Transport phenomena

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Abstract. This tutorial paper describes how various transport phenomena affect the atmospheric structure. These basic principles are applied to the Earth's atmosphere, but can be extended to any other atmosphere. Two types of movements are considered, namely global movements which affects all constituents and minor constituents movements which depend on the nature of the atmospheric components. Since the atmospheric composition depends on the actual hydrodynamical regime, the transition from perfect mixing to molecular diffusion is analyzed as well as the transition from collisional dominated heterosphere to the exosphere where almost no interaction occurs between atmospheric components.

1. INTRODUCTION

The construction of a three–dimensional time dependent atmospheric model is an extremely difficult task. In principle, one has to solve, *for each constituent*, a continuity equation, a momentum conservation equation and an energy conservation equation. To my knowledge, it has never been proven mathematically that a solution of such a coupled partial differential equations system exists. We know, however, that there is at least one solution, since the atmosphere exits. In order to obtain a more or less accurate solution, we have always to introduce simplifying assumptions.

For example, the continuity equation is solved for the total atmospheric density. But, when chemical reactions play a role, one has to treat a continuity equation for each constituent. This point of view is adopted in the present chapter. When the momentum equation is solved for the whole atmosphere one obtains global movements affecting simultaneously all species. The energy conservation equation is not considered in this chapter, although a coupling with the continuity and momentum equations occurs through the temperature.

Section 2 deals with the global atmospheric structure to show why transport phenomena must be considered. Global transport affecting all atmospheric components is discussed in section 3. As shown in section 4, minor constituents transport requires a special treatment and section 5 develops some useful approximations for minor components. Section 6 describes how and why the transition between the homosphere and the heterosphere occurs. As altitude increases, collisions become less and less frequent and the transition between the heterosphere and the exosphere is discussed in section 7 with a short description how particles can definitively escape for the Earth's gravitational attraction. The reference list is far from being exhaustive and it should be considered as a guide.

2. ATMOSPHERIC STRUCTURE

The global structure of the Earth's atmosphere has been extensively modeled using satellite drag data, mass spectrometric data, incoherent scattering observations and optical data. Several semi-empirical models based on spherical harmonics have been developed. At present time, the most widely used models are those of Hedin [1–2] and Berger *et al.* [3].

Figure 1 shows the atmospheric nomenclature based on the vertical temperature distribution. The two curves on Figure 1 correspond respectively to low and high solar activity and reflect the variation of solar EUV fluxes (see [4]).
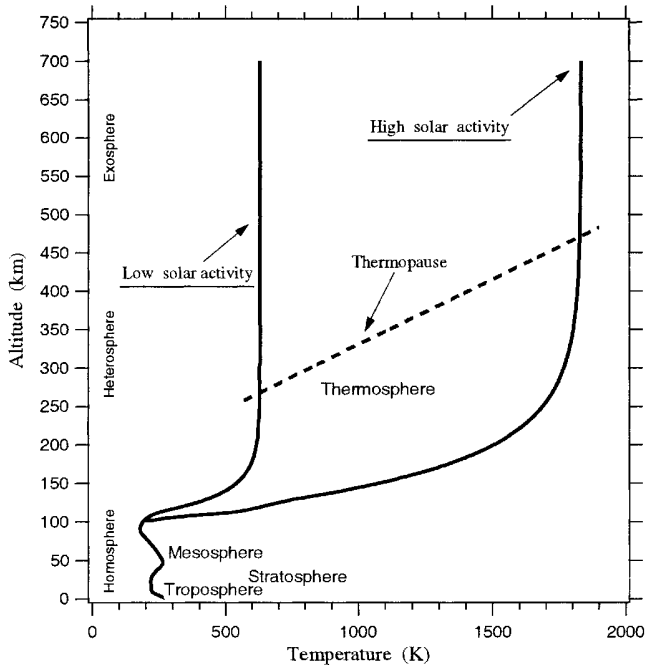

