

PTY544: Physics of the high atmosphere

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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 (\mathbf{r}, \mathbf{v}) at time t is

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

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

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

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

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

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

It is convenient to write the random thermal velocity as

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

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

$$\mathbf{u}(t, \mathbf{r}) = \frac{\int d^3v \mathbf{v} F(t, \mathbf{r}, \mathbf{v})}{\int d^3v F(t, \mathbf{r}, \mathbf{v})}. \quad (5)$$

Repeating the derivation of the Boltzmann equation in Gombosi (1994) with $\mathbf{c}(t, \mathbf{r})$ yields the transformations

$$\frac{\partial F(t, \mathbf{r}, \mathbf{v})}{\partial t} \rightarrow \frac{\partial F(t, \mathbf{r}, \mathbf{c})}{\partial t} - \frac{\partial u_i(t, \mathbf{r})}{\partial t} \frac{\partial F(t, \mathbf{r}, \mathbf{c})}{\partial c_i} \quad (6)$$

$$\frac{\partial F(t, \mathbf{r}, \mathbf{v})}{\partial x_j} \rightarrow \frac{\partial F(t, \mathbf{r}, \mathbf{c})}{\partial x_j} - \frac{\partial u_i(t, \mathbf{r})}{\partial x_j} \frac{\partial F(t, \mathbf{r}, \mathbf{c})}{\partial c_i} \quad (7)$$

$$\frac{\partial F(t, \mathbf{r}, \mathbf{v})}{\partial v_j} \rightarrow \frac{\partial F(t, \mathbf{r}, \mathbf{c})}{\partial c_j} \quad (8)$$

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

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

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

$$dN_1 = I_1 S(\mathbf{g}, \mathbf{g}') d\Omega \quad (10)$$

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 $\mathbf{g} + d\mathbf{g}$ 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 χ 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 ϵ around the direction of \mathbf{g} . Therefore, the differential cross section is $S(\mathbf{g}, \mathbf{g}') = S(g, \chi)$ 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 $I_1 = g F(t, \mathbf{r}, \mathbf{v}_1) d^3 \mathbf{v}_1$ and we have

$$dN_1 = g S(g, \chi) \sin \chi d\chi d\epsilon F(t, \mathbf{r}, \mathbf{v}_1) d^3 \mathbf{v}_1. \quad (11)$$

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

$$dN_{12} = g S(g, \chi) \sin \chi d\chi d\epsilon F(t, \mathbf{r}, \mathbf{v}_1) F(t, \mathbf{r}, \mathbf{v}_2) d^3 \mathbf{v}_1 d^3 \mathbf{v}_2 \quad (12)$$

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 \mathbf{v}_1 and $\mathbf{v}_1 + d\mathbf{v}_1$ inside the phase space volume element at a given location i.e.,

$$\frac{\delta F}{\delta t} = \left(\frac{\delta F}{\delta t} \right)^+ - \left(\frac{\delta F}{\delta t} \right)^-. \quad (13)$$

We divide equation (12) by $d^3\mathbf{v}_1$ and integrate to obtain the rate of change in F ($m^{-6} \text{ s}^3 \text{ s}^{-1}$) due to collisions that deplete particles with velocities between \mathbf{v}_1 and $\mathbf{v}_1 + d\mathbf{v}_1$:

$$\left(\frac{\delta F}{\delta t} \right)^- = \int d^3v_2 \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi) g F(t, \mathbf{r}, \mathbf{v}_1) F(t, \mathbf{r}, \mathbf{v}_2) \quad (14)$$

where the total collision cross section is defined as

$$\sigma(g) = \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi). \quad (15)$$

The rate of change in F due to collisions that replenish particles with velocities between \mathbf{v}_1 and $\mathbf{v}_1 + d\mathbf{v}_1$ can be written as

$$\left(\frac{\delta F}{\delta t} \right)^+ = \int d^3v_2 \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi) g F(t, \mathbf{r}, \mathbf{v}'_1) F(t, \mathbf{r}, \mathbf{v}'_2) \quad (16)$$

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

$$\frac{\delta F}{\delta t} = \int d^3v_2 \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi) g (F'F'_2 - FF_2), \quad (17)$$

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

$$\frac{\delta F}{\delta t} = \int d^3c_2 \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi) g (F'F'_2 - FF_2), \quad (18)$$

where the phase space distribution functions are $F = F(t, \mathbf{r}, \mathbf{c}_1)$ and $F_2 = F(t, \mathbf{r}, \mathbf{c}_2)$. Also, for a single species s in a multi-species gas, the collision integral is

$$\frac{\delta F_s}{\delta t} = \sum_t \int d^3 c_t \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin \chi S(g, \chi) g (F'_s F'_t - F_s F_t) \quad (19)$$

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

$$\frac{\partial F}{\partial t} + (u_i + c_i) \frac{\partial F}{\partial x_i} - \left[\frac{\partial u_i}{\partial t} + (u_j + c_j) \frac{\partial u_i}{\partial x_j} - a_i \right] \frac{\partial F}{\partial c_i} = 0, \quad (20)$$

which means that $F'F'_2 = FF_2$ i.e, that $\ln F$ 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):

$$F(t, \mathbf{r}, \mathbf{c}) = n(\mathbf{r}) \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left(-\frac{mc^2}{2kT} \right) \quad (21)$$

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:

$$dN_{12} = gS(g, \chi) \sin \chi d\chi d\epsilon n_1 n_2 f(\mathbf{v}_1) f(\mathbf{v}_2) d^3 \mathbf{v}_1 d^3 \mathbf{v}_2 \quad (22)$$

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

$$f(\mathbf{r}, \mathbf{v}) = \frac{F(\mathbf{r}, \mathbf{v})}{n(\mathbf{r})}, \quad (23)$$

which normalizes to

$$\int d^3 \mathbf{v} f(\mathbf{r}, \mathbf{v}) = \frac{1}{n(\mathbf{r})} \int d^3 \mathbf{v} F(\mathbf{r}, \mathbf{v}) = 1 \quad (24)$$

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

$$N_{12} = \kappa_{12} n_1 n_2 \int d^3 \mathbf{v}_1 \int d^3 \mathbf{v}_2 g \sigma(g) f(\mathbf{v}_1) f(\mathbf{v}_2) \quad (25)$$

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

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

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

$$\sigma(g) = \sigma_0 H(g - g_0) \quad (27)$$

where H is the Heaviside step function and

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

Thus, we can integrate equation (26) to obtain

$$Z_{12} = \kappa_{12}\sigma_0 n_1 n_2 \sqrt{\frac{8kT}{\pi m_{12}}} \exp\left(-\frac{U_0}{kT}\right) \left(1 + \frac{U_0}{kT}\right). \quad (29)$$

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

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

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

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

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

$$k_{12} \approx Q \langle v_T \rangle \quad (32)$$

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

$$\langle W \rangle = \frac{1}{n} \int d^3c W(\mathbf{c}) F(t, \mathbf{r}, \mathbf{c}). \quad (33)$$

Setting $W = 1$ then gives the obvious result that

$$n = \int F d^3c \quad (34)$$

and setting $W = \mathbf{c}$ is

$$\int c_i F d^3c = 0 \quad (35)$$

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 $W(\mathbf{c})$ by writing:

$$\int d^3c W(\mathbf{c}) \left\{ \frac{\partial F}{\partial t} + (u_i + c_i) \frac{\partial F}{\partial x_i} - \left[\frac{\partial u_i}{\partial t} + (u_j + c_j) \frac{\partial u_i}{\partial x_j} - a_i \right] \frac{\partial F}{\partial c_i} \right\} = \int d^3c W(\mathbf{c}) \frac{\delta F}{\delta t}. \quad (36)$$

Here, we write

$$\int d^3c W(\mathbf{c}) \frac{\partial F}{\partial t} = \frac{\partial}{\partial t} \int d^3c W(\mathbf{c}) F = \frac{\partial}{\partial t} (n \langle W \rangle) \quad (37)$$

$$\int d^3c W(\mathbf{c}) u_i \frac{\partial F}{\partial x_i} = u_i \frac{\partial}{\partial x_i} (n \langle W \rangle) \quad (38)$$

$$\int d^3c W(\mathbf{c}) c_i \frac{\partial F}{\partial x_i} = \frac{\partial}{\partial x_i} (n \langle c_i W \rangle) \quad (39)$$

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

$$\int d^3c W(\mathbf{c}) \frac{\partial F}{\partial c_i} = \int d^3c \frac{\partial(WF)}{\partial c_i} - \int d^3c F \frac{\partial W}{\partial c_i} = -n \left\langle \frac{\partial W}{\partial c_i} \right\rangle \quad (40)$$

because the first term in the middle is a perfect differential and $F \rightarrow 0$ at $c_i = \pm\infty$. Employing the same logic, we also obtain

$$\int d^3c W(\mathbf{c}) a_i \frac{\partial F}{\partial c_i} = -n \left\langle a_i \frac{\partial W}{\partial c_i} \right\rangle \quad (41)$$

$$\int d^3c W(\mathbf{c}) c_j \frac{\partial F}{\partial c_i} = -n \left\langle c_j \frac{\partial W}{\partial c_i} \right\rangle - n \delta_{ij} \langle W \rangle. \quad (42)$$

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),

$$\begin{aligned} \int d^3c W(\mathbf{c}) \frac{\delta F}{\delta t} &= \frac{\delta W}{\delta t} = \Delta[W] \\ &= \frac{1}{2} \int d^3c \int d^3c_2 \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin\chi \mathcal{S}(g, \chi) g(W' + W'_2 - W - W_2) F F_2. \end{aligned} \quad (43)$$

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

$$\frac{\delta W_s}{\delta t} = \sum_t \int d^3c_s \int d^3c_t \int_0^{2\pi} d\epsilon \int_0^\pi d\chi \sin\chi \mathcal{S}(g, \chi) g(W'_s - W_s) F_s F_t \quad (44)$$

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

$$\begin{aligned} \frac{\partial}{\partial t} (n\langle W \rangle) + \frac{\partial}{\partial x_i} (n u_i \langle W \rangle) + \frac{\partial}{\partial x_i} (n \langle c_i W \rangle) + n \left\langle \frac{\partial W}{\partial c_i} \right\rangle \left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) \\ + n \left\langle c_j \frac{\partial W}{\partial c_i} \right\rangle \frac{\partial u_i}{\partial x_j} - n \left\langle a_i \frac{\partial W}{\partial c_i} \right\rangle = \Delta[W], \end{aligned} \quad (45)$$

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

$$\frac{\partial}{\partial t} (\rho_s) + \frac{\partial}{\partial x_i} (\rho_s u_i) = P_s - L_s \quad (46)$$

because $\langle c_{si} \rangle = 0$, the derivatives of m_s with respect to c_{si} 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

$$\frac{\partial c_{sk}}{\partial c_{si}} = \delta_{ki}. \quad (47)$$

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

$$\rho_s \left(\frac{\partial u_{si}}{\partial t} + u_{sj} \frac{\partial u_{si}}{\partial x_j} \right) + \frac{\partial P_{sik}}{\partial x_i} - \rho_s \langle a_{si} \rangle = \frac{\delta M_{si}}{\delta t} \quad (48)$$

where

$$P_{sik} = \rho_s \langle c_{si} c_{sk} \rangle \quad (49)$$

is the pressure tensor, the acceleration is

$$\langle \mathbf{a}_s \rangle = \mathbf{g} + \frac{e_s}{m_s} \langle \mathbf{E} + \mathbf{u}_s \times \mathbf{B} + \mathbf{c}_s \times \mathbf{B} \rangle = \mathbf{g} + \frac{e_s}{m_s} (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}), \quad (50)$$

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

$$\rho_s \left(\frac{\partial u_{si}}{\partial t} + u_{sj} \frac{\partial u_{si}}{\partial x_j} \right) + \frac{\partial P_{sik}}{\partial x_i} - \rho_s g_i - n_s e_s (E_i + \epsilon_{ijl} u_{sj} B_l) = \frac{\delta M_{si}}{\delta t} \quad (51)$$

where ϵ_{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

$$P_{sik} = p_s \delta_{ik} + \tau_{sik} \quad (52)$$

where the trace of the deviatoric stress tensor τ_{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

$$\begin{aligned} & \frac{\partial P_{skl}}{\partial t} + P_{skl} \frac{\partial u_{si}}{\partial x_i} + u_{si} \frac{\partial P_{skl}}{\partial x_i} + \frac{\partial Q_{sikl}}{\partial x_i} + P_{slj} \frac{\partial u_{sk}}{\partial x_j} + P_{skj} \frac{\partial u_{sl}}{\partial x_j} \\ & - \rho_s \langle a_{sk} c_{sl} + a_{sl} c_{sk} \rangle = \frac{\delta P_{skl}}{\delta t} \end{aligned} \quad (53)$$

where

$$Q_{sikl} = \rho_s \langle c_{si} c_{sk} c_{sl} \rangle \quad (54)$$

is the heat flow tensor, $\delta P_{skl}/\delta t$ is the pressure tensor collision integral and we used

$$\left\langle \frac{\partial(c_{sk}c_{sl})}{\partial c_{si}} \right\rangle = \langle \delta_{ki}c_{sl} + \delta_{li}c_{sk} \rangle = 0 \quad (55)$$

$$\rho_s \langle c_{sj} \frac{\partial(c_{sk}c_{sl})}{\partial c_{si}} \rangle \frac{\partial u_{si}}{\partial x_j} = \rho_s \langle \delta_{ki}c_{sl}c_{sj} + \delta_{li}c_{sk}c_{sj} \rangle \frac{\partial u_{si}}{\partial x_j} = P_{slj} \frac{\partial u_{sk}}{\partial x_j} + P_{skj} \frac{\partial u_{sl}}{\partial x_j}. \quad (56)$$

