximum production:

$$\exp \left( \frac{z_{max} - z_0}{H} \right) = \frac{\sigma_\nu n(z_0)H}{\mu}. $$  \hspace{1cm} (123)

Given that the vertical optical depth is

$$\tau_\nu(z) = \sigma_\nu n(z_0)H \exp \left( -\frac{z-z_0}{H} \right),$$  \hspace{1cm} (124)

we find that maximum production occurs at the altitude where $\tau_\nu/\mu = 1$.

Substituting equation (123) into equation (119) gives the maximum production rate as

$$q_\nu(z_{\max}, \mu) = \frac{F_{\infty \nu} \mu}{eH}$$  \hspace{1cm} (125)

where $e$ is Euler’s number. Based on this, equation (113) for a single-valued frequency gives

$$n_{e}^{max} = \left( \frac{F_{\infty \nu}}{\alpha eH} \right)^{1/2} \mu^{1/2},$$  \hspace{1cm} (126)
which shows the dependency of the peak electron density with solar zenith angle in the Chapman theory. Furthermore, our final expression for the Chapman production function can be written as

\[
q_\nu(z, \mu) = q_{\nu M} \exp \left[ 1 - \frac{z - z_M}{H} - \frac{1}{\mu} \exp \left( - \frac{z - z_M}{H} \right) \right]
\] (127)

where

\[
q_{\nu M} = \frac{F_{\infty \nu}}{eH}
\] (128)

is the peak production rate for the overhead sun (\(\mu = 1\)) and

\[
\exp \left( \frac{z_M - z_0}{H} \right) = \sigma_{\nu n(z_0)} H
\] (129)

where it must be noted that \(z_M\) generally depends on frequency.

### 2.2 Simplified Ohm’s law and the conductivity tensor (Week 13)

The Ohm’s law in atmospheric theory is based on the momentum equations for ions, electrons and neutrals. A comprehensive derivation with minimum loss of generality is outlined by Leake et al. (2014). Such a derivation, however, does not easily provide physical insight to the basic ideas underlying the conductivity tensor. Instead, we summarize the derivation of the simplified Ohm’s law given by Schunk and Nagy (2000) here and highlight the assumptions involved. We note that this form of the Ohm’s law is commonly used in almost all solar system planetary ionosphere models.

The vector form of the 13-moment momentum equation (72) for species \(s\) in a rotating frame of a planet is

\[
\rho_s \frac{D\mathbf{u}_s}{Dt} + \nabla P_s - n_s \mathbf{e}_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) - \rho_s (g - 2\Omega \times \mathbf{u}_s - \Omega \times \Omega \times \mathbf{r}) = \sum_t \nu_{st} (\mathbf{u}_s - \mathbf{u}_t) + \frac{\nu_{st}}{kT_{st}} \left( \mathbf{q}_s - \frac{\rho_s}{\rho_t} \mathbf{q}_t \right)
\] (130)

where \(\Omega\) is the angular rotation vector of the planet the meaning of the rest of the terms is explained in Section 1.5.3. In order to derive the simplified Ohm’s law, we assume that the charged particle momentum equations in the direction perpendicular to the local magnetic field reduce to

\[
\frac{e_s}{m_s} (\mathbf{E}_\perp + \mathbf{u}_s \times \mathbf{B}) = \sum_t \nu_{st} (\mathbf{u}_s - \mathbf{u}_t).
\] (131)

One can recognize this as a rather severe assumption, which ignores advection, pressure gradients, stress, gravity and Coriolis forces. It is also useful to recognize that at the
limit of no collisions, the charged particle motion here reduces to

\[ u_{\perp,s} = \frac{E \times B}{B^2} , \]  

which is the electric drift, identical for both electrons and ions.

Equation (131) is further simplified by assuming that the neutral density is much higher than the plasma density and only including ion-neutral collisions:

\[ \frac{e_i}{m_i} (E_{\perp} + u_i \times B) = \sum_i \nu_{in} (u_i - u_n) = \nu_i (u_i - u_n) \]  

(133)

where we use subscript \( i \) to denote an ion and assume that the neutrals have equal velocities. We transform this equation to a frame moving with the neutral atmosphere by writing \( u_i = u'_i + u_n \), which leads to

\[ \frac{e_i}{m_i} E'_{\perp} + \frac{\omega_i}{\nu_i} u'_i \times b = u'_i \]  

(134)

where \( E'_\perp = E_{\perp} + u_n \times B \) is the electric field in the frame moving with the neutrals, \( \omega_i \) is the ion gyrofrequency and \( b \) is the magnetic field unit vector. Taking the cross product with \( b \) on the left side and re-organizing gives

\[ u'_i \times b = -\frac{e_i}{m_i \nu_i} b \times E'_{\perp} - \frac{\omega_i}{\nu_i} u'_{i\perp} , \]  

(135)

which can be substituted back to equation (134) to obtain

\[ u'_i \left( 1 + \frac{\omega_i^2}{\nu_i^2} \right) = \frac{e_i}{m_i} \left( \frac{E'_{\perp}}{\nu_i} - \frac{\omega_i}{\nu_i} b \times E'_{\perp} \right) \]

\[ \rightarrow u'_{i\perp} = \frac{e_i}{m_i \nu_i} \left( \frac{\nu_i^2}{\nu_i^2 + \omega_i^2} E'_{\perp} + \frac{\nu_i \omega_i}{\nu_i^2 + \omega_i^2} E'_{\perp} \times b \right) . \]  

(136)

Similar developments yield the perpendicular electron velocity

\[ u'_{e\perp} = -\frac{e_e}{m_e \nu_e} \left( \frac{\nu_e^2}{\nu_e^2 + \omega_e^2} E'_{\perp} - \frac{\nu_e \omega_e}{\nu_e^2 + \omega_e^2} E'_{\perp} \times b \right) \]  

(137)

where \( \nu_e = \sum_n \nu_{en} \) where only electron-neutral collisions are included for.