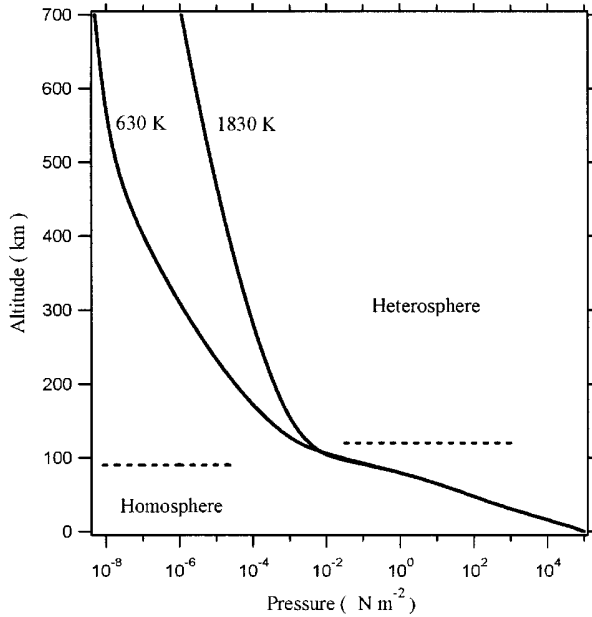**Figure 1.** Vertical temperature distribution for low and high solar activity.

This figure has been computed using Hedin's [2] model. It is interesting to note that the *mesopause* is around 100 km altitude and not around 85 km where it is generally placed. This is in agreement with the recent experimental studies of Berger and von Zahn [5] based on lidar observations.

Another way to look at the atmospheric structure, is to consider the vertical distribution of the total pressure. Figure 2 gives the pressure distribution corresponding to the two temperature profiles of Figure .

Besides the variation with solar activity in the *heterosphere* above 100 km altitude, it is clear on Figure 2 that the pressure gradient in the *homosphere*, below 100 km altitude, is much steeper. In the homosphere the pressure decreases by approximately a factor 10^6 between ground level and 100 km altitude. A similar decrease in the heterosphere occurs only after several hundreds km depending on the solar activity. Such a behavior is directly related to different dynamical regimes in these two regions.

The most simple, but incomplete, approach to explain Figure 2 is to consider the atmosphere as a perfect gas where the total pressure p is given by

$$p = n \times k \times T \tag{1}$$

Figure 2. Vertical pressure distribution for low and high solar activity.

In equation (1) n is the total concentration, usually in cm^{-3}, k is Boltzmann's constant and T is the absolute temperature. When this equation is combined with the hydrostatic law

$$\frac{dp}{dz} = -\rho \times g \qquad (2)$$

where z, ρ, g are respectively the geometric altitude, the total mass density and the acceleration of gravity, one obtains

$$\frac{dp}{p} = -\frac{dz}{H} \qquad (3)$$

In equation (3) H is the atmospheric scale height associated to the pressure p. It is given by

$$H = \frac{k \times T}{m \times g} \qquad (4)$$

where $m = \rho/n$ is the mean molecular mass.

Integration of equation (3) leads to

$$p(z) = p(z_o) \times \exp[-\int_{z_o}^{z} \frac{dz}{H}] \qquad (5)$$

where z_0 is a reference altitude.

In order to explain the less steeper pressure gradient in the heterosphere (see Figure 2), equation (5) indicates that the atmospheric scale height H should be larger in the heterosphere than in the homosphere. From the definition of H given by equation (4), two possibilities can lead to an increase of the scale height: an increase of the temperature with height and/or a decrease of the mean molecular mass. Both mechanisms occur in the heterosphere. The temperature increases as a result of solar EUV heating and the mean molecular mass decreases as a result of a transport phenomena, namely molecular diffusion. This possibility will be discussed in detail in section 4. It should be
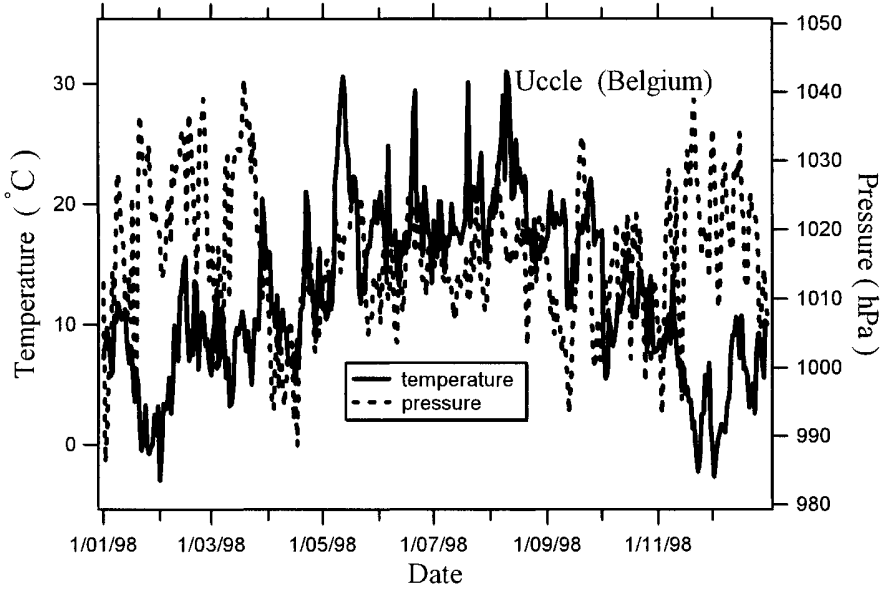
Figure 3. Atmospheric pressure reduced to sea level and temperature in Uccle as a function of time.