Let us now evaluate the acceleration terms. We have

$$\begin{aligned} \langle a_{sk}c_{sl} \rangle &= \langle g_k c_{sl} + \frac{e_s}{m_s} E_k c_{sl} + \frac{e_s}{m_s} (\epsilon_{kab} c_{sa} B_b + \epsilon_{kab} u_{sa} B_b) c_{sl} \rangle \\ &= \left\langle \frac{e_s}{m_s} \epsilon_{kab} c_{sl} c_{sa} B_b \right\rangle = \frac{e_s}{m_s} \epsilon_{kab} P_{sla} B_b = \frac{e_s}{m_s} \mathbf{P}_s \times \mathbf{B} \end{aligned} \quad (57)$$

$$\langle a_{sl}c_{sk} \rangle = -\frac{e_s}{m_s} \epsilon_{lab} B_a P_{sbk} = -\frac{e_s}{m_s} \mathbf{B} \times \mathbf{P}_s. \quad (58)$$

because $\langle c_{sl} \rangle = 0$. Thus, the pressure tensor equation is

$$\begin{aligned} \frac{\partial P_{skl}}{\partial t} + P_{skl} \frac{\partial u_{si}}{\partial x_i} + u_{si} \frac{\partial P_{skl}}{\partial x_i} + \frac{\partial Q_{sikl}}{\partial x_i} + P_{slj} \frac{\partial u_{sk}}{\partial x_j} + P_{skj} \frac{\partial u_{sl}}{\partial x_j} \\ - \frac{e_s}{m_s} (\epsilon_{kab} P_{sla} B_b - \epsilon_{kab} B_a P_{sbl}) = \frac{\delta P_{skl}}{\delta t}. \end{aligned} \quad (59)$$

The pressure tensor contains 9 elements but only 6 are independent because the deviatoric 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

$$P_{sii} = \rho_s \langle c_s^2 \rangle = 3p_s = 3n_s kT_s, \quad (60)$$

which means that temperature can be obtained from

$$\frac{3}{2} kT_s = \frac{1}{2} m_s \langle c_s^2 \rangle. \quad (61)$$

We now recognize that the energy equation can simply be extracted as the trace of the pressure tensor equation i.e., setting $k = l$:

$$3 \frac{\partial p_s}{\partial t} + 3p_s \frac{\partial u_{si}}{\partial x_i} + 3u_{si} \frac{\partial p_s}{\partial x_i} + 2 \frac{\partial q_{si}}{\partial x_i} + 2P_{sij} \frac{\partial u_{si}}{\partial x_j} = 3 \frac{\delta p_s}{\delta t}. \quad (62)$$

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

$$q_{si} = \frac{1}{2} \rho_s \langle c_{si} c_s^2 \rangle = \frac{1}{2} Q_{sijj}. \quad (63)$$

Thus, we obtain the energy equation

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_s \right) + u_{si} \frac{\partial}{\partial x_i} \left(\frac{3}{2} p_s \right) + \frac{5}{2} p_s \frac{\partial u_{si}}{\partial x_i} + \frac{\partial q_{si}}{\partial x_i} + \tau_{sij} \frac{\partial u_{si}}{\partial x_j} = \frac{3}{2} \frac{\delta p_s}{\delta t} \quad (64)$$

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

$$\frac{3}{2} p_s = \frac{3}{2} \frac{k}{m_s} \rho_s T_s = c_v \rho_s T_s \quad (65)$$

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 up 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:

$$F(t, \mathbf{r}, \mathbf{c}) = F_0(t, \mathbf{r}, \mathbf{c}) \left[1 + A_i(t, \mathbf{r}) c_i + B_{ij}(t, \mathbf{r}) c_i c_j + D_{ijk}(t, \mathbf{r}) c_i c_j c_k \right] \quad (66)$$

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):

$$B_{ii} = 0 \quad (67)$$

$$A_i + \left(\frac{3kT}{m} \right) D_{ijj} = 0. \quad (68)$$

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

$$F_s = F_{s0} \left[1 + \frac{\rho_s}{2p_s^2} \tau_{sij} c_{si} c_{sj} + \frac{\rho_s^2}{p_s^3} \left(\frac{c_s^2}{5} - \frac{p_s}{\rho_s} \right) q_{si} c_{si} \right], \quad (69)$$

which is the 13-moment phase space distribution function.

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

$$Q_{sijk} = \rho_s \langle c_{si} c_{sk} c_{sl} \rangle,$$

which is

$$Q_{sikl} = \frac{2}{5} (\delta_{ik} q_{sl} + \delta_{il} q_{sk} + \delta_{kl} q_{si}), \quad (70)$$

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

$$\mu_{sik} = \frac{1}{2} \rho_s \langle c_s^2 c_{si} c_{sk} \rangle = \frac{5 k T_s}{2 m_s} \left(p_s \delta_{ik} + \frac{7}{5} \tau_{sik} \right). \quad (71)$$

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

$$\rho_s \left(\frac{\partial u_{si}}{\partial t} + u_{sj} \frac{\partial u_{si}}{\partial x_j} \right) + \frac{\partial p_s}{\partial x_i} + \frac{\partial \tau_{sji}}{\partial x_j} - \rho_s g_i - n_s e_s (E_i + \epsilon_{ijl} u_{sj} B_l) = \frac{\partial M_{si}}{\partial t} \quad (72)$$

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

$$\frac{\delta M_{si}}{\delta t} = \sum_t \rho_s \nu_{st} (u_{ti} - u_{si}) - \sum_t \nu_{st} \frac{z_{st} m_{st}}{k T_{st}} \left(\frac{\rho_s}{\rho_t} q_{ti} - q_{si} \right). \quad (73)$$

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:

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

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

$$\frac{3}{2} \frac{\delta p_s}{\delta t} = \sum_t \frac{\rho_s \nu_{st}}{m_s + m_t} [3k(T_t - T_s) + m_t(u_s - u_t)^2]. \quad (74)$$

1.5.5 Stress tensor equation

We start with the 13-moment pressure tensor equation

$$\begin{aligned} & \frac{\partial p_s}{\partial t} \delta_{kl} + \frac{\partial \tau_{skl}}{\partial t} + (p_s \delta_{kl} + \tau_{skl}) \frac{\partial u_{si}}{\partial x_i} + u_{si} \left(\frac{\partial p_s}{\partial x_i} \delta_{kl} + \frac{\partial \tau_{skl}}{\partial x_i} \right) + \frac{2}{5} \left(\frac{\partial q_{sk}}{\partial x_l} + \frac{\partial q_{sl}}{\partial x_k} + \frac{\partial q_{si}}{\partial x_i} \delta_{kl} \right) \\ & + (p_s \delta_{lj} + \tau_{slj}) \frac{\partial u_{sk}}{\partial x_j} + (p_s \delta_{kj} + \tau_{skj}) \frac{\partial u_{sl}}{\partial x_j} - \frac{e_s}{m_s} (\epsilon_{kab} \tau_{sla} \mathbf{B}_b - \epsilon_{kab} \mathbf{B}_a \tau_{sbl}) = \frac{\delta}{\delta t} (p \delta_{kl} + \tau_{kl}) \end{aligned}$$

where we used the fact that

$$\frac{\partial Q_{sikl}}{\partial x_i} = \frac{2}{5} \left(\frac{\partial q_{sk}}{\partial x_l} + \frac{\partial q_{sl}}{\partial x_k} + \frac{\partial q_{si}}{\partial x_i} \delta_{kl} \right). \quad (75)$$

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

$$\begin{aligned} & \frac{\partial \tau_{skl}}{\partial t} + (p_s \delta_{kl} + \tau_{skl}) \frac{\partial u_{si}}{\partial x_i} + u_{si} \frac{\partial \tau_{skl}}{\partial x_i} - \frac{10}{6} p_s \delta_{kl} \frac{\partial u_{si}}{\partial x_i} + \frac{2}{5} \left(\frac{\partial q_{sk}}{\partial x_l} + \frac{\partial q_{sl}}{\partial x_k} + \frac{\partial q_{si}}{\partial x_i} \delta_{kl} \right) \\ & - \frac{2}{3} \frac{\partial q_{si}}{\partial x_i} \delta_{kl} + p_s \frac{\partial u_{sk}}{\partial x_l} + \tau_{slj} \frac{\partial u_{sk}}{\partial x_j} + p_s \frac{\partial u_{sl}}{\partial x_k} + \tau_{skj} \frac{\partial u_{sl}}{\partial x_j} - \frac{e_s}{m_s} (\epsilon_{kab} \tau_{sla} \mathbf{B}_b - \epsilon_{kab} \mathbf{B}_a \tau_{sbl}) \\ & - \frac{2}{3} \tau_{sij} \frac{\partial u_{si}}{\partial x_j} \delta_{kl} = \frac{\delta \tau_{skl}}{\delta t}, \end{aligned}$$

which gives the result:

$$\begin{aligned} & \frac{\partial \tau_{skl}}{\partial t} + u_{si} \frac{\partial \tau_{skl}}{\partial x_i} + \tau_{skl} \frac{\partial u_{si}}{\partial x_i} - \frac{e_s}{m_s} (\epsilon_{kab} \tau_{sla} \mathbf{B}_b - \epsilon_{kab} \mathbf{B}_a \tau_{sbl}) \\ & + \frac{2}{5} \left(\frac{\partial q_{sk}}{\partial x_l} + \frac{\partial q_{sl}}{\partial x_k} - \frac{2}{3} \frac{\partial q_{si}}{\partial x_i} \delta_{kl} \right) + p_s \left(\frac{\partial u_{sk}}{\partial x_l} + \frac{\partial u_{sl}}{\partial x_k} - \frac{2}{3} \frac{\partial u_{si}}{\partial x_i} \delta_{kl} \right) \\ & + \tau_{slj} \frac{\partial u_{sk}}{\partial x_j} + \tau_{skj} \frac{\partial u_{sl}}{\partial x_j} - \frac{2}{3} \tau_{sij} \frac{\partial u_{si}}{\partial x_j} \delta_{kl} = \frac{\delta \tau_{skl}}{\delta t}. \end{aligned} \quad (76)$$

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

$$\begin{aligned} & \frac{\partial q_{sk}}{\partial t} + u_{si} \frac{\partial q_{sk}}{\partial x_i} + q_{si} \frac{\partial u_{sk}}{\partial x_i} + q_{sk} \frac{\partial u_{si}}{\partial x_i} + Q_{skij} \frac{\partial u_{sj}}{\partial x_i} + \frac{\partial \mu_{sik}}{\partial x_i} \\ & + \left[\frac{\partial u_{sl}}{\partial t} + u_{sl} \frac{\partial u_{sl}}{\partial x_i} - g_l - \frac{e_s}{m_s} (E_l + \epsilon_{lij} u_{si} B_j) \right] \left(\tau_{slk} + \frac{5}{2} p_s \delta_{lk} \right) \\ & - \frac{e_s}{m_s} \epsilon_{kij} q_{si} B_j = \frac{\delta q_{sk}}{\delta t} \end{aligned} \quad (77)$$

where μ_{sik} is the higher order stress tensor given by equation (71). Noting that

$$\frac{\partial \mu_{sik}}{\partial x_i} = \frac{5}{2} \frac{k}{m_s} \left[\frac{\partial (T_s p_s)}{\partial x_k} + \frac{7}{5} \frac{\partial (T_s \tau_{sik})}{\partial x_i} \right], \quad (78)$$

we obtain

$$\begin{aligned} & \frac{\partial q_{sk}}{\partial t} + u_{si} \frac{\partial q_{sk}}{\partial x_i} + q_{si} \frac{\partial u_{sk}}{\partial x_i} + q_{sk} \frac{\partial u_{si}}{\partial x_i} + Q_{skij} \frac{\partial u_{sj}}{\partial x_i} + \frac{5}{2} \frac{k}{m_s} \left[\frac{\partial (T_s p_s)}{\partial x_k} + \frac{7}{5} \frac{\partial (T_s \tau_{sik})}{\partial x_i} \right] \\ & + \left[\frac{\partial u_{sl}}{\partial t} + u_{sl} \frac{\partial u_{sl}}{\partial x_i} - g_l - \frac{e_s}{m_s} (E_l + \epsilon_{lij} u_{si} B_j) \right] \left(\tau_{slk} + \frac{5}{2} p_s \delta_{lk} \right) \\ & - \frac{e_s}{m_s} \epsilon_{kij} q_{si} B_j = \frac{\delta q_{sk}}{\delta t}. \end{aligned} \quad (79)$$