The perpendicular current density is defined as

\[ j_{\perp} = j_{e\perp} + \sum_i j_{i\perp} = \sum_i n_i e_i u'_i - n_e e u'_{e\perp} + \left( \sum_i n_i e_i - n_e e \right) u_{n\perp} \]  

(138)

where the last term cancels under charge neutrality. Thus, we have

\[ j_{\perp} = \sigma_p E'_{\perp} - \sigma_H E'_{\perp} \times b \]  

(139)

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where the Pedersen and Hall conductivities are

\[
\sigma_P = \sum_i \sigma_i \frac{\nu_i^2}{\nu_i^2 + \omega_i^2} + \sigma_e \frac{\nu_e^2}{\nu_e^2 + \omega_e^2}
\]  
(140)

\[
\sigma_H = -\sum_i \sigma_i \frac{\nu_i \omega_i}{\nu_i^2 + \omega_i^2} + \sigma_e \frac{\nu_e \omega_e}{\nu_e^2 + \omega_e^2}
\]  
(141)

where

\[
\sigma_s = \frac{n_s e_s^2}{m_s \nu_s}
\]  
(142)

We can also write the conductivities as

\[
\sigma_P = \sum_i \sigma_i \frac{1}{1+k_i^2} + \sigma_e \frac{1}{1+k_e^2}
\]  
(143)

\[
\sigma_H = -\sum_i \sigma_i \frac{k_i}{1+k_i^2} + \sigma_e \frac{k_e}{1+k_e^2}
\]  
(144)

where \(k_s = \omega_s / \nu_s\) is the magnetization parameter.

The electron momentum equation in the direction parallel to the magnetic field, consistent with the assumptions above, is

\[
en_e E_\parallel = \sum_t \rho_t \nu_{et} (u_t - u_e)_\parallel.
\]  
(145)

The electron velocity along the magnetic field is typically much faster than ion or neutral velocities and we can estimate

\[
u_e' = \sum_i \nu_{ei} + \sum_n \nu_{en}
\]  
(147)

The current density is

\[
j_\parallel \approx -en_e u_e_\parallel = \sigma_\parallel E_\parallel
\]  
(148)

where

\[
\sigma_\parallel = \frac{n_e e^2}{m_e \nu_e'}
\]  
(149)

Collecting all the terms together, the Ohm’s law is

\[
j = \sigma_\parallel (E' \cdot b) b + \sigma_P (b \times E' \times b) - \sigma_H (E' \times b),
\]  
(150)

which is valid in any coordinate system or our choice, as long as the plasma density is small compared to the neutral density.
3 Molecular and eddy diffusion

We will use the 5-moment momentum equation to derive the diffusive equilibrium density profile for a minor species $s$. This level of approximation is comparable to the Euler equations of fluid flow, except for the momentum transfer collision term, and it excludes the so called thermal diffusion that we will return to later. The starting point is (e.g., Schunk and Nagy, 2000):

$$\rho_s \left[ \frac{\partial \mathbf{u}_s}{\partial t} + (\mathbf{u}_s \cdot \nabla) \mathbf{u}_s \right] + \nabla \cdot \mathbf{p}_s - \rho_s \mathbf{g} - n_s q_s \mathbf{E} = - \sum_{t \neq s} \rho_s \nu_{st} (\mathbf{u}_s - \mathbf{u}_t)$$

(151)

where $\rho_s$ is the mass density, $\mathbf{u}_s$ is the species velocity, $p_s = n_s k T_s$ is the partial pressure, $\mathbf{g}$ is gravity, $n_s$ is the species number density, $q_s$ is the electric charge, $\mathbf{E}$ is the atmospheric electric field and $\nu_{st}$ is the momentum transfer collision frequency with species $t$. We retained some generality in this equation for future use. If there is no magnetic field or for a neutral species, this equation applies to the vertical (radial) direction. If there is a magnetic field, the equation holds parallel to the magnetic field for ions.

3.1 Diffusive equilibrium for a neutral species (Week 2)

We write equation (151) with $q_s = 0$ along the radial direction:

$$\rho_s \left( \frac{\partial w_s}{\partial t} + w_s \frac{\partial w_s}{\partial r} \right) + \frac{\partial p_s}{\partial r} + \rho_s g(r) = - \sum_{t \neq s} \rho_s \nu_{st} (w_s - w_t)$$

(152)

where $w_s$ is the vertical velocity. Using the scale height of the atmosphere as the vertical length scale, we find that the ratio of advection terms to the pressure gradient is approximately $w_s / c_s$, where $c_s = kT_s / m_s$ is the thermal velocity, so we can ignore the advection terms for subsonic flow. Thus, we have

$$\frac{\partial p_s}{\partial r} + \rho_s g(r) = - \sum_{t \neq s} \rho_s \nu_{st} (w_s - w_t)$$

(153)

which is

$$\frac{\partial p_s}{\partial r} - \frac{\rho_s}{\rho} \frac{\partial p}{\partial r} = - \sum_{t \neq s} \rho_s \nu_{st} (w_s - w_t)$$

(154)

under hydrostatic equilibrium. We divide this equation by $p_s$ to write

$$\frac{1}{p_s} \frac{\partial p_s}{\partial r} - \frac{m_s}{m} \frac{\partial \ln p}{\partial r} = - \sum_{t \neq s} \frac{x_t}{D_{st}} (w_s - w_t)$$

(155)
where $x_t = n_t/n$ and

$$D_{st} = \frac{x_t kT}{m_s \nu_{st}}$$  \hspace{1cm} (156)

is the coefficient of diffusion based on collisions between species $s$ and $t$.