pointed out that the perfect gas law given by equation (1) is only valid in a static medium. This is clearly demonstrated in Figure 3. Data of Figure 3 were kindly provided by the Royal Meteorological Institute of Belgium. The pressure is reduced to sea level and the temperature is measured 2 m above the ground. If the perfect gas law could be used, a pressure increase or decrease should correspond respectively to a temperature increase or decrease. It is obvious from Figure that this is not the case. The fundamental reason for such a situation results from the fact that the perfect gas law is not a solution of the three conservation equations, mass, momentum and energy. From a meteorological point of view, the perfect gas law does not account for winds, condensation and evaporation phenomena, clouds .... This is the reason why the momentum conservation equation has to be used for the global transport discussed in next section.

3. GLOBAL TRANSPORT

Since the atmosphere is a compressible fluid with several components, two type of movements are to be considered: firstly the global movements which affect simultaneously all components and secondly the individual movements which are specific to a given component. These specific movements are discussed in section 4.

Global transport can be estimated from the momentum conservation equation. There are many derivations of this equation (see [6]–[9]). Two reference frames can be used: the *Eulerian* frame which is fixed with respect to the space coordinates and the *Lagrangian* frame which is moving with the fluid. An excellent discussion of differences between these two approaches is given by Garcia *et al.* [10].

Any conservation equation can be derived from Boltzmann's equation by computing the appropriate moment (see [11–12]). The first order moment leads to

$$\frac{D\boldsymbol{v}_a}{Dt} + \frac{1}{\rho}\,\boldsymbol{\nabla}\,p - \frac{\mu}{\rho}\,\boldsymbol{\nabla}^2\,\boldsymbol{v}_a = \frac{1}{\rho}\sum_j n_j\,\boldsymbol{X}_j \qquad (6)$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + v_a \, \nabla$ is sometimes called the derivative along the movement, v_a is the atmospheric velocity vector, ρ in g cm^{-3} is the total density, p is the atmospheric pressure and μ is the dynamical viscosity of air measured in g cm^{-1} s^{-1}. The dynamical viscosity μ should not be confused with the kinematic viscosity η which is defined by $\eta = \mu/\rho$ in cm^2 s^{-1}. Vectors X_j represents all external forces acting on particles of type j. These external forces can be split into two categories: the forces common to all species, i.e. gravitational effects and rotational effects, and the forces specific to the individual species. Therefore, vectors X_j can be written as

$$X_j = [g - 2\omega \times v_a - \omega \times (\omega \times r)] \, m_j + F_j \tag{7}$$

where g is the gravitational acceleration vector, ω is the angular Earth's rotation vector and r is the geocentric distance. F_j represents any other external force acting on particle j. Symbol $\times$ is used for a vector product.

Numerical solutions of equation (6) are far from being a simple task, since the momentum equation is coupled to the continuity equation through individual number densities and another coupling occurs with the energy conservation equation through the temperature. Usually simplifying assumptions are always required depending on the problem to tackle.

When everything is neglected in equation (6) except the pressure gradient and the acceleration of gravity, one obtains immediately the hydrostatic equation (2). This confirms the discussion presented for Figure 3 in section 2.