Next, we write

$$Q_{skij} \frac{\partial u_{sj}}{\partial x_i} = \frac{2}{5} (\delta_{ki} q_{sj} + \delta_{kj} q_{si} + \delta_{ij} q_{sk}) \frac{\partial u_{sj}}{\partial x_i} = \frac{2}{5} \left(\frac{\partial u_{sj}}{\partial x_k} q_{sj} + q_{si} \frac{\partial u_{sk}}{\partial x_i} + q_{sk} \frac{\partial u_{si}}{\partial x_i} \right) \quad (80)$$

and note that the momentum equation gives us

$$\frac{\partial u_{sl}}{\partial t} + u_{sj} \frac{\partial u_{sl}}{\partial x_j} - g_l - \frac{e_s}{m_s} (E_l + \epsilon_{lij} u_{si} B_j) = \frac{1}{\rho_s} \left(\frac{\partial M_{sl}}{\partial t} - \frac{\partial p_s}{\partial x_l} - \frac{\partial \tau_{sil}}{\partial x_i} \right). \quad (81)$$

Based on these, the heat flow equation is

$$\begin{aligned} & \frac{\partial q_{sk}}{\partial t} + u_{si} \frac{\partial q_{sk}}{\partial x_i} + \frac{7}{5} q_{si} \frac{\partial u_{sk}}{\partial x_i} + \frac{7}{5} q_{sk} \frac{\partial u_{si}}{\partial x_i} + \frac{2}{5} \frac{\partial u_{sj}}{\partial x_k} q_{sj} + \frac{5}{2} \frac{k p_s}{m_s} \frac{\partial T_s}{\partial x_k} \\ & + \frac{5}{2} \frac{k}{m_s} \left[T_s \frac{\partial p_s}{\partial x_k} + \frac{7}{5} \frac{\partial (T_s \tau_{sik})}{\partial x_i} \right] + \left[\frac{1}{\rho_s} \left(-\frac{\partial p_s}{\partial x_l} - \frac{\partial \tau_{sil}}{\partial x_i} \right) \right] \left(\tau_{slk} + \frac{5}{2} p_s \delta_{lk} \right) \\ & - \frac{e_s}{m_s} \epsilon_{kij} q_{si} B_j = \frac{\delta q_{sk}}{\delta t} - \frac{1}{\rho_s} \frac{\partial M_{sl}}{\partial t} \left(\tau_{lk} + \frac{5}{2} p_s \delta_{lk} \right), \end{aligned}$$

which, after some manipulation, gives us the result

$$\begin{aligned}
& \frac{\partial q_{sk}}{\partial t} + u_{si} \frac{\partial q_{sk}}{\partial x_i} + \frac{7}{5} q_{si} \frac{\partial u_{sk}}{\partial x_i} + \frac{7}{5} q_{sk} \frac{\partial u_{si}}{\partial x_i} + \frac{2}{5} \frac{\partial u_{sj}}{\partial x_k} q_{sj} + \frac{5}{2} \frac{k p_s}{m_s} \frac{\partial T_s}{\partial x_k} \\
& + \frac{1}{\rho_s} \frac{\partial \tau_{sil}}{\partial x_i} (p_s \delta_{kl} - \tau_{slk}) + \left(\frac{7}{2} \frac{k}{m_s} \frac{\partial T_s}{\partial x_l} - \frac{1}{\rho_s} \frac{\partial p_s}{\partial x_l} \right) \tau_{slk} \\
& - \frac{e_s}{m_s} \epsilon_{kij} q_{si} B_j = \frac{\delta q_{sk}}{\delta t} - \frac{1}{\rho_s} \frac{\partial M_{sl}}{\partial t} \left(\tau_{lk} + \frac{5}{2} p_s \delta_{lk} \right). \tag{82}
\end{aligned}$$

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:

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

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

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

$$\frac{\delta F}{\delta t} = -\frac{F - F_0}{\tau_0} = \frac{F_0}{\tau_0} \left[\frac{\rho}{2p^2} \tau_{ij} c_i c_j + \frac{\rho^2}{p^3} \left(\frac{c^2}{5} - \frac{p}{\rho} \right) q_i c_i \right], \tag{85}$$

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 τ_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 τ_0 . Inspecting equations (76) and (82) then yields:

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{3}{2} p \right) + u_i \frac{\partial}{\partial x_i} \left(\frac{3}{2} p \right) + \frac{5}{2} p \frac{\partial u_i}{\partial x_i} &= \frac{\partial}{\partial x_i} \left(\kappa \frac{\partial T}{\partial x_i} \right) \\ + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \frac{\partial u_i}{\partial x_j}. \end{aligned} \quad (94)$$

These equations agree with the classical equations of motion for a Newtonian fluid. It should be noted that the equations are only valid when τ_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

$$Re = \frac{LU}{\nu} \quad (95)$$

where L is the length scale of interest, U is the typical flow speed and

$$\nu = \frac{\mu}{\rho} \quad (96)$$

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

$$Pe = \frac{LU}{\alpha} \quad (97)$$

where the thermal diffusivity is

$$\alpha = \frac{\kappa}{\rho c_p} \quad (98)$$

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

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

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

$$\begin{aligned} \sum_n \frac{D_n \mathbf{u}_n}{Dt} &= \sum_n \rho_n \frac{\partial \mathbf{u}_n}{\partial t} + \sum_n \rho_n (\mathbf{u}_n \cdot \nabla) \mathbf{u}_n \\ &= \sum_n \left[\frac{\partial}{\partial t} (\rho_n \mathbf{u}_n) - \mathbf{u}_n \frac{\partial \rho_n}{\partial t} \right] + \sum_n \rho_n (\mathbf{u}_n \cdot \nabla) \mathbf{u}_n \\ &= \frac{\partial}{\partial t} (\rho \mathbf{u}) + \sum_n \mathbf{u}_n \nabla \cdot (\rho_n \mathbf{u}_n) + \sum_n \rho_n (\mathbf{u}_n \cdot \nabla) \mathbf{u}_n \\ &= \frac{\partial}{\partial t} (\rho \mathbf{u}) + \sum_n \nabla \cdot (\rho_n \mathbf{u}_n \mathbf{u}_n) \end{aligned} \quad (100)$$

where we used the center of mass velocity

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

and the continuity equation

$$\frac{\partial \rho_n}{\partial t} + \nabla \cdot (\rho_n \mathbf{u}_n) = 0. \quad (102)$$

In order to write the sum over the pressure tensor term, we write the pressure tensor as

$$\mathbf{P}_s = \mathbf{P}_s^* - \rho_s \mathbf{w}_s \mathbf{w}_s \quad (103)$$

where we used subscript s instead of n to retain generality at this point. Here $\mathbf{w}_s = \mathbf{u}_s - \mathbf{u}$ is the diffusion velocity of species s and the thermal velocity with respect to center of mass flow is $\mathbf{c}_s^* = \mathbf{v}_s - \mathbf{u}$ so that $\mathbf{c}_s = \mathbf{v}_s - \mathbf{u}_s = \mathbf{c}_s^* - \mathbf{w}_s$. Therefore,

$$\begin{aligned} \sum_n \nabla \cdot \mathbf{P}_n &= \nabla \cdot \left[\sum_n \mathbf{P}_n^* - \sum_n \rho_n (\mathbf{u}_n - \mathbf{u})(\mathbf{u}_n - \mathbf{u}) \right] \\ &= \nabla \cdot \mathbf{P} - \sum_n \nabla \cdot (\rho_n \mathbf{u}_n \mathbf{u}_n) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}). \end{aligned} \quad (104)$$

With these expressions, the neutral momentum equation is

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot \mathbf{P} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) - \rho \mathbf{g} = \sum_n \sum_t \rho_n \nu_{nt} (\mathbf{u}_t - \mathbf{u}_n) \quad (105)$$

Using the equation of mass continuity yields

$$\rho \frac{D\mathbf{u}}{Dt} + \nabla \cdot \mathbf{P} - \rho \mathbf{g} = \sum_n \sum_t \rho_n \nu_{nt} (\mathbf{u}_t - \mathbf{u}_n) = - \sum_n \sum_t \rho_t \nu_{tn} (\mathbf{u}_n - \mathbf{u}_t) \quad (106)$$

where $\mathbf{P} = \sum_n \mathbf{P}_n^*$ and $\rho_n \nu_{nt} = \rho_t \nu_{tn}$.

We approximate the collision term by assuming that the charged particle momentum equation is given by

$$-\frac{e_t}{m_t} (\mathbf{E} + \mathbf{u}_t \times \mathbf{B}) = \sum_n \rho_t \nu_{tn} (\mathbf{u}_n - \mathbf{u}_t) \quad (107)$$

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

$$\mathbf{u}_E = \frac{\mathbf{E} \times \mathbf{B}}{B^2} \quad (108)$$

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):

$$\rho \frac{D\mathbf{u}}{Dt} + \nabla \cdot \mathbf{P} - \rho \mathbf{g} = \sum_t n_t e_t (\mathbf{E} + \mathbf{u}_t \times \mathbf{B}) = \left(\sum_i n_i e_i \mathbf{u}_i - n_e e \mathbf{u}_e \right) \times \mathbf{B}. \quad (109)$$

Thus, the neutral bulk flow momentum equation is

$$\rho \frac{D\mathbf{u}}{Dt} + \nabla \cdot \mathbf{P} - \rho \mathbf{g} - \mathbf{j} \times \mathbf{B} = 0 \quad (110)$$

where the current density is

$$\mathbf{j} = \sum_i n_i e_i \mathbf{u}_i - n_e e \mathbf{u}_e \quad (111)$$

and $\mathbf{j} \times \mathbf{B}$ 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

$$\frac{dn_i}{dt} = q_i - \alpha n_i n_e \quad (112)$$

where n_i is the number density of ion i , q_i is the production rate, α 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

$$n_e = \sqrt{\frac{q_i}{\alpha}}. \quad (113)$$

For example, on Venus q_i is the photoionization rate of CO_2 and α is the rate coefficient for dissociative recombination of O_2^+ .

We shall assume plane parallel geometry and obtain the production rate q_ν at altitude z and cosine of the solar zenith angle $\mu = \cos \chi$ as

$$q_\nu(z, \mu) dz = \mu \frac{dI_\nu}{h\nu} = \sum_s \sigma_{s\nu} n_s(z) \frac{I_\nu}{h\nu} dz \quad (114)$$

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_ν is the intensity of radiation at (z, μ) . For a single parent species, the production rate is

$$q_\nu(z, \mu) = \sigma_\nu n(z) F_{\infty\nu} \exp \left[- \int_z^\infty \frac{n(z') \sigma_\nu dz'}{\mu'} \right] \quad (115)$$

where $F_{\infty\nu}$ is the solar photon flux ($m^{-2} s^{-1}$) above the atmosphere. Note that μ depends on z along the line of sight according to (e.g., Rees, 1989):

$$\mu' = \sqrt{1 - \left(\frac{R+z}{R+z'} \right)^2 \sin^2 \chi} \quad (116)$$

where μ applies at z . This means that $\mu' \approx \mu$ when $\chi \lesssim 75^\circ$, which we shall assume hereafter.