Using hydrostatic equilibrium, we write equation (155) as

$$\frac{1}{p_s} \frac{\partial p_s}{\partial r} + \frac{1}{H_s} = -\sum_{t \neq s} x_t D_{st} (w_s - w_t)$$  \hspace{1cm} (157)

where $H_s = kT / (m_s g)$. We now assume that the background atmosphere undergoes turbulent motions that act to mix the atmosphere and write

$$w_t = w_K = -K_{zz} \frac{1}{x_s} \frac{\partial x_s}{\partial r}$$  \hspace{1cm} (158)

where $K_{zz}$ is the eddy mixing coefficient. Thus, we write

$$w_s = w_K - D_s \left( \frac{1}{p_s} \frac{\partial p_s}{\partial r} + \frac{1}{H_s} \right)$$  \hspace{1cm} (159)

where we defined the ‘mean’ diffusion coefficient for species $s$ as

$$\frac{1}{D_s} = \sum_{t \neq s} x_t D_{st}.$$  \hspace{1cm} (160)

Noting that

$$\frac{1}{x_s} \frac{\partial x_s}{\partial r} = \frac{1}{p_s} \frac{\partial p_s}{\partial r} + \frac{1}{H}$$  \hspace{1cm} (161)

where $H$ is the pressure scale height, we obtain

$$w_s = -K_{zz} \left( \frac{1}{p_s} \frac{\partial p_s}{\partial r} + \frac{1}{H} \right) - D_s \left( \frac{1}{p_s} \frac{\partial p_s}{\partial r} + \frac{1}{H_s} \right).$$  \hspace{1cm} (162)

In steady state (diffusive equilibrium), $w_s = 0$ and we can write equation (162) as

$$\frac{1}{p_s} \frac{\partial p_s}{\partial r} = -(1 + \Lambda_s)^{-1} \left( \frac{1}{H_s} + \frac{\Lambda_s}{H} \right)$$  \hspace{1cm} (163)

where $\Lambda_s = K_{zz}/D_s$, i.e.,

$$p_s(r) = p_s(r_0) \exp \left[ -\int_{r_0}^{r} \frac{dr'}{1+\Lambda_s} \left( \frac{1}{H_s} + \frac{\Lambda_s}{H} \right) \right].$$  \hspace{1cm} (164)

In other words, if $K_{zz} \gg D_s$, $\Lambda_s \gg 1$ and the partial pressure of species $s$ decreases with altitude based on the pressure scale height of the atmosphere. If, on the other hand,
\( K_{zz} \ll D_s, \Lambda_s \ll 1 \) and the partial pressure of species \( s \) decreases with altitude based on its own scale height \( H_s \). The homopause, where \( D_s = K_{zz} \) by definition, is in the transition regime.

A common form of the diffusion equation is given in terms of the mixing ratio \( x_s \). This is obtained from equation (155) by using equation (161), and it is given by

\[
\frac{\partial x_s}{\partial r} + \left( x_s - \frac{\rho_s}{\rho} \right) \frac{\partial \ln p}{\partial r} = - \sum_{i \neq s} x_s x_i \frac{w_s - w_i}{D_{st}}. \tag{165}
\]

We can also incorporate eddy and thermal diffusion here by writing

\[
(1 + \Lambda_s) \frac{\partial x_s}{\partial r} + \left( x_s - \frac{\rho_s}{\rho} \right) \frac{\partial \ln p}{\partial r} + \frac{\alpha_s x_s}{T} \frac{\partial T}{\partial r} = - \sum_{i \neq s} x_s x_i \frac{w_s - w_i}{D_{st}} \tag{166}
\]

where \( \alpha_s \) is the thermal diffusion coefficient for species \( s \). Assuming that \( w_i = 0 \), we obtain the diffusion velocity of species \( s \) as (e.g., Chamberlain and Hunten, 1987):

\[
w_s = -D_s \left( \frac{1}{n_s} \frac{\partial n_s}{\partial r} + \frac{1}{H_s} + \frac{1 + \alpha_s}{T} \frac{\partial T}{\partial r} \right) + K_{zz} \left( \frac{1}{n_s} \frac{\partial n_s}{\partial r} + \frac{1}{H_s} + \frac{1}{T} \frac{\partial T}{\partial r} \right). \tag{167}
\]

Equation (156) gives a formula for the diffusion coefficient but in most applications, tabulated values are used (e.g., Marrero and Mason, 1972). In the absence of readily available values for neutral species, the equation

\[
D_{st} = \frac{1.52 \times 10^{24}}{n} \sqrt{\frac{1}{M_s} + \frac{1}{M_i}} T, \tag{168}
\]

where \( n \) is the total number density of the atmosphere and \( M \) is the molecular weight in amu, is a reasonable approximation.