To close this section, we will now briefly discuss the major difference between the horizontal circulation in the homosphere and in the heterosphere.

By neglecting viscosity, F_j forces, temporal variations and the vertical component in equation (6) one obtains

$$\frac{1}{\rho} \, \nabla_h \, p = -2 \, \omega \, \times \, v_{ah} \tag{8}$$

where subscript h means that the corresponding vector has only two horizontal components along the x and y axis oriented towards South and East respectively.

If φ represent geographic latitude the two components of equation (8) can be written

$$\frac{1}{\rho} \frac{\partial p}{\partial x} \;=\; 2 \, v_{ay} \, \omega \, \sin \varphi \tag{9}$$

$$\frac{1}{\rho} \frac{\partial p}{\partial y} \;=\; -2 \, v_{ax} \, \omega \, \sin \varphi \tag{10}$$

where $2\omega \sin \varphi$ is often called as th Coriolis parameter.

Multiplying equation (9) by v_{ax} and equation (10) by v_{ay} and summing the results, one sees that v_{ah} is *perpendicular* to the pressure gradient since

$$v_{ah}.\nabla p = 0 \tag{11}$$

This is called the *geostrophic* approximation which implies that horizontal winds are blowing parallel to isobars. In the Northern hemisphere wind is blowing clockwise around high pressure zones and anticlockwise around low pressure zones. A reversed situation occurs in the Southern hemisphere since the Coriolis parameter changes its sign.

In the homosphere, above 1 km altitude and for latitudes greater than 10°, the crude Coriolis approximation leads to realistic results.

In the heterosphere, above 100 km, external forces F_j are progressively dominated by interactions between the neutral atmosphere and the ionosphere. Considering only external forces and the pressure gradient, equation (6) can than be written as

$$\frac{1}{\rho} \, \nabla p = \nu_{ni} \, (v_i - v_a) \tag{12}$$

where ν_{ni} is the collision frequency between neutral particles and ionized species characterized by a velocity $\boldsymbol{v}_i$. Equation (12) shows that the neutral wind is now parallel to the pressure gradient and blows from a high pressure zone to a low pressure zone perpendicularly to the isobars. Such a situation is completely different from what occurs in the homosphere. Although Coriolis force also exists in the heterosphere, its magnitude is much smaller than the force in equation (12) which is called *ion drag* when the ions produce a drag of the neutral atmosphere. When the neutral atmosphere drags the ions, it is called *atmospheric drag.*

Above 100 km altitude, horizontal winds can easily exceed 100 m s^{-1}. Although the abundance of ions and electrons is always much smaller than the neutral concentration, ion drag is generally sufficient to decrease the intensity of the neutral wind. Zonal and meridional winds are usually smaller during day time since ionized particles are more abundant.

Ionized particles can also be driven by external electric fields. This is particularly true in the auroral regions. In this case ions and electrons can accelerate the neutral atmosphere and the neutral wind can reach values as high as 1000 m s^{-1} (see [12]).

The dynamical behavior of the homosphere and the heterosphere are essentially different as a result of different transport phenomena.

4. MINOR CONSTITUENTS TRANSPORT

The distribution of individual constituents can be influenced by photochemical processes and relative movements are possible. This type of transport is analyzed using a time–dependent continuity equation for each constituent such as

$$\frac{\partial n_i}{\partial t} + \operatorname{div}\left(n_i \, \boldsymbol{W}_i\right) = P_i - n_i \times L_i \tag{13}$$

where P_i represents the production rate (cm^{-3} s^{-1}) of species i, L_i is the loss rate (s^{-1}) of species i with concentration n_i (cm^{-3}). The total transport velocity $\boldsymbol{W}_i$ is given by

$$\boldsymbol{W}_i = \boldsymbol{v}_a + \boldsymbol{v}_{iD} + \boldsymbol{v}_{iK} \tag{14}$$

In this equation, $\boldsymbol{v}_a$ is the global transport velocity discussed in section 3, $\boldsymbol{v}_{iD}$ is the molecular diffusion velocity and $\boldsymbol{v}_{iK}$ is the turbulent diffusion velocity, also called eddy diffusion velocity.