We assume an isothermal atmosphere:

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

and write

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

or

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

If we write

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

the derivative of the production rate is

$$\frac{\partial q_\nu}{\partial z} = \sigma_\nu n(z_0) F_{\infty\nu} \frac{\partial A}{\partial z} \left\{ \exp\left[-\frac{\sigma_\nu n(z_0) H}{\mu} A(z)\right] \right. \quad (121)$$

$$\left. -A(z) \frac{\sigma_\nu n(z_0) H}{\mu} \exp\left[-\frac{\sigma_\nu n(z_0) H}{\mu} A(z)\right] \right\}. \quad (122)$$

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

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

Given that the vertical optical depth is

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

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

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

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

$$n_e^{max} = \left(\frac{F_{\infty\nu}}{\alpha e H}\right)^{1/2} \mu^{1/2}, \quad (126)$$

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

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

where

$$q_{\nu M} = \frac{F_{\infty \nu}}{eH} \quad (128)$$

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

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

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

$$\begin{aligned} & \rho_s \frac{D_s \mathbf{u}_s}{Dt} + \nabla \mathbf{P}_s - n_s e_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) - \rho_s (\mathbf{g} - 2\boldsymbol{\Omega} \times \mathbf{u}_s - \boldsymbol{\Omega} \times \boldsymbol{\Omega} \times \mathbf{r}) \\ & = \sum_t \rho_s \nu_{st} (\mathbf{u}_t - \mathbf{u}_s) + \sum_t \nu_{st} \frac{z_{st} \mu_{st}}{kT_{st}} \left(\mathbf{q}_s - \frac{\rho_s}{\rho_t} \mathbf{q}_t \right) \end{aligned} \quad (130)$$

where $\boldsymbol{\Omega}$ 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

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

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

$$\mathbf{u}_{\perp s} = \frac{\mathbf{E} \times \mathbf{B}}{B^2}, \quad (132)$$

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:

$$\frac{e_i}{m_i} (\mathbf{E}_{\perp} + \mathbf{u}_i \times \mathbf{B}) = \sum_t \nu_{in} (\mathbf{u}_i - \mathbf{u}_n) = \nu_i (\mathbf{u}_i - \mathbf{u}_n) \quad (133)$$

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 $\mathbf{u}_i = \mathbf{u}'_i + \mathbf{u}_n$, which leads to

$$\frac{e_i}{m_i \nu_i} \mathbf{E}'_{\perp} + \frac{\omega_i}{\nu_i} \mathbf{u}'_i \times \mathbf{b} = \mathbf{u}'_i \quad (134)$$

where $\mathbf{E}'_{\perp} = \mathbf{E}_{\perp} + \mathbf{u}_n \times \mathbf{B}$ is the electric field in the frame moving with the neutrals, ω_i is the ion gyrofrequency and \mathbf{b} is the magnetic field unit vector. Taking the cross product with \mathbf{b} on the left side and a re-organizing gives

$$\mathbf{u}'_i \times \mathbf{b} = -\frac{e_i}{m_i \nu_i} \mathbf{b} \times \mathbf{E}'_{\perp} - \frac{\omega_i}{\nu_i} \mathbf{u}'_{i\perp}, \quad (135)$$

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

$$\begin{aligned} \mathbf{u}'_{i\perp} \left(1 + \frac{\omega_i^2}{\nu_i^2}\right) &= \frac{e_i}{m_i} \left(\frac{\mathbf{E}'_{\perp}}{\nu_i} - \frac{\omega_i}{\nu_i^2} \mathbf{b} \times \mathbf{E}'_{\perp}\right) \\ \rightarrow \mathbf{u}'_{i\perp} &= \frac{e_i}{m_i \nu_i} \left(\frac{\nu_i^2}{\nu_i^2 + \omega_i^2} \mathbf{E}'_{\perp} + \frac{\nu_i \omega_i}{\nu_i^2 + \omega_i^2} \mathbf{E}'_{\perp} \times \mathbf{b}\right). \end{aligned} \quad (136)$$

Similar developments yield the perpendicular electron velocity

$$\mathbf{u}'_{e\perp} = -\frac{e}{m_e \nu_e} \left(\frac{\nu_e^2}{\nu_e^2 + \omega_e^2} \mathbf{E}'_{\perp} - \frac{\nu_e \omega_e}{\nu_e^2 + \omega_e^2} \mathbf{E}'_{\perp} \times \mathbf{b}\right) \quad (137)$$

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

The perpendicular current density is defined as

$$\mathbf{j}_{\perp} = \mathbf{j}_{e\perp} + \sum_i \mathbf{j}_{i\perp} = \sum_i n_i e_i \mathbf{u}'_{i\perp} - n_e e \mathbf{u}'_{e\perp} + \left(\sum_i n_i e_i - n_e e\right) \mathbf{u}_{n\perp} \quad (138)$$

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

$$\mathbf{j}_{\perp} = \sigma_P \mathbf{E}'_{\perp} - \sigma_H \mathbf{E}'_{\perp} \times \mathbf{b} \quad (139)$$

where the Pedersen and Hall conductivities are

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

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

where

$$\sigma_s = \frac{n_s e^2}{m_s \nu_s}. \quad (142)$$

We can also write the conductivities as

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

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

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

$$en_e \mathbf{E}_{\parallel} = \sum_t \rho_e \nu_{et} (\mathbf{u}_t - \mathbf{u}_e)_{\parallel}. \quad (145)$$

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

$$\mathbf{u}_{e\parallel} \approx -\frac{e}{m_e \nu'_e} \mathbf{E}_{\parallel}. \quad (146)$$

where we now retain electron-ion collisions i.e.,

$$\nu'_e = \sum_i \nu_{ei} + \sum_n \nu_{en} \quad (147)$$

The current density is

$$\mathbf{j}_{\parallel} \approx -en_e \mathbf{u}_{e\parallel} = \sigma_{\parallel} \mathbf{E}_{\parallel} \quad (148)$$

where

$$\sigma_{\parallel} = \frac{n_e e^2}{m_e \nu'_e}. \quad (149)$$

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

$$\mathbf{j} = \sigma_{\parallel} (\mathbf{E}' \cdot \mathbf{b}) \mathbf{b} + \sigma_P (\mathbf{b} \times \mathbf{E}' \times \mathbf{b}) - \sigma_H (\mathbf{E}' \times \mathbf{b}), \quad (150)$$

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

2.3 Electron transport

Here, we follow the derivation of the suprathermal electron transport equation given by Stamnes and Rees (1983) since this formulation has significant legacy in Earth and solar system planetary science. Gombosi (1998) give a more complete version of the general transport equation for energetic particles. We begin by writing the Boltzmann equation for suprathermal electrons as

$$\frac{\partial F}{\partial t} + v_i \frac{\partial F}{\partial x_i} + \frac{\partial}{\partial v_i} (a_i F) = \eta \quad (151)$$

where F is the phase space distribution function ($m^{-6} s^3$) and the function η captures the impact of elastic and inelastic collisions with ions and neutrals. The latter function does not include Coulomb collisions between suprathermal and thermal electrons that heat the thermal electron population. Instead, we describe this interaction by defining a frictional dissipative force:

$$ma_i = -n_e \frac{L(E)v_i}{v} \quad (152)$$

where the stopping cross section $L(E)$ is a function of the suprathermal electron energy E and n_e is the thermal electron density. Typically, $L(E)$ is given in units of $eV cm^2$ and it can be calculated from (Swartz et al., 1971):

$$L(E) = \frac{3.37 \times 10^{-12}}{n_e^{0.03} E^{0.94}} \left(\frac{E - E_e}{E - 0.53E_e} \right)^{2.36} \quad (153)$$

where $E_e = 8.618 \times 10^{-5} T_e$ is the thermal electron energy in eV. We note that the quantity $n_e L(E)$ has units of $eV m^{-1}$ and describes the deposition of energy per unit distance along the electron path. Therefore $\Lambda_{pe} = E/(n_e L)$ is a measure of the length scale of suprathermal electron energy deposition through Coulomb collisions.

According to the above, the acceleration term in the Boltzmann equation is

$$\begin{aligned} \frac{\partial}{\partial v_i} (a_i F) &= -n_e \frac{\partial}{\partial v_i} \left[L(E) \frac{v_i}{mv} F \right] = -n_e \frac{\partial}{\partial v_i} \left[L(E) \frac{v^2}{m} F \frac{v_i}{v^3} \right] \\ &= -n_e \left\{ \frac{v_i}{v^3} \frac{\partial}{\partial v_i} \left[L(E) \frac{v^2}{m} F \right] - L(E) \frac{v^2}{m} F \frac{\partial}{\partial v_i} \left(\frac{v_i}{v^3} \right) \right\} \\ &= -n_e \frac{v_i}{v^3} \frac{\partial}{\partial E} \left[L(E) \frac{v^2}{m} F \right] \frac{\partial E}{\partial v_i} = -n_e \frac{m}{v} \frac{\partial}{\partial E} \left[L(E) \frac{v^2}{m} F \right] \end{aligned} \quad (154)$$

because

$$\frac{\partial E}{\partial v_i} = mv_i.$$

Therefore, we can multiply the Boltzmann equation by v/m and write it as

$$\frac{v}{m} \frac{\partial F}{\partial t} + \frac{v}{m} v_i \frac{\partial F}{\partial x_i} - n_e \frac{\partial}{\partial E} \left[L(E) \frac{v^2}{m} F \right] = \Pi \quad (155)$$

where $\Pi = (v/m)\eta$.

We now define the suprathermal electron intensity ($m^{-2} s^{-1} sr^{-1} J^{-1}$) as

$$I(\mathbf{r}, E, \Omega, t) = \frac{v^2}{m} F(t, \mathbf{r}, \mathbf{v}) \quad (156)$$

where $\Omega = \mathbf{v}/v$, which for steady state conditions $\partial F/\partial t = 0$ yields the transport equation

$$\frac{v_i}{v} \frac{\partial I}{\partial x_i} - n_e \frac{\partial}{\partial E} [L(E)I] = \Pi. \quad (157)$$

For electrons drifting parallel to the magnetic field, we have $v_i/v = v_{\parallel}/v = \cos \alpha$ where α is the pitch angle, defined by

$$\tan \alpha = \frac{v_{\perp}}{v_{\parallel}} \quad (158)$$

where v_{\perp} is the electron velocity perpendicular to the magnetic field. Thus, the electron transport equation can be written as

$$\mu \frac{dI}{dz} = n_e \frac{\partial}{\partial E} [L(E)I] + \Pi \quad (159)$$

where $\mu = \cos \alpha$.

2.3.1 Elastic and inelastic interactions

The term Π encapsulates most of the important physics in electron transport, including elastic scattering, excitation of discrete atomic and molecular transitions, molecular dissociation and secondary ionization. The general rate expression for these processes under azimuthal symmetry is

$$\Pi = 2\pi \sum_s \sum_j \int_E dE_{1,2} \int_{-1}^1 d\mu_{1,2} R_{s,j}(E_1, E_2; \mu_1, \mu_2) I(z, E_{1,2}, \mu_{1,2}) \quad (160)$$

where s denotes other species, j denotes different processes associated with interactions involving species s (say, different transitions for excited states), $R_{s,j}$ is the redistribution function that maps electrons with initial energy and direction E_1 and μ_1 to final energy and direction E_2 and μ_2 .

The redistribution function for the loss of electrons from the initial beam $I(z, E, \mu)$ due to elastic scattering can be written formally as

$$R_s(E, E'; \mu, \mu') = \frac{P_{el}(E; \mu, \mu')}{4\pi} n_s(z) \sigma_{es}(E) \delta(E' - E) \quad (161)$$

where the elastic scattering phase function $P_{el}(E; \mu, \mu')$ captures the change in direction, $n_s(z)$ is the density of the collision partner s , $\sigma_{es}(E)$ is the elastic scattering cross section and $\delta(E' - E)$ is the Kronecker delta function. The energy mapping is a delta function because there is effectively no energy change in elastic scattering. The loss term due to elastic scattering is

$$\Pi_{el}^L = -2\pi \sum_s \int dE' \int_{-1}^1 d\mu' R_s(E, E'; \mu, \mu') I(z, E, \mu) \quad (162)$$

where primed variables refer to the final state of the lost photoelectron. Given that E and μ are considered fixed for our beam of electrons and the integrals are over the primed quantities, we may write, by using the delta function for energy mapping:

$$\Pi_{el}^L = - \sum_s n_s(z) \sigma_{es}(E) I(z, E, \mu) \frac{1}{2} \int_{-1}^1 d\mu' P_{el}(E; \mu, \mu') \quad (163)$$

where we recognize the standard normalization of the phase function

$$\frac{1}{2} \int_{-1}^1 d\mu' P_{el}(E; \mu, \mu') = 1, \quad (164)$$

which gives us

$$\Pi_{el}^L = - \sum_s n_s(z) \sigma_{es}(E) I(z, E, \mu) \quad (165)$$

as the final, intuitive expression for the loss of electrons from our beam due to elastic scattering. Correspondingly, elastic scattering of electrons into our beam (production) from all other directions is

$$\Pi_{el}^P = \sum_s n_s(z) \sigma_{es}(E) \frac{1}{2} \int_{-1}^1 d\mu' P_{el}(E; \mu', \mu) I(z, E, \mu') \quad (166)$$

where the primed quantities denote the initial electron direction and therefore, $I(z, E, \mu')$ cannot be moved outside of the integral because we wish to evaluate the sum of all electrons scattered to μ from all directions μ' . Note that in our convention, primed quantities always denote electrons that are not a part of the beam at fixed (E, μ) .

Next, we consider loss of electrons with (E, μ) to (E', μ') due to the excitation of discrete states with excitation energy W_j . Energy conservation requires that $E' = E - W_j$ and we can write the redistribution function as

$$R_{sj}(E, E'; \mu, \mu') = \frac{P_j^d(E; \mu, \mu')}{4\pi} n_s(z) \sigma_{sj}^d(E) \delta(E - E' - W_j) \quad (167)$$

where the phase function P_j^d again captures the change in direction and $\sigma_{sj}^d(E)$ is the excitation cross section for species s and transition j . It is easy to show that the loss term due to discrete excitation has the same form as the elastic scattering term:

$$\Pi_d^L = - \sum_s n_s(z) \sigma_{sj}^d(E) I(z, E, \mu). \quad (168)$$

The corresponding production term i.e.,

$$\Pi_d^P = \sum_s \sum_j n_s(z) \sigma_{es}(E + W_j) \frac{1}{2} \int_{-1}^1 d\mu' P_{el}(E + W_j; \mu', \mu) I(z, E + W_j, \mu') \quad (169)$$

represents the mapping of electrons from $(E + W_j, \mu')$ to (E, μ) .