### 3.2 Major ion diffusive equilibrium, no magnetic field (Week 4)

Consider a single major ion in charge balance, so that the electron density \( n_e = n_i = n_p \) where \( n_p \) is referred to as the plasma density. We write the steady state ion momentum equation as

\[
\nabla \cdot \mathbf{p}_i - n_i e \mathbf{E} = -\rho_i \mathbf{v}_i (\mathbf{u}_i - \mathbf{u}_e) - \sum_s \rho_i \nu_{is} (\mathbf{u}_i - \mathbf{u}_s) \tag{169}
\]

which applies parallel to the magnetic field lines or in the vertical direction. The parallel current density is

\[
\mathbf{j}_\parallel = \sum_i n_i q_i \mathbf{u}_i \tag{170}
\]
where $q_i$ is ion charge. Assuming zero current conditions for a major ion implies that $(\mathbf{u}_i - \mathbf{u}_e)_{\parallel} = 0$ and the major ion equation becomes

$$\nabla_{\parallel} p_i - n_i e \mathbf{E}_{\parallel} - \rho_i g_{\parallel} = -\rho_i \nu_{in} (\mathbf{u}_i - \mathbf{u}_n),$$

(171)

where we further assumed that collisions with one neutral species $n$ dominate.

The polarization electric field is obtained from the electron momentum equation under the zero current assumption and ignoring any terms including the small electron mass $m_e$. Thus, it is given by

$$e \mathbf{E}_{\parallel} = -\frac{1}{n_e} \nabla_{\parallel} p_e.$$

(172)

Substituting this into equation (171) gives:

$$\nabla_{\parallel} (p_i + p_e) - \rho_i g_{\parallel} = -\rho_i \nu_{in} (\mathbf{u}_i - \mathbf{u}_n).$$

(173)

In diffusive equilibrium and in the absence of a magnetic field, we have

$$\frac{\partial}{\partial r} (p_i + p_e) + \rho_i g = 0,$$

(174)

which we can write as

$$\frac{1}{n_i k T_p} \frac{\partial}{\partial r} (n_i k T_p) + \frac{m_i g}{2 k T_p} = 0$$

(175)

where the plasma temperature is

$$T_p = \frac{T_i + T_e}{2}$$

(176)

and $T_{i,e}$ are the ion and electron temperatures, respectively. Thus,

$$n_i(r) = n_i(r_0) \exp \left( -\frac{r-r_0}{H_p} \right)$$

(177)

is the diffusive equilibrium density profile for a major ion, provided that $T_p$ and $g$ are constant with altitude. The plasma scale height is

$$H_p = \frac{2 k T_p}{m_i g},$$

(178)

which is equivalent to twice the scale height of a neutral species with the same mass as the major ion in collision-dominated media for which $T_e = T_i = T_n$.  

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3.3 Major ion diffusion with magnetic field

We make the same assumptions as in the last section, up to equation (173):

\[ \nabla \parallel (p_i + p_e) - \rho_i g_\parallel = -\rho_i \nu_{in} (u_i - u_n) \parallel. \]

Note that we ignore electrodynamic drift and parallel currents. We also assume that the ions are tied to the field lines i.e., magnetization

\[ k_i = \frac{q_i B}{m_i \nu_{in}} \gg 1, \tag{179} \]

which means that the ion gyrofrequency is much larger than the ion-neutral collision frequency. We do not consider ion-ion collisions because the equations here are valid for a single major ion only.

We rewrite the equation above as

\[ (u_i - u_n) \parallel = -2D_i \left[ \frac{1}{n_i} \nabla \parallel n_i + \frac{1}{T_p} \nabla \parallel T_p - \frac{m_i g_\parallel}{2kT_p} \right] \tag{180} \]

where \( T_p \) is the plasma temperature and the diffusion coefficient is

\[ D_i = \frac{kT_p}{m_i \nu_{in}}. \tag{181} \]

Cast in magnetic dipole coordinates, the gradient operator is (Swisdak, 2006, and Section 5.1)

\[ \nabla f = q \frac{\delta}{r^3} \frac{\partial f}{\partial q} + p \frac{\delta}{\sin^3 \theta} \frac{\partial f}{\partial p} + e_\phi \frac{1}{r \sin \theta} \frac{\partial f}{\partial \phi}, \tag{182} \]

which means that

\[ \nabla \parallel f = q \frac{\delta}{r^3} \frac{\partial f}{\partial q}. \tag{183} \]

where for a south to north (Earth-style) centered dipole

\[ q = -\left( \frac{2 \cos \theta}{\delta} e_r + \frac{\sin \theta}{\delta} e_\phi \right) \tag{184} \]

With this, the major ion drift equation is

\[ (u_i - u_n) q = -2D_i \left[ \frac{1}{n_i} \frac{\delta n_i}{r^3 q} + \frac{1}{T_p} \frac{\delta T_p}{r^3 q} - \frac{m_i g_\parallel}{2kT_p} \right] q. \tag{185} \]

We extract the radial component of this equation by taking the dot product with \( e_r \), noting that

\[ q \cdot e_r = -\frac{2 \cos \theta}{\delta} \tag{186} \]
and thus we have

$$u_{ir} + u_{nq} \frac{2 \cos \theta}{\delta} = 2D_i \left[ \frac{1}{n_i} \frac{\delta n_i}{\delta q} + \frac{1}{T_p} \frac{\delta T_p}{\delta q} - \frac{m_i g}{2kT_p} \right] \frac{2 \cos \theta}{\delta}$$

(187)

where

$$u_{ir} = -\frac{2 \cos \theta}{\delta} u_i$$

(188)

is the radial component of the ion velocity.

Using coordinate transformations for the dipole coordinate system, we can write

$$\frac{\partial}{\partial q} = \frac{\partial}{\partial r} \frac{\partial r}{\partial q} = -\frac{2r^2 \cos \theta}{\delta^2} \frac{\partial}{\partial r}.$$  

(189)

Also, gravity along the magnetic field line is

$$g_q = -g e_r \cdot q = \frac{2g \cos \theta}{\delta}.$$  

(190)

Finally, zonal winds do not have a component along the dipole magnetic field lines and vertical winds are much slower than meridional winds. Based on this, we assume that

$$u_n = u_n \mathbf{e}_\theta \rightarrow u_{nq} = u_n \cdot q = -\frac{\sin \theta}{\delta} u_n.$$  

(191)

Now, the expression for the ion drift becomes

$$u_{ir} = \frac{2 \cos \theta \sin \theta}{\delta} u_n = -2D_i \frac{4 \cos^2 \theta}{\delta^2} \left[ \frac{1}{n_i} \frac{\partial n_i}{\partial r} + \frac{1}{T_p} \frac{\partial T_p}{\partial q} + \frac{m_i g}{2kT_p} \right].$$

(192)

We move to define the magnetic dip angle $I$ as the angle between the magnetic field vector and the meridional unit vector. Thus, we have

$$\sin I = q \times e_\theta = q_r = -\frac{2 \cos \theta}{\delta}$$

(193)

$$\cos I = q \cdot e_\theta = q_\theta = -\frac{\sin \theta}{\delta}$$

(194)

and with these definitions,

$$u_{ir} = u_n \cos I \sin I - 2D_i \sin^2 I \left[ \frac{1}{n_i} \frac{\partial n_i}{\partial r} + \frac{1}{T_p} \frac{\partial T_p}{\partial q} + \frac{m_i g}{2kT_p} \right].$$

(195)

is a basic form of the ion drift equation.

It should be noted that equation (195) ignores ion motion perpendicular to the field lines, assumes zero field-aligned currents and does not include electrodynamic drift. As
an example of the latter, we may consider the eastward equatorial electric field in the
dayside ionosphere of the Earth. This electric field is generated by a wind dynamo in
the E region and communicated along the field lines to the F region where $k_i \gg 1$. The
ion drift based on this field has the form

$$\mathbf{v}_{id} = \frac{\mathbf{E} \times \mathbf{B}}{B}.$$

(196)

For an eastward electric field, the component in the vertical direction is

$$u_{idr} = \frac{E}{B} \cos I,$$

(197)

leading to an equatorial F region drift equation given by

$$u_n = \frac{E}{B} \cos I + u_n \cos I \sin I - 2D_i \sin^2 I \left[ \frac{1}{n_i} \frac{\partial n_i}{\partial r} + \frac{1}{T_p} \frac{\partial T_p}{\partial q} + \frac{m_i g}{2kT_p} \right].$$

(198)

The dynamo field thus produces upwelling around the equator, which is balanced by
downwelling at mid-latitudes. This effect that modifies the equatorial electron density
profiles is known as the Appleton fountain.

4 Energy balance

4.1 Exospheric temperature (Week 1)

Assume that the thermosphere is heated from above by solar EUV flux $F_\infty$ and that the
globally averaged effective heat flux $F_E$ is

$$F_E = \frac{1}{4} \epsilon F_\infty$$

(199)

where $\epsilon$ is the heating efficiency parameter (more on that later). Assume that heating
is balanced by downward heat conduction to the mesopause where the energy is reradi-
ated to space in the infrared. Then, the outgoing flux at the mesopause is equal to the
downward heat flux by conduction:

$$F_E = \kappa \frac{dT}{dr}$$

(200)

where $\kappa$ is the coefficient of heat conduction. This coefficient is given by

$$\kappa = AT^s$$

(201)
where $A$ [W m$^{-1}$ K$^{-(s+1)}$] and $s$ are constants that depend on the relevant atmospheric constituents. Gombosi (1994) gives the following expression based on the mean free path method:

$$\kappa = \frac{2k}{\sigma} \sqrt{\frac{k}{\pi m} T^{1/2}} \tag{202}$$

where $k$ is the Boltzmann constant, $\sigma$ is the total cross section of molecular collisions and $m$ is the molecular weight of the constituent. In practical applications, however, we use tabulated values of $A$ and $s$ for different species rather than this expression.

We use hydrostatic equilibrium to write

$$dr = -H \frac{dp}{p} \tag{203}$$

and thus equation (200) is

$$F_E \frac{TH_0}{T_0} \frac{dp}{p} = -AT^s dT \tag{204}$$

where we also assumed that

$$H = \frac{T}{T_0} H_0 \tag{205}$$

where $T_0$ and $H_0$ are the temperature and pressure scale height at the mesopause. We now proceed to integrate this equation from the mesopause roughly to the level of the EUV heating peak:

$$F_E \int_{p_0}^{p} \frac{dp'}{p'} = -\frac{AT_0}{H_0} \int_{T_0}^{T_\infty} T^{s-1} dT \tag{206}$$

where we labeled the exospheric temperature as $T_\infty$. Thus, we obtain

$$F_E \ln \left( \frac{p}{p_0} \right) = -\frac{AT_0}{sH_0} (T_\infty^s - T_0^s) \tag{207}$$

and finally, the result is

$$T_\infty^s = T_0^s + \frac{seF_{EUV}H_0}{4AT_0} \ln \left( \frac{p_0}{p} \right). \tag{208}$$

The obvious trouble with this equation is that we do not have \textit{a priori} knowledge of the appropriate value of $p$. One solution is to write (Chamberlain and Hunten, 1987)

$$\frac{p_0}{p} \approx \frac{\tau_0}{< \mu >} \tag{209}$$

where $\tau_0$ is the optical depth (for global average) at the mesopause to radiation in the $\sim$20–100 nm band and the cosine of the solar zenith angle $< \mu >$ = 1/2.
4.2 Energy-limited escape (Week 13)