Secondary ionization leads to a number of complications. We will begin by considering the loss of (primary) electrons from our beam with (E, μ) due to secondary ionization. This leads to the production of primary electrons with (E', μ') and the production of a secondary electron with energy E_{sec} . Energy conservation places the constraint

$$E = E' + E_{sec} + I_{pj} \quad (170)$$

where I_{pj} is the threshold energy for ionization path j . Here, we ignore the ion energies, assuming that the excess energy of the photon goes entirely to the secondary electron. Formally, the redistribution function is

$$R_{sj}(E, E'; \mu, \mu') = \frac{P_j^I(E; \mu, \mu')}{4\pi} n_s(z) \sigma_{sj}^I(E, E') \quad (171)$$

where $\sigma_{sj}^I(E, E')$ is the differential cross section for reducing the primary electron energy from E to E' so that the secondary electron energy is $E_{sec} = E - E' - I_{pj}$. Therefore, the loss function is

$$\Pi_I^L = - \sum_s \sum_j n_s(z) I(z, E, \mu) \int_0^{E - I_{pj}} \sigma_{sj}^I(E, E') dE'. \quad (172)$$

In reality, differential cross sections are measured for secondary electron production (see Rees, 1989) i.e., they are given as $\sigma_{sj}^I(E, E_{sec})$. We note that $dE_{sec} = -dE$, with $E_{sec} = 0$ for $E' = E - I_{pj}$ and $E_{sec} = E - I_{pj}$ for $E' = 0$. Thus, the loss function can be written as

$$\Pi_I^L = - \sum_s \sum_j n_s(z) I(z, E, \mu) \int_0^{E - I_{pj}} \sigma_{sj}^I(E, E_{sec}) dE_{sec} \quad (173)$$

where

$$\sigma_{sj}^I(E) = \int_0^{E-I_{pj}} \sigma_{sj}^I(E, E_{sec}) dE_{sec} \quad (174)$$

is the total ionization cross section and the loss function has the same form as elastic scattering and excitation of discrete states above.

Following the same philosophy as above, it is possible to write the expression for the production of electrons with (E, μ) due to secondary ionization by electrons with $(E' = E + E_{sec} + I_{pj}, \mu')$. This expression is

$$\Pi_I^P = \sum_s \sum_j n_s(z) \frac{1}{2} \int_{-1}^1 P_j^I(E'; \mu', \mu) \int_{E-I_{pj}}^{\infty} \sigma_{sj}^I(E', E) I(z, E', \mu') dE' d\mu'. \quad (175)$$

Finally, we also have to consider the production of secondary electrons with energy $E = E_{sec}$ based on secondary ionization by primary electron with E'_p , which is reduced to energy E_p . The redistribution function is

$$R_{sj}(E'_p, E; \mu', \mu_{sec}) = \frac{P_j^{sec}(E; \mu', \mu_{sec})}{4\pi} n_s(z) \sigma_{sj}^I(E'_p, E) \quad (176)$$

where it should be noted that the phase function is to a good approximation isotropic i.e., $P_j^{sec}(E; \mu', \mu_{sec}) = 1$. Therefore, we have

$$\Pi_{sec} = \frac{1}{2} \sum_s \sum_j n_s(z) \int_{-1}^1 \int_{I_{pj}}^{\infty} \sigma_{sj}^I(E', E) I(z, E', \mu') dE' d\mu'. \quad (177)$$

as the production rate of secondary electrons that are added to our beam with (E, μ) . So far, we have not considered molecular dissociation, which has the same mathematical form as ionization although it does not result in the production of secondary electrons. We shall not consider it further here and it is left as an exercise.

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):

$$\rho_s \left[\frac{\partial \mathbf{u}_{\parallel s}}{\partial t} + (\mathbf{u}_s \cdot \nabla \mathbf{u}_s)_{\parallel} \right] + \nabla_{\parallel} p_s - \rho_s \mathbf{g}_{\parallel} - n_s q_s \mathbf{E}_{\parallel} = - \sum_{t \neq s} \rho_s \nu_{st} (\mathbf{u}_s - \mathbf{u}_t)_{\parallel} \quad (178)$$

where ρ_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 ν_{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 (178) with $q_s = 0$ along the radial direction:

$$\rho_s \left(\frac{\partial w_s}{\partial t} + w_s \frac{\partial w_s}{\partial r} \right) + \frac{\partial p_s}{\partial r} + \rho_s g(r) = - \sum_{t \neq s} \rho_s \nu_{st} (w_s - w_t) \quad (179)$$

where w_s is the vertical velocity. We exclude the time derivative and the advection terms on the left-hand side for now. An explicit justification for this is provided in Section 3.4. Thus, we have

$$\frac{\partial p_s}{\partial r} + \rho_s g(r) = - \sum_{t \neq s} \rho_s \nu_{st} (w_s - w_t), \quad (180)$$

which is

$$\frac{\partial p_s}{\partial r} - \frac{\rho_s}{\rho} \frac{\partial p}{\partial r} = - \sum_{t \neq s} \rho_s \nu_{st} (w_s - w_t), \quad (181)$$

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

$$\frac{1}{p_s} \frac{\partial p_s}{\partial r} - \frac{m_s}{m} \frac{\partial \ln p}{\partial r} = - \sum_{t \neq s} \frac{x_t}{D_{st}} (w_s - w_t) \quad (182)$$

where $x_t = n_t/n$ and

$$D_{st} = \frac{x_t k T}{m_s \nu_{st}} \quad (183)$$

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

Using hydrostatic equilibrium, we write equation (182) as

$$\frac{1}{p_s} \frac{\partial p_s}{\partial r} + \frac{1}{H_s} = - \sum_{t \neq s} \frac{x_t}{D_{st}} (w_s - w_t) \quad (184)$$

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

$$w_t = w_K = -K_{zz} \frac{1}{x_s} \frac{\partial x_s}{\partial r} \quad (185)$$

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

$$w_s = w_K - D_s \left(\frac{1}{p_s} \frac{\partial p_s}{\partial r} + \frac{1}{H_s} \right) \quad (186)$$

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

$$\frac{1}{D_s} = \sum_{t \neq s} \frac{x_t}{D_{st}}. \quad (187)$$

Noting that

$$\frac{1}{x_s} \frac{\partial x_s}{\partial r} = \frac{1}{p_s} \frac{\partial p_s}{\partial r} + \frac{1}{H} \quad (188)$$

where H is the pressure scale height, we obtain

$$w_s = -K_{zz} \left(\frac{1}{p_s} \frac{\partial p_s}{\partial r} + \frac{1}{H} \right) - D_s \left(\frac{1}{p_s} \frac{\partial p_s}{\partial r} + \frac{1}{H_s} \right). \quad (189)$$

In steady state (diffusive equilibrium), $w_s = 0$ and we can write equation (189) as

$$\frac{1}{p_s} \frac{\partial p_s}{\partial r} = -(1 + \Lambda_s)^{-1} \left(\frac{1}{H_s} + \frac{\Lambda_s}{H} \right) \quad (190)$$

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

$$p_s(r) = p_s(r_0) \exp \left[- \int_{r_0}^r \frac{dr'}{1 + \Lambda_s} \left(\frac{1}{H_s} + \frac{\Lambda_s}{H} \right) \right]. \quad (191)$$

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 (182) by using equation (188), and it is given by

$$\frac{\partial x_s}{\partial r} + \left(x_s - \frac{\rho_s}{\rho}\right) \frac{\partial \ln p}{\partial r} = - \sum_{t \neq s} x_s x_t \frac{w_s - w_t}{D_{st}}. \quad (192)$$

We can also incorporate eddy and thermal diffusion here by writing

$$(1 + \Lambda_s) \frac{\partial x_s}{\partial r} + \left(x_s - \frac{\rho_s}{\rho}\right) \frac{\partial \ln p}{\partial r} + \frac{\alpha_s x_s}{T} \frac{\partial T}{\partial r} = - \sum_{t \neq s} x_s x_t \frac{w_s - w_t}{D_{st}} \quad (193)$$

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

$$w_s = -D_s \left(\frac{1}{n_s} \frac{\partial n_s}{\partial r} + \frac{1}{H_s} + \frac{1 + \alpha_s}{T} \frac{\partial T}{\partial r} \right) + K_{zz} \left(\frac{1}{n_s} \frac{\partial n_s}{\partial r} + \frac{1}{H} + \frac{1}{T} \frac{\partial T}{\partial r} \right). \quad (194)$$

Equation (183) 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

$$D_{st} = \frac{1.52 \times 10^{18}}{n} \sqrt{\left(\frac{1}{M_s} + \frac{1}{M_t} \right) T} \text{ cm}^2 \text{ s}^{-1}, \quad (195)$$

where n is the total number density of the atmosphere in cm^{-3} 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

$$\nabla_{\parallel} p_i - n_i e \mathbf{E}_{\parallel} - \rho_i \mathbf{g}_{\parallel} = -\rho_i \nu_{ie} (\mathbf{u}_i - \mathbf{u}_e)_{\parallel} - \sum_s \rho_i \nu_{is} (\mathbf{u}_i - \mathbf{u}_s)_{\parallel}, \quad (196)$$

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

$$\mathbf{j}_{\parallel} = \sum_i n_i q_i \mathbf{u}_{i\parallel} - n_e e \mathbf{u}_{e\parallel} \quad (197)$$

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

$$\nabla_\parallel p_i - n_i e \mathbf{E}_\parallel - \rho_i \mathbf{g}_\parallel = -\rho_i \nu_{in} (\mathbf{u}_i - \mathbf{u}_n)_\parallel, \quad (198)$$

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

$$e \mathbf{E}_\parallel = -\frac{1}{n_e} \nabla_\parallel p_e. \quad (199)$$

Substituting this into equation (198) gives:

$$\nabla_\parallel (p_i + p_e) - \rho_i \mathbf{g}_\parallel = -\rho_i \nu_{in} (\mathbf{u}_i - \mathbf{u}_n)_\parallel. \quad (200)$$

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

$$\frac{\partial}{\partial r} (p_i + p_e) + \rho_i g = 0, \quad (201)$$

which we can write as

$$\frac{1}{n_i k T_p} \frac{\partial}{\partial r} (n_i k T_p) + \frac{m_i g}{2 k T_p} = 0 \quad (202)$$

where the plasma temperature is

$$T_p = \frac{T_i + T_e}{2} \quad (203)$$

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

$$n_i(r) = n_i(r_0) \exp\left(-\frac{r-r_0}{H_p}\right) \quad (204)$$

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

$$H_p = \frac{2kT_p}{m_i g}, \quad (205)$$

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 $T_e = T_i = T_n$.

3.3 Major ion diffusion with magnetic field

We make the same assumptions as in the last section, up to equation (200):

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

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

$$k_i = \frac{q_i B}{m_i \nu_{in}} \gg 1, \quad (206)$$

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

$$(\mathbf{u}_i - \mathbf{u}_n)_{\parallel} = -2D_i \left[\frac{1}{n_i} \nabla_{\parallel} n_i + \frac{1}{T_p} \nabla_{\parallel} T_p - \frac{m_i \mathbf{g}_{\parallel}}{2kT_p} \right] \quad (207)$$

where T_p is the plasma temperature and the diffusion coefficient is

$$D_i = \frac{kT_p}{m_i \nu_{in}}. \quad (208)$$

Cast in magnetic dipole coordinates, the gradient operator is (Swisdak, 2006, and Section 6.1)

$$\nabla f = \mathbf{q} \frac{\delta}{r^3} \frac{\partial f}{\partial q} + \mathbf{p} \frac{\delta}{\sin^3 \theta} \frac{\partial f}{\partial p} + \mathbf{e}_{\phi} \frac{1}{r \sin \theta} \frac{\partial f}{\partial \phi}, \quad (209)$$

which means that

$$\nabla_{\parallel} f = \mathbf{q} \frac{\delta}{r^3} \frac{\partial f}{\partial q}. \quad (210)$$

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

$$\mathbf{q} = - \left(\frac{2 \cos \theta}{\delta} \mathbf{e}_r + \frac{\sin \theta}{\delta} \mathbf{e}_{\theta} \right) \quad (211)$$

With this, the major ion drift equation is

$$(u_i - u_{nq}) \mathbf{q} = -2D_i \left[\frac{1}{n_i} \frac{\delta}{r^3} \frac{\partial n_i}{\partial q} + \frac{1}{T_p} \frac{\delta}{r^3} \frac{\partial T_p}{\partial q} - \frac{m_i \mathbf{g}_q}{2kT_p} \right] \mathbf{q}. \quad (212)$$

We extract the radial component of this equation by taking the dot product with \mathbf{e}_r , noting that

$$\mathbf{q} \cdot \mathbf{e}_r = -\frac{2 \cos \theta}{\delta} \quad (213)$$

and thus we have

$$u_{ir} + u_{nq} \frac{2 \cos \theta}{\delta} = 2D_i \left[\frac{1}{n_i} \frac{\delta}{r^3} \frac{\partial n_i}{\partial q} + \frac{1}{T_p} \frac{\delta}{r^3} \frac{\partial T_p}{\partial q} - \frac{m_i g_q}{2kT_p} \right] \frac{2 \cos \theta}{\delta} \quad (214)$$

where

$$u_{ir} = -\frac{2 \cos \theta}{\delta} u_i \quad (215)$$

is the radial component of the ion velocity.

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

$$\frac{\partial}{\partial q} = \frac{\partial}{\partial r} \frac{\partial r}{\partial q} = -\frac{2r^3 \cos \theta}{\delta^2} \frac{\partial}{\partial r}. \quad (216)$$

Also, gravity along the magnetic field line is

$$g_q = -g \mathbf{e}_r \cdot \mathbf{q} = \frac{2g \cos \theta}{\delta}. \quad (217)$$

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

$$\mathbf{u}_n = u_n \mathbf{e}_\theta \rightarrow u_{nq} = \mathbf{u}_n \cdot \mathbf{q} = -\frac{\sin \theta}{\delta} u_n. \quad (218)$$

Now, the expression for the ion drift becomes

$$u_{ir} - \frac{2 \cos \theta \sin \theta}{\delta} u_n = -2D_i \frac{4 \cos^2 \theta}{\delta^2} \left[\frac{1}{n_i} \frac{\partial n_i}{\partial r} + \frac{1}{T_p} \frac{\partial T_p}{\partial r} + \frac{m_i g}{2kT_p} \right]. \quad (219)$$

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

$$\sin I = \mathbf{q} \times \mathbf{e}_\theta = q_r = -\frac{2 \cos \theta}{\delta} \quad (220)$$

$$\cos I = \mathbf{q} \cdot \mathbf{e}_\theta = q_\theta = -\frac{\sin \theta}{\delta} \quad (221)$$

and with these definitions,

$$u_{ir} = u_n \cos I \sin I - 2D_i \sin^2 I \left[\frac{1}{n_i} \frac{\partial n_i}{\partial r} + \frac{1}{T_p} \frac{\partial T_p}{\partial r} + \frac{m_i g}{2kT_p} \right] \quad (222)$$

is a basic form of the ion drift equation.

It should be noted that equation (222) 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

$$\mathbf{v}_{id} = \frac{\mathbf{E} \times \mathbf{B}}{B}. \quad (223)$$

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

$$u_{idr} = \frac{E}{B} \cos I, \quad (224)$$

leading to an equatorial F region drift equation given by

$$u_{ir} = \frac{E}{B} \cos I + u_n \cos I \sin I - 2D_i \sin^2 I \left[\frac{1}{n_i} \frac{\partial n_i}{\partial r} + \frac{1}{T_p} \frac{\partial T_p}{\partial r} + \frac{m_i g}{2kT_p} \right]. \quad (225)$$

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.

3.4 Generalized diffusion (Week 13)

3.4.1 The diffusion approximation

The purpose of this section is to examine the nature of the diffusion approximation and related equations above in some more detail and derive an expression that can be solved to obtain the different species velocities. We start from the continuity equation (178) in the radial direction for an unmagnetized atmosphere, for convenience with $K_{zz} = 0$:

$$\rho_s \left(\frac{\partial w_s}{\partial t} + w_s \frac{\partial w_s}{\partial r} \right) + \frac{\partial p_s}{\partial r} - \rho_s g(r) - n_s e_s E = - \sum_{t \neq s} \rho_s \nu_{st} (w_s - w_t). \quad (226)$$

We now use the so-called diffusion approximation i.e., write the species velocities as $w_s = w + w'_s$ where the center of mass (bulk flow) velocity is

$$w = \frac{1}{\rho} \sum_k \rho_k w_k \quad (227)$$

where the sum is over all species k . The definition of bulk flow velocity means that

$$\sum_k \rho_k w'_k = 0. \quad (228)$$

Substituting the expression for w_s to the momentum equation yields

$$\begin{aligned} \rho_s \left[\frac{\partial}{\partial t} (w + w'_s) + w \frac{\partial w}{\partial r} + w'_s \frac{\partial w}{\partial r} + w \frac{\partial w'_s}{\partial r} \right] + \frac{\partial p_s}{\partial r} \\ - \rho_s g(r) - n_s e_s E = - \sum_{t \neq s} \rho_s \nu_{st} (w'_s - w'_t). \end{aligned} \quad (229)$$

where we excluded terms second order in w'_s . Note that the momentum equation for bulk flow is

$$\rho \left(\frac{\partial w}{\partial t} + w \frac{\partial w}{\partial r} \right) + \frac{\partial p}{\partial r} - \rho g(r) = 0 \quad (230)$$

and thus we can write the diffusion equation as

$$-\frac{\rho_s}{\rho} \frac{\partial p}{\partial r} + \frac{\partial p_s}{\partial r} + \rho_s \left(w \frac{\partial w'_s}{\partial r} + w'_s \frac{\partial w}{\partial r} \right) - n_s e_s E = - \sum_{t \neq s} \rho_s \nu_{st} (w'_s - w'_t). \quad (231)$$

Writing the species pressure gradient in terms of x_s and p gives:

$$\frac{\partial x_s}{\partial r} + \left(x_s - \frac{\rho_s}{\rho} \right) \frac{\partial (\ln p)}{\partial r} - \frac{n_s e_s E}{p} + \frac{\rho_s}{p} \left(w \frac{\partial w'_s}{\partial r} + w'_s \frac{\partial w}{\partial r} \right) = - \sum_{t \neq s} x_s x_t \frac{w'_s - w'_t}{D_{st}}. \quad (232)$$

Now, we can ignore the species advection terms as long as

$$\left| \frac{D_s n_s}{H} \left(1 - \frac{m_s}{m} \right) \right| \gg \left| \frac{D_s n_s}{H} \frac{m_s}{kT} w'_s w \right| \quad (233)$$

where we multiplied the diffusion equation by nD_s and used the pressure scale height H as the vertical scale length.

For example, we consider a situation for which $m_s > m$. Then the above condition is

$$\frac{m_s}{m} - 1 \gg \frac{m_s}{kT} w'_s w \gg \frac{w w'_s}{c_{ss}^2} \quad (234)$$

where $c_{ss}^2 = kT/m_s$. If $w = 0$ (static atmosphere), this condition is always satisfied for $m_s > m$. The reverse condition for $m_s < m$ is also always satisfied. Now, let us assume that $w = c_{ss}$. In this case,

$$\frac{m_s}{m} - 1 \gg \frac{w'_s}{c_{ss}}.$$

This means that diffusion conditions is only violated if the perturbation velocity $w'_s > c_{ss} = w$, a situation that is obviously impossible for a heavier minor species. Following the same logic, we can set $w = c_s$ for bulk flow and note that the condition is only violated if $w'_s > c_s$, another impossible situation. We conclude that the standard diffusion equation

$$\frac{\partial x_s}{\partial r} + \left(x_s - \frac{\rho_s}{\rho} \right) \frac{\partial (\ln p)}{\partial r} - \frac{n_s e_s E}{p} = - \sum_{t \neq s} x_s x_t \frac{w'_s - w'_t}{D_{st}} \quad (235)$$

is valid for a wide variety of situations, including non-zero bulk flow.

3.4.2 Solving for the diffusion velocities

We denote the left-hand side of equation (235) as d_s so that we can write

$$d_s = - \sum_{t \neq s}^{N-1} x_s x_t \frac{w'_s - w'_t}{D_{st}} - \frac{x_s x_N}{D_{sN}} (w'_s - w'_N) \quad (236)$$

where N is pre-selected as the ‘remainder’ species. Given the condition of zero diffusive mass flux, we have

$$w'_N = - \frac{1}{\rho_N} \sum_k^{N-1} \rho_k w'_k = - \frac{1}{\rho_N} \left(\rho_s w'_s - \sum_{t \neq s}^{N-1} \rho_t w'_t \right) \quad (237)$$

which we can substitute to the equation above:

$$d_s = - \left[\sum_{j \neq s}^{N-1} \frac{x_s x_j}{D_{sj}} + \frac{x_s x_N}{D_{sN}} \left(1 + \frac{m_s x_s}{m_N x_N} \right) \right] w'_s + \sum_{t \neq s}^{N-1} \left[\left(\frac{x_s x_t}{D_{st}} - \frac{m_t x_s x_t}{m_N D_{sN}} \right) \right] w'_t \quad (238)$$

or

$$d_s = M_{st} w'_t \quad (239)$$

$$M_{st} = - \left[\sum_{j \neq s}^{N-1} \frac{x_s x_j}{D_{sj}} + \frac{x_s x_N}{D_{sN}} \left(1 + \frac{m_s x_s}{m_N x_N} \right) \right] \delta_{st} \quad (239)$$

$$+ \sum_{t \neq s}^{N-1} \left[\left(\frac{x_s x_t}{D_{st}} - \frac{m_t x_s x_t}{m_N D_{sN}} \right) \right] (1 - \delta_{st}), \quad (240)$$

which we can invert to solve for w'_s .

3.5 Diffusion-limited escape (Week 13)

Here, we consider some interesting limits of the generalized diffusion equation that are used to describe the escape of minor species from planetary atmospheres. Consider a situation in which a light minor species is escaping in the background of a stationary heavier major species. In this case, $m_s < m$, $w = 0$ and we set $w'_t \sim 0$. In this case, we can write the flux of species s in hydrostatic equilibrium as

$$f_s = n_s w_s = \frac{n_s D_s}{H} \left(1 - \frac{m_s}{m} \right) - n (D_s + K_{zz}) \frac{\partial x_s}{\partial r} \quad (241)$$

where the diffusion-limited flux is defined as (Hunten, 1973)

$$f_L = \frac{n_s D_s}{H} \left(1 - \frac{m_s}{m} \right). \quad (242)$$

Thus, we have an expression for the gradient of the volume mixing ratio:

$$\frac{\partial x_s}{\partial r} = \frac{1}{n(D_s + K_{zz})} (f_L - f_s). \quad (243)$$

In other words, if $f_s < f_L$, the mixing ratio gradient is positive, as expected for a lighter minor species. When $f_s = f_L$, the mixing ratio of the species is constant with altitude and the upward flux reaches a maximum. For $f_s > f_L$, the mixing ratio gradient becomes negative and the upward flux decreases until it settles back to $f_s = f_L$. Note that the diffusion limit is an upper limit for the escape of the light minor species from an atmosphere dominated by stationary heavy species.

3.6 Cross-over mass (Week 14)

The concept of the cross-over mass was developed to describe the behavior of a heavier minor species in an atmosphere where the dominant lighter species is undergoing rapid escape such as hydrodynamic escape (although the latter is not required). In this case, we consider a 2-species system with $m_2 < m_1$ and non-zero bulk flow enabled originally by the escape of species 1. At altitudes of interest, we assume that $K_{zz} = 0$. If the atmosphere remains close to hydrostatic equilibrium (layers below the sonic point), we can write the diffusion equation as

$$\begin{aligned} \frac{1}{x_2} \frac{\partial x_2}{\partial r} &= \frac{mg}{kT} - \frac{m_2 g}{kT} + \frac{1}{nD_{12}} \left(f_1 - \frac{x_1}{x_2} f_2 \right) \\ &= \frac{1}{nD_{12}} \left(f_1 - \frac{x_1}{x_2} f_2 \right) - (m_2 - m_1) \frac{x_1 g}{kT} \end{aligned} \quad (244)$$

where $m = x_1 m_1 + x_2 m_2$, $x_2 - 1 = -x_1$ and $T = T_1 = T_2$. We start by considering a situation in which the mixing ratio gradient for species 2 vanishes. This gives

$$f_2 = \frac{x_2}{x_1} f_1 \left[1 - \frac{nD_{12} x_1 g}{kT f_1} \right]. \quad (245)$$

In other words, if the mass of the heavier species is

$$m_2 < m_c = m_1 + \frac{kT f_1}{nD_{12} x_1 g}, \quad (246)$$

where m_c is the cross-over mass (Hunten et al., 1987), $f_2 > 0$ and the heavier species undergoes escape due to drag forces from the escaping lighter species 1. In this case, the escape flux of species 2 is given by

$$f_2 = \frac{x_2}{x_1} f_1 \left(\frac{m_c - m_2}{m_c - m_1} \right) \quad (247)$$

If, on the other hand, $m_2 > m_c$, $f_2 < 0$ and the mixing ratio begins to decrease with altitude, as expected for a heavier minor species in diffusive equilibrium. The limiting case is $m_2 = m_c$ for which $f_2 = 0$.

4 Energy balance

4.1 Exospheric temperature (Week 1)

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

$$F_E = \frac{1}{4}\epsilon F_\infty \quad (248)$$

where ϵ 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 reradiated to space in the infrared. Then, the outgoing flux at the mesopause is equal to the downward heat flux by conduction:

$$F_E = \kappa \frac{dT}{dr} \quad (249)$$

where κ is the coefficient of heat conduction. This coefficient is given by

$$\kappa = AT^s \quad (250)$$

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

$$\kappa = \frac{2k}{\sigma} \sqrt{\frac{k}{\pi m}} T^{1/2} \quad (251)$$

where k is the Boltzmann constant, σ 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

$$dr = -H \frac{dp}{p} \quad (252)$$

and thus equation (249) is

$$F_E \frac{TH_0}{T_0} \frac{dp}{p} = -AT^s dT \quad (253)$$

where we also assumed that

$$H = \frac{T}{T_0} H_0 \quad (254)$$

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:

$$F_E \int_{p_0}^p \frac{dp'}{p'} = -\frac{AT_0}{H_0} \int_{T_0}^{T_\infty} T^{s-1} dT \quad (255)$$

where we labeled the exospheric temperature as T_∞ . Thus, we obtain

$$F_E \ln \left(\frac{p}{p_0} \right) = -\frac{AT_0}{sH_0} (T_\infty^s - T_0^s) \quad (256)$$

and finally, the result is

$$T_\infty^s = T_0^s + \frac{s\epsilon F_{\text{EUV}} H_0}{4AT_0} \ln \left(\frac{p_0}{p} \right). \quad (257)$$

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

$$\frac{p_0}{p} \approx \frac{\tau_0}{\langle \mu \rangle} \quad (258)$$

where τ_0 is the optical depth (for global average) at the mesopause to radiation in the $\sim 20\text{--}100$ nm band and the cosine of the solar zenith angle $\langle \mu \rangle = 1/2$.