The derivation of the exospheric temperature above is based on a simple balance between net heating, downward conduction and re-radiation of the absorbed energy back to space at the mesopause. An alternative balance that has gained popularity among exoplanet modelers is the so-called energy-limited escape. We write the Navier-Stokes energy equation in the radial direction as (e.g., Koskinen et al., 2013b)

\[
\frac{\partial}{\partial t} (\rho c_v T) + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho c_v T w \right) = \rho Q_R - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa \frac{\partial}{\partial r} \right) + \Phi_V \tag{210}
\]

where \( w \) is the radial bulk flow speed, \( Q_R \) is the net radiative heating term (sum of heating and cooling), \( \kappa \) is the coefficient of heat conduction and \( \Phi_V \) is the viscous dissipation functional. By using the continuity and momentum equations, we can write this equation in steady state as:

\[
\frac{\partial}{\partial r} \left[ F_{\rho} \left( c_p T + \frac{1}{2} w^2 + \phi_g \right) \right] = \rho r^2 Q_R + \frac{\partial}{\partial r} \left( r^2 \kappa \frac{\partial}{\partial r} \right) + r^2 \Phi_V \tag{211}
\]

where the radial mass flux constant \( F_{\rho} = \rho w r^2 \) and \( \phi_g \) is the gravitational potential.

We assume that conduction is negligible (\( \kappa = 0 \)) and ignore the viscous dissipation functional. Integrating equation (211) from \( r_0 \) to infinity then leads to

\[
-F_{\rho} \left( c_p T_0 - \frac{1}{2} w^2 + \phi_{g0} \right) = \epsilon F_E r_E^2 \tag{212}
\]

where we assumed that \( T \to 0 \) at infinity, \( w \to 0 \) at \( r_0 \) and \( \phi_g \) vanishes at infinity. Furthermore, we can define the product

\[
\epsilon F_E r_E^2 = \int_{r_0}^{\infty} r^2 \alpha(r) q(r) dr \tag{213}
\]

where \( F_E \) is the effective (radiative) heat flux at the top of the atmosphere, \( r_E \) is the effective peak altitude of the heating function, \( \epsilon \) is the column-averaged heating efficiency, \( \alpha \) is the altitude-dependent heating efficiency and \( q \) is the altitude-dependent total energy deposition rate.

We can divide the potential term in equation (212) by the specific enthalpy term for monatomic gas

\[
\frac{\phi_{g0}}{c_p T_0} = \frac{2m |\phi_{g0}|}{5k T_0} = \frac{2}{5} X_0 \tag{214}
\]

where \( X_0 \) is the thermal escape parameter. In other words, as long as \( X_0 > 5/2 \) at \( r_0 \), the specific enthalpy term is negligible, a condition that is almost always satisfied at the
base of the thermosphere. In most cases, the kinetic energy flux can also be ignored, and this gives

\[ F_p = \frac{\epsilon r_E^2 F_E^2}{\phi_{g0}}. \]  

(215)

The standard formula for energy-limited global mass loss is obtained by setting \( \phi_{g0} = -GM_p/r_0 \) and assuming that \( F_E = F_{XUV}/4 \) for a global average i.e.,

\[ \dot{M}_E = 4\pi F_p = \frac{\epsilon \pi r_{XUV}^2 F_{XUV} R_p}{GM_p} \]

(216)

where \( F_{XUV} \) is the stellar XUV flux at the top of the atmosphere, \( R_p \) is the radius of the planet and \( M_p \) is the mass of the planet.

It should be noted that this equation implies a balance between the net radiative heating term in the energy equation and the thermal (adiabatic) expansion term

\[ p \frac{\partial}{\partial r} (r^2 w) = \frac{\partial}{\partial r} \left( p w r^2 \right) + w r^2 \frac{\partial p}{\partial r} \]

(217)

where the second term on the right-hand side

\[ w r^2 \frac{\partial p}{\partial r} = - \left[ w \frac{\partial}{\partial r} \left( p w^2 r^2 \right) + w r^2 \frac{\partial \phi_g}{\partial r} \right] \]

(218)

is obtained from the steady-state radial momentum equation.

5 Supporting topics

5.1 Magnetic dipole coordinates

Magnetic dipole coordinates \( p \) and \( q \) are given by (e.g., Swisdak, 2006):

\[ p = \frac{r}{\sin^2 \theta} \]

(219)

\[ q = \frac{\cos \theta}{r^2} \]

(220)

where \( r \) is radial distance, \( \theta \) is co-latitude, \( p \) is constant along magnetic field lines and \( q \) is constant in the direction perpendicular to the magnetic field lines. The reader may wonder where these expressions come from. The starting point is the dipole magnetic field centered at the planet:

\[ B = \frac{\mu_0}{4\pi} \frac{\mu_M}{r^3} \left( 2\cos \theta \mathbf{e}_r + \sin \theta \mathbf{e}_\theta \right) \]

(221)
where $\mu_0 = 4\pi \times 10^{-7}$ N A$^{-2}$ is the permeability of free space and $\mu_M$ is the magnetic moment in units of A m$^2$. An alternative expression for magnetic moment $m$ is

$$m = \frac{\mu_0}{4\pi} \mu_M,$$  \hspace{1cm} (222)

which has units of T m$^3$. Finally, the magnitude of the dipole field is

$$B = \frac{\mu_0 \mu_M \delta}{4\pi r^3},$$  \hspace{1cm} (223)

$$\delta = \sqrt{1 + 3 \cos^2 \theta}. \hspace{1cm} (224)$$

Now, consider a path length element parallel to the magnetic field i.e.,

$$\mathbf{ds} \times \mathbf{B} = 0.$$  \hspace{1cm} (225)