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)

$$\frac{\partial}{\partial t} (\rho c_v T) + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho c_v T w) = \rho Q_R - p \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 w) + \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \kappa \frac{\partial}{\partial r} \right) + \Phi_V \quad (259)$$

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

$$\frac{\partial}{\partial r} \left[F_\rho \left(c_p T + \frac{1}{2} w^2 + \phi_g \right) \right] = \rho r^2 Q_R + \frac{\partial}{\partial r} \left(r^2 \kappa \frac{\partial}{\partial r} \right) + r^2 \Phi_V \quad (260)$$

where the radial mass flux constant $F_\rho = \rho w r^2$ and ϕ_g is the gravitational potential.

We assume that conduction is negligible ($\kappa = 0$) and ignore the viscous dissipation functional. Integrating equation (260) from r_0 to infinity then leads to

$$-F_\rho \left(c_p T_0 - \frac{1}{2} w^2 + \phi_{g0} \right) = \epsilon F_E r_E^2 \quad (261)$$

where we assumed that $T \rightarrow 0$ at infinity, $w \rightarrow 0$ at r_0 and ϕ_g vanishes at infinity. Furthermore, we can define the product

$$\epsilon F_E r_E^2 = \int_{r_0}^{\infty} r^2 \alpha(r) q(r) dr \quad (262)$$

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, ϵ is the column-averaged heating efficiency, α is the altitude-dependent heating efficiency and q is the altitude-dependent total energy deposition rate.

We can divide the potential term in equation (261) by the specific enthalpy term for monatomic gas

$$\frac{|\phi_{g0}|}{c_p T_0} = \frac{2m|\phi_{g0}|}{5kT_0} = \frac{2}{5} X_0 \quad (263)$$

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

$$F_\rho = \frac{\epsilon r_E^2 F_E^2}{|\phi_{g0}|}. \quad (264)$$

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.,

$$\dot{M}_E = 4\pi F_\rho = \frac{\epsilon \pi r_{XUV}^2 F_{XUV} R_p}{GM_p} \quad (265)$$

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

$$p \frac{\partial}{\partial r} (r^2 w) = \frac{\partial}{\partial r} (p w r^2) + w r^2 \frac{\partial p}{\partial r} \quad (266)$$

where the second term on the right-hand side

$$w r^2 \frac{\partial p}{\partial r} = - \left[w \frac{\partial}{\partial r} (\rho w^2 r^2) + w r^2 \frac{\partial \phi_g}{\partial r} \right] \quad (267)$$

is obtained from the steady-state radial momentum equation.

5 Numerical methods

5.1 Photochemical models (Week 14)

Photochemical models solve the continuity equations for multiple species, typically including chemical reactions and diffusion. The solution techniques are very different from chemical equilibrium models and we will briefly cover some basic principles here. We will follow the solution used by Lavvas et al. (2008) in their model of neutral photochemistry for Titan's atmosphere. In order to highlight the usual assumptions regarding diffusion in neutral photochemical models, we start from equation (193) above:

$$\left(1 + \frac{K_{zz}}{D_s}\right) \frac{\partial x_s}{\partial r} + \left(x_s - \frac{\rho_s}{\rho}\right) \frac{\partial \ln p}{\partial r} + \frac{\alpha_s x_s}{T} \frac{\partial T}{\partial r} = - \sum_{t \neq s} x_s x_t \frac{w_s - w_t}{D_{st}}.$$

Assuming a stationary background ($w_t = 0$), we multiply equation (193) by nD_s and re-organize to get the flux of species s

$$f_s = \frac{nD_s}{H} \left(1 - \frac{m_s}{m} - \alpha_T \frac{H}{T} \frac{\partial T}{\partial r}\right) x_s - n(D_s + K_{zz}) \frac{\partial x_s}{\partial r} \quad (268)$$

where we also replaced the pressure gradient with

$$\frac{\partial \ln p}{\partial r} = -\frac{1}{H}. \quad (269)$$

Based on this, the continuity equation in the absence of vertical advection is

$$\frac{\partial n_s}{\partial t} = -\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 f_s) + P_s - L_s \quad (270)$$

where we included the chemical production (P_s) and loss (L_s) rates. The production rate can include chemical reactions, photo-ionization, photolysis and impact ionization/dissociation. Note, however, that these equations ignore electric and magnetic fields, so the diffusion formulation is not suitable for models of the ionosphere. The loss term can include chemical reactions, condensation and surface processes.

We can write the divergence of flux as

$$-\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 f_s) = \frac{p}{H} \frac{\partial f_s}{\partial p} - \frac{2}{r} f_s \quad (271)$$

where

$$\frac{\partial f_s}{\partial r} = \frac{\partial f_s}{\partial p} \frac{\partial p}{\partial r} = -\frac{p}{H} \frac{\partial f_s}{\partial p}. \quad (272)$$

Expressing the flux as

$$f_s = C_{1s} x_s + C_{2s} \frac{\partial x_s}{\partial p} \quad (273)$$

where

$$C_{1s}(p, T) = \frac{pD_s}{kTH} \left(1 - \frac{m_s}{m} + \alpha_T \frac{p}{T} \frac{\partial T}{\partial p} \right) \quad (274)$$

$$C_{2s}(p, T) = (D_s + K_{zz}) \frac{p^2}{kTH}, \quad (275)$$

we can further write the divergence of flux as

$$-\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 f_s) = D_{1s} x_s + D_{2s} \frac{\partial x_s}{\partial p} + D_{3s} \frac{\partial^2 x_s}{\partial p^2} \quad (276)$$

where

$$D_{1s} = \frac{p}{H} \frac{\partial C_{1s}}{\partial p} - \frac{2}{r} C_{1s} \quad (277)$$

$$D_{2s} = \frac{p}{H} \left(C_{1s} + \frac{\partial C_{2s}}{\partial p} \right) - \frac{2C_{2s}}{r} \quad (278)$$

$$D_{3s} = \frac{p}{H} C_{2s}. \quad (279)$$

We note that the time derivative of number density at a fixed pressure p is

$$\frac{\partial n_s}{\partial t} = \frac{\partial (nx_s)}{\partial t} = n \frac{\partial x_s}{\partial t} - \frac{x_s p}{kT^2} \frac{\partial T}{\partial t} = n \frac{\partial x_s}{\partial t} \quad (280)$$

for constant temperature over time. We may now write the continuity equation for species s at pressure level n as

$$\frac{\partial x_{s,n}}{\partial t} = a_{s,n} x_{s,n} + b_{s,n} \frac{\partial x_{s,n}}{\partial p} + c_{s,n} \frac{\partial^2 x_{s,n}}{\partial p^2} + u_{s,n}(\mathbf{x}_n) - v_{s,n}(\mathbf{x}_n) \quad (281)$$

where we highlight that the values for a, b, c depend on both the species and the pressure level, and the production and loss rates depend on the mixing ratios of all the species at level n . Here, the variables are

$$a_{s,n} = \frac{D_{1s,n}}{n_n}, \quad b_{s,n} = \frac{D_{2s,n}}{n_n}, \quad c_{s,n} = \frac{D_{3s,n}}{n_n}, \quad u_{s,n} = \frac{P_{s,n}}{n_n}, \quad v_{s,n} = \frac{L_{s,n}}{n_n}. \quad (282)$$

where the subscripts should not be confused with the tensor summation convention.

To complete the continuity equation at level n , we use second order central finite difference approximation to express the partial derivatives:

$$\begin{aligned} \frac{\partial x_{s,n}}{\partial t} &= u_{s,n}(\mathbf{x}_n) - v_{s,n}(\mathbf{x}_n) + a_{s,n} x_{s,n} + b_{s,n} (d_{n-1} x_{s,n-1} + d_n x_{s,n} + d_{n+1} x_{s,n+1}) \\ &\quad + c_{s,n} (e_{n-1} x_{s,n-1} + e_n x_{s,n} + e_{n+1} x_{s,n+1}). \end{aligned} \quad (283)$$

We can write this as

$$\frac{\partial x_{s,n}}{\partial t} = Q_{s,n}(\mathbf{x}_n) + a_{s,n}(p_n, T_n)x_{s,n} + w_{s,n}(x_{s,n-1}, x_{s,n}, x_{s,n+1}; p_n, T_n) \quad (284)$$

where

$$\begin{aligned} w_{s,n} &= (d_{n-1}b_{s,n} + e_{n-1}c_{s,n})x_{s,n-1} + (d_nb_{s,n} + e_nc_{s,n})x_{s,n} + (d_{n+1}b_{s,n} + e_{n+1}c_{s,n})x_{s,n+1} \\ &= \alpha_{s,n-1}x_{s,n-1} + \beta_{s,n}x_{s,n} + \gamma_{s,n+1}x_{s,n+1} \end{aligned} \quad (285)$$

with the first derivative terms

$$\begin{aligned} d_{n-1} &= -\frac{p_{n+1} - p_n}{(p_n - p_{n-1})(p_{n+1} - p_{n-1})} \\ d_n &= -(d_{n+1} + d_{n-1}) \\ d_{n+1} &= \frac{p_n - p_{n-1}}{(p_{n+1} - p_n)(p_{n+1} - p_{n-1})} \end{aligned} \quad (286)$$

and the second derivative terms

$$\begin{aligned} e_{n-1} &= \frac{2}{(p_n - p_{n-1})(p_{n+1} - p_{n-1})} \\ e_n &= -\frac{2}{(p_{n+1} - p_n)(p_n - p_{n-1})} \\ e_{n+1} &= \frac{2}{(p_{n+1} - p_n)(p_{n+1} - p_{n-1})}. \end{aligned} \quad (287)$$

Finally, the general form of the continuity equation is

$$\frac{\partial x_{s,n}}{\partial t} = H_{s,n}(t; \mathbf{x}_n; x_{s,n-1}, x_{s,n}, x_{s,n+1}; p_n, T_n). \quad (288)$$

At this point it is a good idea to examine the variable and array dependencies of this equation. Through the production and loss rates, the mixing ratio of species s depends on the abundances of all the other species at level n , often in a complex, non-linear manner. The transport terms, on the other hand, depend on the species s mixing ratios on adjacent levels while there is no direct dependency on the other species at adjacent levels. We may therefore expect the numerical solution of this equation to constitute a complex matrix inversion problem.

The presence of the transport terms forces us to set spatial boundary conditions that would not be required in the absence of the mixing ratio derivatives. The boundary conditions are handled by introducing imaginary points above the upper boundary and below the lower boundary. For Titan, Lavvas et al. (2008) assumed zero gradient in the mixing ratio at the boundary, which for second order central differences gives

$$d_0x_{s0} + d_1x_{s1} + d_2x_{s2} = 0 \rightarrow d_0x_{s0} = -d_1x_{s1} - d_2x_{s2}, \quad (289)$$

which can be used to eliminate d_0x_{s0} from the continuity equation. At the upper boundary, they assumed zero second derivative for the mixing ratio x_s .

We note that the function $H_{s,n}$ encapsulates processes with wildly different timescales and a straightforward solution is not possible. For this reason, equation (288) is a ‘stiff’ equation. This equation is often solved by using the backward Euler technique with Newton-Raphson iteration. Consider, for example,

$$\mathbf{x}'(t) = \mathbf{f}[t, \mathbf{x}(t)]. \quad (290)$$

The forward Euler step for this equation would be

$$\mathbf{x}(t+h) = \mathbf{x}(t) + h\mathbf{f}[t, \mathbf{x}(t)] \quad (291)$$

which usually leads to instabilities in photochemical models. Instead, the backward Euler step is

$$\mathbf{x}(t+h) = \mathbf{x}(t) + h\mathbf{f}[t+h, \mathbf{x}(t+h)]. \quad (292)$$

If we call $\mathbf{k} = \mathbf{x}(t+h) - \mathbf{x}(t)$, it is clear that we need to solve the equation

$$\mathbf{k} = h\mathbf{f}(t+h, \mathbf{x}+\mathbf{k}) \quad (293)$$

to take the backward Euler step.