Using spherical polar coordinates and setting $d\phi = 0$ gives

$$B_\theta dr = B_r r dr \rightarrow \frac{dr}{B_\theta} = \frac{d\theta}{B_r} \rightarrow \frac{dr}{r} = \frac{2du}{u} \hspace{1cm} (226)$$

where we used the radial and meridional components of the magnetic field from above and substituted $u = \sin \theta$. Integrating from the equator where $u = 1$ to some radial distance $r$ leads to

$$\ln \left( \frac{r}{r_{eq}} \right) = 2 \ln u, \hspace{1cm} (227)$$

which gives us the magnetic field line equation:

$$r = r_{eq} \sin^2 \theta \hspace{1cm} (228)$$

where $p = r_{eq}$ is the equatorial radius corresponding to a given field line. Thus $p$ is constant along the magnetic field line. This coordinate is related to the so-called $L$ value of a given field line by

$$p = LR_0 \hspace{1cm} (229)$$

where $R_0$ is an equatorial reference radius.

Similarly, we consider a path length element perpendicular to the field line i.e.,

$$\mathbf{ds} \cdot \mathbf{B} = B_r dr + B_\theta r d\theta = 0,$$ \hspace{1cm} (230)

which leads to

$$\frac{dr}{r} = \frac{d(\cos \theta)}{2\cos \theta} \hspace{1cm} (231)$$

and gives the dipole coordinate $q$ as a constant of integration

$$qr^2 = \cos \theta. \hspace{1cm} (232)$$

For example, at the poles $\cos \theta = 1$ and $q = 1/r^2$. Thus, the coordinate $q$ is constant in the direction perpendicular to the magnetic field line.
5.2 Hydromagnetic theorem

Consider a fully ionized plasma where Hall currents are negligible, for example the solar wind. The Ohm’s law for the current density can be written as

\[ j = \sigma_e (E + u \times B) \]  

(233)

where

\[ \eta_e = \frac{1}{\sigma_e} = \frac{m_e \nu_c}{n_e e^2} \]  

(234)

is the plasma resistivity i.e, the inverse of conductivity, and \( \nu_c \) is the Coulomb collision frequency. The velocity is

\[ u = \frac{\sum_s m_s n_s u_s}{\rho} \]  

(235)

where \( \rho \) is total mass density and the sum is over all species \( s \) with number density \( n_s \) and mass \( m_s \). For a single ion plasma, we have

\[ u_i \approx u \]  

(236)

\[ u_e \approx u - \frac{j}{en_e} \]  

(237)

because of the small electron mass.

Taking the curl of equation (233), assuming constant \( \eta_e \) and using Faraday’s and Ampere’s laws (without the displacement current) gives

\[ \frac{\partial B}{\partial t} + \nabla \times (u \times B) = \frac{\eta_e}{\mu_0} \nabla \times (\nabla \times B). \]  

(238)

We use the Levi-Civita symbol (see Section 5.4) to write the cross product:

\[ [\nabla \times (\nabla \times B)]_m = \epsilon_{mnk} \epsilon_{ijk} \frac{\partial}{\partial x_n} \left( \frac{\partial B_k}{\partial x_j} \right). \]  

(239)

An even permutation of the Levi-Civita symbol gives

\[ [\nabla \times (\nabla \times B)]_m = \epsilon_{mnk} \epsilon_{ijk} \frac{\partial}{\partial x_n} \left( \frac{\partial B_k}{\partial x_j} \right) \]  

(240)

and therefore, we have

\[ [\nabla \times (\nabla \times B)]_m = \left( \delta_{jm} \delta_{kn} - \delta_{jn} \delta_{km} \right) \frac{\partial}{\partial x_n} \left( \frac{\partial B_k}{\partial x_j} \right) \]

\[ = \frac{\partial}{\partial x_n} \left( \frac{\partial B_m}{\partial x_j} \right) - \frac{\partial}{\partial x_n} \left( \frac{\partial B_j}{\partial x_m} \right) \]

\[ = \frac{\partial}{\partial x_m} \left( \frac{\partial B_n}{\partial x_j} \right) - \frac{\partial}{\partial x_n} \left( \frac{\partial B_m}{\partial x_j} \right) \]  

(241)

34
or
\[ \nabla \times (\nabla \times \mathbf{B}) = \nabla (\nabla \cdot \mathbf{B}) - \nabla^2 \mathbf{B} = -\nabla^2 \mathbf{B}. \] 
(242)

Using this vector identity, we obtain the induction equation
\[ \frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}) + \frac{\eta}{\mu_0} \nabla^2 \mathbf{B}. \] 
(243)

If the magnetic Reynold’s number
\[ R_m = \mu_0 \sigma u L_B >> 1, \] 
(244)

where \( L_B \) is the length scale of spatial variations within the magnetic field, the second term on the right-hand side of the induction equation (magnetic diffusion) can be neglected and we obtain the hydromagnetic theorem:
\[ \frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}). \] 
(245)

This is equivalent to zero electric field in the rest frame of the plasma (i.e., infinite conductivity):
\[ \mathbf{E} + \mathbf{u} \times \mathbf{B} = 0, \] 
(246)

which implies that ions and electrons drift with the same velocity
\[ \mathbf{u} = \frac{\mathbf{E} \times \mathbf{B}}{B} \] 
(247)

perpendicular to both the electric and magnetic fields and that the magnetic field is frozen-in to the plasma.