We package the problem as

$$\mathbf{G}(\mathbf{k}) = \mathbf{k} - h\mathbf{f}(t+h, \mathbf{x}+\mathbf{k}) = 0. \quad (294)$$

For this, the Newton step is

$$\begin{aligned} \mathbf{G}(\mathbf{k} + \Delta\mathbf{k}) &= 0 \\ \rightarrow \mathbf{G}(\mathbf{k}) + \nabla\mathbf{G}(\mathbf{k})\Delta\mathbf{k} &= 0 \\ \rightarrow \nabla\mathbf{G}(\mathbf{k})\Delta\mathbf{k} &= -\mathbf{G}(\mathbf{k}). \end{aligned} \quad (295)$$

Here

$$\nabla\mathbf{G}(\mathbf{k}) = \nabla[\mathbf{k} - h\mathbf{f}(t+h, \mathbf{x}+\mathbf{k})] = \mathbf{I} - h\nabla_{\mathbf{x}}\mathbf{f}(t+h, \mathbf{x}+\mathbf{k}) \quad (296)$$

where

$$\mathbf{f}(t+h, \mathbf{x}+\mathbf{k}) \approx \mathbf{f}(t+h, \mathbf{x}) + \mathbf{k}\nabla_{\mathbf{x}}\mathbf{f}(t+h, \mathbf{x}+\mathbf{k})$$

is consistent with the backward Euler step. Thus, the Newton step is

$$[\mathbf{I} - h\nabla_{\mathbf{x}}\mathbf{f}(t+h, \mathbf{x}+\mathbf{k})] \Delta\mathbf{k} = h\mathbf{f}(t+h, \mathbf{x}+\mathbf{k}) - \mathbf{k}, \quad (297)$$

which we invert to obtain $\Delta\mathbf{k}$ in order to update \mathbf{k} . The initial value of \mathbf{k} can be taken to be zero or obtained by taking the forward Euler step.

Let us now apply this theory to the continuity equation in photochemical models. We may write

$$x_{s,n}(t_{m+1}) = x_{s,n}(t_m) + h_m H_{s,n}(t_{m+1}; \mathbf{x}_{m+1}; x_{m+1,s,n-1}, x_{m+1,s,n}, x_{m+1,s,n+1}). \quad (298)$$

In this case, the function \mathbf{G} is

$$G = x_{s,n}(t_{m+1}) - x_{s,n}(t_m) - h_m H_{s,n}(t_{m+1}; \mathbf{x}_{m+1,n}; x_{m+1,s,n-1}, x_{m+1,s,n}, x_{m+1,s,n+1}) = 0 \quad (299)$$

and we identify

$$k_{s,n} = x_{s,n}(t_{m+1}) - x_{s,n}(t_m) \quad (300)$$

so that $\mathbf{x}_{m+1} = \mathbf{x}_m + \mathbf{k}$. Discarding transport terms would allow us to derive separate equations for each pressure level:

$$G = k_s - h_m H_s(t_{m+1}; \mathbf{x}_{m+1}) = 0. \quad (301)$$

Application of the Newton step i.e., equation (297), then yields

$$\left(\delta_{sj} - h_m \frac{\partial Q_s}{\partial x_j} \right) \Delta k_j = h_m H(t_{m+1}; x_{m+1,s}) - k_s = -\epsilon_s \quad (302)$$

where Einstein summation convention is assumed.

Including the transport terms complicates the solution because it relates the equations for different levels to the two adjacent levels and makes it tempting to consider operator-splitting. This, however, is not used in typical photochemical models and instead Lavvas et al. (2008) include the transport terms in the Newton iteration. Some mental gymnastics are required to follow this procedure. The main difference is that H is a function of the mixing ratio x_s at three different pressure levels through the numerical first and second derivative. Therefore, we need to write

$$\frac{\partial H_{s,n}}{\partial x_{j,n-1}} = \alpha_{j,n-1} \delta_{sj} \quad (303)$$

$$\frac{\partial H_{s,n}}{\partial x_{j,n}} = a_{j,n} \delta_{sj} + \beta_{j,n} \delta_{sj} - \frac{\partial Q_s}{\partial x_j} \quad (304)$$

$$\frac{\partial H_{s,n}}{\partial x_{j,n+1}} = \gamma_{j,n+1} \delta_{sj} \quad (305)$$

to account for the total derivative of $H_{s,n}$ in $\nabla_{\mathbf{x}} \mathbf{H}$. Therefore, the Newton step now gives

$$h_m \alpha_{s,n-1} \delta_{sj} \Delta k_{j,n-1} + h_m \left(\frac{\delta_{sj}}{h_m} + a_{j,n} \delta_{sj} + \beta_{j,n} \delta_{sj} - \frac{\partial Q_{s,n}}{\partial x_j} \right) \Delta k_{j,n} + \gamma_{j,n+1} \delta_{sj} \Delta k_j = -\epsilon_n, \quad (306)$$

which can be written as block tridiagonal matrix and inverted to obtain $\Delta \mathbf{k}_n$.

6 Supporting topics

6.1 Magnetic dipole coordinates

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

$$p = \frac{r}{\sin^2 \theta} \quad (307)$$

$$q = \frac{\cos \theta}{r^2} \quad (308)$$

where r is radial distance, θ 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:

$$\mathbf{B} = \frac{\mu_0 \mu_M}{4\pi r^3} (2 \cos \theta \mathbf{e}_r + \sin \theta \mathbf{e}_\theta) \quad (309)$$

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

$$m = \frac{\mu_0}{4\pi} \mu_M, \quad (310)$$

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

$$\mathbf{B} = \frac{\mu_0 \mu_M}{4\pi r^3} \delta \quad (311)$$

$$\delta = \sqrt{1 + 3 \cos^2 \theta}. \quad (312)$$

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

$$d\mathbf{s} \times \mathbf{B} = 0. \quad (313)$$

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

$$B_\theta dr = B_r r d\theta \rightarrow \frac{dr}{B_r} = \frac{r d\theta}{B_\theta} \rightarrow \frac{dr}{r} = \frac{2 du}{u} \quad (314)$$

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

$$\ln \left(\frac{r}{r_{\text{eq}}} \right) = 2 \ln u, \quad (315)$$

which gives us the *magnetic field line equation*:

$$r = r_{\text{eq}} \sin^2 \theta \quad (316)$$

where $p = r_{\text{eq}}$ 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

$$p = LR_0 \quad (317)$$

where R_0 is an equatorial reference radius.

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

$$ds \cdot \mathbf{B} = B_r dr + B_\theta r d\theta = 0, \quad (318)$$

which leads to

$$\frac{dr}{r} = \frac{d(\cos \theta)}{2 \cos \theta} \quad (319)$$

and gives the dipole coordinate q as a constant of integration

$$qr^2 = \cos \theta. \quad (320)$$

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.

6.2 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

$$\mathbf{j} = \sigma_e (\mathbf{E} + \mathbf{u} \times \mathbf{B}) \quad (321)$$

where

$$\eta_e = \frac{1}{\sigma_e} = \frac{m_e \nu_c}{n_e e^2} \quad (322)$$

is the plasma resistivity i.e, the inverse of conductivity, and ν_c is the Coulomb collision frequency. The velocity is

$$\mathbf{u} = \frac{\sum_s m_s n_s \mathbf{u}_s}{\rho} \quad (323)$$

where ρ 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

$$\mathbf{u}_i \approx \mathbf{u} \quad (324)$$

$$\mathbf{u}_e \approx \mathbf{u} - \frac{\mathbf{j}}{en_e} \quad (325)$$

because of the small electron mass.

Taking the curl of equation (321), assuming constant η_e and using Faraday's and Ampere's laws (without the displacement current) gives

$$-\frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{u} \times \mathbf{B}) = \frac{\eta_e}{\mu_0} \nabla \times (\nabla \times \mathbf{B}). \quad (326)$$

We use the Levi-Civita symbol (see Section 6.4) to write the cross product:

$$[\nabla \times (\nabla \times \mathbf{B})]_m = \epsilon_{mni} \epsilon_{ijk} \frac{\partial}{\partial x_n} \left(\frac{\partial B_k}{\partial x_j} \right). \quad (327)$$

An even permutation of the Levi-Civita symbol gives

$$[\nabla \times (\nabla \times \mathbf{B})]_m = \epsilon_{imn} \epsilon_{ijk} \frac{\partial}{\partial x_n} \left(\frac{\partial B_k}{\partial x_j} \right) \quad (328)$$

and therefore, we have

$$\begin{aligned} [\nabla \times (\nabla \times \mathbf{B})]_m &= (\delta_{jm} \delta_{kn} - \delta_{jn} \delta_{km}) \frac{\partial}{\partial x_n} \left(\frac{\partial B_k}{\partial x_j} \right) \\ &= \frac{\partial}{\partial x_n} \left(\frac{\partial B_n}{\partial x_m} \right) - \frac{\partial}{\partial x_n} \left(\frac{\partial B_m}{\partial x_n} \right) \\ &= \frac{\partial}{\partial x_m} \left(\frac{\partial B_n}{\partial x_n} \right) - \frac{\partial}{\partial x_n} \left(\frac{\partial B_m}{\partial x_n} \right) \end{aligned} \quad (329)$$

or

$$\nabla \times (\nabla \times \mathbf{B}) = \nabla (\nabla \cdot \mathbf{B}) - \nabla^2 \mathbf{B} = -\nabla^2 \mathbf{B}. \quad (330)$$

Using this vector identity, we obtain the induction equation

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}) + \frac{\eta_e}{\mu_0} \nabla^2 \mathbf{B}. \quad (331)$$

If the magnetic Reynold's number

$$R_m = \mu_0 \sigma_e u L_B \gg 1, \quad (332)$$

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:

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}). \quad (333)$$

This is equivalent to zero electric field in the rest frame of the plasma (i.e., infinite conductivity):

$$\mathbf{E} + \mathbf{u} \times \mathbf{B} = 0, \quad (334)$$

which implies that ions and electrons drift with the same velocity

$$\mathbf{u} = \frac{\mathbf{E} \times \mathbf{B}}{B} \quad (335)$$

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

6.3 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):

$$\kappa n_{sw} m_p (\mathbf{n} \cdot \mathbf{v}_{sw})^2 = \frac{1}{2\mu_0} (\mathbf{n} \times \mathbf{B}_p)^2 \quad (336)$$

where \mathbf{n} is a unit vector normal to the magnetopause boundary, n_{sw} is the solar wind plasma density, \mathbf{v}_{sw} is the solar wind velocity, \mathbf{B}_p is the Earth's magnetic field strength, m_p is proton mass and κ 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 \mathbf{n} , we can write

$$\kappa n_{sw} m_p v_{sw}^2 = \frac{B_p^2}{2\mu_0}. \quad (337)$$

Assuming that the magnetic field at the stagnation point can be represented by a distorted dipole field, we obtain

$$n_{sw} m_p v_{sw}^2 = \frac{K B_E^2}{2\mu_0 R_{mp}^6} R_E^6 \quad (338)$$

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

$$R_{mp} = \left(\frac{K B_E^2}{2\mu_0 n_{sw} m_p v_{sw}^2} \right)^{1/6} R_E \quad (339)$$

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

$$R_{mpf} = \left(\frac{KB_E^2}{2\mu_0\gamma n_{sw}kT_{sw}} \right)^{1/6} R_E, \quad (340)$$

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.

6.4 Levi-Civita symbol

6.4.1 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:

$$\begin{aligned} \epsilon_{ij} &= 1 \quad \text{for } (i,j) = (1,2) \\ &= -1 \quad \text{for } (i,j) = (2,1) \\ &= 0 \quad \text{for } i = j. \end{aligned} \quad (341)$$

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,

$$\epsilon_{ij}\epsilon_{mn} = \delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}. \quad (342)$$

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

$$\epsilon_{ij}\epsilon_{in} = \delta_{ii}\delta_{jn} - \delta_{in}\delta_{ji} \quad (343)$$

where repeated indices imply a sum. Thus,

$$\epsilon_{ij}\epsilon_{in} = 2\delta_{jn} - \delta_{1n}\delta_{j1} - \delta_{2n}\delta_{j2} = \delta_{jn}. \quad (344)$$

Finally, we obtain

$$\epsilon_{ij}\epsilon_{ij} = \delta_{jj} = 2 \quad (345)$$

by setting $j = n$.

6.4.2 Rank 3

The Levi-Civita symbol of rank 3 is

$$\begin{aligned}\epsilon_{ijk} &= 0 \text{ for any two indices equal} \\ &= 1 \text{ for even permutations of } (1,2,3) \\ &= -1 \text{ for odd permutations of } (1,2,3)\end{aligned}\tag{346}$$

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

$$\begin{aligned}\epsilon_{ijk}\epsilon_{lmn} &= \delta_{il}\delta_{jm}\delta_{kn} + \delta_{im}\delta_{jn}\delta_{kl} + \delta_{in}\delta_{jl}\delta_{km} \\ &- \delta_{im}\delta_{jl}\delta_{kn} - \delta_{il}\delta_{jn}\delta_{km} - \delta_{in}\delta_{jm}\delta_{kl}.\end{aligned}\tag{347}$$

Setting $i = l$ then gives

$$\epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}\tag{348}$$

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

$$(\mathbf{a} \times \mathbf{b})_i = \epsilon_{ijk}a_jb_k\tag{349}$$

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

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