5.3 Simple magnetopause boundary

The magnetopause is a tangential discontinuity where the pressure of the solar-wind magnetosheath plasma balances the pressure of the Earth’s magnetosphere, the latter being dominated by the pressure of the Earth geomagnetic field. More specifically, around the nose of the magnetopause boundary (Baumjohann and Treumann, 1997):
\[ \kappa n_{sw} m_p (\mathbf{n} \cdot \mathbf{v}_{sw})^2 = \frac{1}{2 \mu_0} (\mathbf{n} \times \mathbf{B}_p)^2 \] 
(248)

where \( \mathbf{n} \) is a unit vector normal to the magnetopause boundary, \( n_{sw} \) is the solar wind plasma density, \( v_{sw} \) is the solar wind velocity, \( \mathbf{B}_p \) is the Earth’s magnetic field strength, \( m_p \) is proton mass and \( \kappa \) is an efficiency factor that accounts for non-specular reflection
of the solar wind plasma. At the stagnation point (nose) where solar wind velocity is parallel to n, we can write
\[ \kappa n_{sw} m_p v_{sw}^2 = \frac{B_p^2}{2\mu_0}. \]  
(249)

Assuming that the magnetic field at the stagnation point can be represented by a distorted dipole field, we obtain
\[ n_{sw} m_p v_{sw}^2 = \frac{KB_E^2}{2\mu_0 n_{sw} m_p v_{sw}^2} R_E^6 \]  
(250)

where \( R_{mp} \) is the stand-off distance and the parameter \( K \) accounts for non-specular reflection and deviation from the dipole configuration driven by the magnetopause current. Based on this, we obtain
\[ R_{mp} = \left( \frac{KB_E^2}{2\mu_0 n_{sw} m_p v_{sw}^2} \right)^{1/6} R_E \]  
(251)

where \( m_p \) is proton mass and \( B_E \) is the Earth’s surface magnetic field strength. With \( K = 2 \), we obtain \( R_{mp} \approx 10 R_E \).

On the magnetopause flanks, the normal component of the solar wind ram pressure is small and solar wind thermal pressure dominates. Thus, we have
\[ R_{mpf} = \left( \frac{KB_E^2}{2\mu_0 \gamma n_{sw} kT_{sw}} \right)^{1/6} R_E, \]  
(252)

where \( \gamma = 5/3 \) and \( T_{sw} \) is the temperature of the solar wind magnetosheath plasma. This expression yields values about 1.8 times larger than \( R_{mp} \) and gives \( \sim 18 R_E \) as the extent of the magnetopause on the flanks. These estimates deviate somewhat from real values (e.g., \( \sim 14 R_E \) for the magnetopause extent on the flanks), but they are good to an order of magnitude and provide useful guidance.

### 5.4 Levi-Civita symbol

#### 5.4.1 Rank 2

The Levi-Civita symbol is a tensor of a rank set to match the dimensions of a given problem. It is helpful to consider the rank 2 case first:
\[ \epsilon_{ij} = \begin{cases} 1 & \text{for } (i,j) = (1,2) \\ -1 & \text{for } (i,j) = (2,1) \\ 0 & \text{for } i = j. \end{cases} \]  
(253)
We now wish to write the product of two symbols $\epsilon_{ij}\epsilon_{mn}$ by using Kronecker delta symbols. We recognize that any combination where $i = m$ and $j = n$ at the same time must give 1 (product of the same sign) while for this case, it is also clear that $i \neq n$ and $j \neq m$. The opposite is true for the (1,2)(2,1) combination. Therefore,

$$\epsilon_{ij}\epsilon_{mn} = \delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}. \quad (254)$$

For example, we can set $i = m$ to obtain

$$\epsilon_{ij}\epsilon_{in} = \delta_{ii}\delta_{jn} - \delta_{in}\delta_{ji} \quad (255)$$

where repeated indices imply a sum. Thus,

$$\epsilon_{ij}\epsilon_{in} = 2\delta_{jn} - \delta_{in}\delta_{j1} - \delta_{2n}\delta_{j2} = \delta_{jn}. \quad (256)$$

Finally, we obtain

$$\epsilon_{ij}\epsilon_{ij} = \delta_{jj} = 2 \quad (257)$$

by setting $j = n$.

### 5.4.2 Rank 3

The Levi-Civita symbol of rank 3 is

$$\epsilon_{ijk} = \begin{cases} 0 & \text{for any two indices equal} \\ 1 & \text{for even permutations of (1,2,3)} \\ -1 & \text{for odd permutations of (1,2,3)} \end{cases} \quad (258)$$

where a permutation refers to the swap of any two indices and even permutation is obtained by an even number of swaps. By using the same logic as we did for symbols of rank 2, the product of two symbols of rank 3 is

$$\epsilon_{ijk}\epsilon_{lmn} = \begin{align*} \delta_{il}\delta_{jm}\delta_{kn} + \delta_{im}\delta_{jn}\delta_{kl} + \delta_{in}\delta_{jl}\delta_{km} \\ - \delta_{im}\delta_{jl}\delta_{kn} - \delta_{il}\delta_{jn}\delta_{km} - \delta_{in}\delta_{jm}\delta_{kl}. \end{align*} \quad (259)$$

Setting $i = l$ then gives

$$\epsilon_{ijk}\epsilon_{lmn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km} \quad (260)$$

where repeated indices again indicate a sum. The symbol is useful for writing operations involving cross products. It is easy to demonstrate that

$$(\mathbf{a} \times \mathbf{b})_i = \epsilon_{ijk}a_jb_k \quad (261)$$

is the $i$th component of the cross product of two vectors.
References