The physical meaning of these last two velocities can easily be understood if one define the *mean velocity* $\overline{\boldsymbol{v}}_i$ of constituent i by

$$\overline{\boldsymbol{v}}_i = \frac{1}{n_i} \int \boldsymbol{v}_i \, f(\boldsymbol{v}_i, t) \, d\boldsymbol{v}_i \tag{15}$$

where $f(\boldsymbol{v}_i, t)$ is the velocity distribution function. Integration is made over velocity space. The *mean mass velocity* $\boldsymbol{v}_a$, entering in the momentum equation is then given by

$$\boldsymbol{v}_a = \frac{1}{\rho} \sum_i n_i \, m_i \, \overline{\boldsymbol{v}}_i \tag{16}$$

where $\rho = \sum_i n_i \, m_i$ is the total density and m_i the molecular or atomic mass of species *ie* i. For an atmosphere with a single constituent, it is obvious that $\boldsymbol{v}_a = \overline{\boldsymbol{v}}_i$.

The *diffusion velocity* $\boldsymbol{V}_i$ is defined by relation

$$\boldsymbol{V}_i = \overline{\boldsymbol{v}}_i - \boldsymbol{v}_a \tag{17}$$

and is equal to zero for an atmosphere with a single constituent.

Using equations (15) and (16), one finds that

$$\sum_i n_i \, m_i \, \boldsymbol{V}_i = 0 \tag{18}$$

i.e. the vectorial sum of the mass fluxes is always zero. This relation expresses total mass conservation.

From the above considerations, one sees that the molecular diffusion and turbulent diffusion velocities introduced in equation (14) are simply a decomposition of the general diffusion velocity given by equation (17). This approach is used since gas kinetic theory leads to an analytical expression for molecular diffusion, whereas a phenomenological expression must be used for turbulent diffusion. We consider only vertical expressions for these quantities since horizontal diffusion is usually negligible compared to horizontal winds.

From gas kinetic theory [6–7], the molecular diffusion velocity in the vertical direction z for a constituent i with concentration n_i is given by

$$v_{iD} = -D_i \times \left(\frac{1}{n_i} \frac{\partial n_i}{\partial z} + \frac{1}{H_i} + \frac{1+\alpha_i}{T} \frac{\partial T}{\partial z} \right) \tag{19}$$

In this equation, $H_i = kT/m_i g$ is the scale height associated to the partial pressure of constituent i, α_i is the *thermal diffusion factor* which has no dimension. This factor represents a mass transport resulting from temperature gradients independently of any other gradients. For atomic hydrogen and helium $\alpha = -0.38$, for argon $\alpha = +0.18$ and it can be taken to zero for all other constituents. The molecular diffusion coefficient ($cm^2 s^{-1}$) is expressed as

$$D_i = \frac{A_i \times T^x}{n} \tag{20}$$

where n is the total concentration and A_i is a constant which can be deduced experimentally. The exponent x is usually of the order of 0.7. More precise values can be found in [13–14]. When no experimental values are available, one can use a theoretical result strictly valid only when particles are considered as rigid spheres

$$D_i = 1.52 \times 10^{18} \left(\frac{1}{M_i} + \frac{1}{M} \right)^{1/2} \times \frac{T^{1/2}}{n} \tag{21}$$

where M_i and M are respectively the molecular mass of species i and the mean atmospheric molecular mass expressed in atomic mass units.

By analogy with equation (19), the turbulent diffusion velocity v_{iK} is given by

$$v_{iK} = -\frac{K}{f_i} \frac{\partial f_i}{\partial z} = -K \times \left(\frac{1}{n_i} \frac{\partial n_i}{\partial z} + \frac{1}{H} + \frac{1}{T} \frac{\partial T}{\partial z} \right) \tag{22}$$

where $f_i = n_i/n$ is the volume mixing ratio of constituent i and H is the atmospheric scale height associated with the total pressure.

There is no analytical expression for the turbulent (or eddy) diffusion coefficient K in $cm^2 s^{-1}$ which is actually defined by expression (22). In two or three–dimensional models K can be considered as a tensor. Usually an identical value is used for all constituents.

Molecular diffusion and turbulent diffusion are two competitive processes. Molecular diffusion tends to separate gases according to their mass and turbulent diffusion tends to mix all gases such that their volume mixing ratio remains constant with height. It is, therefore, important to estimate their relative importance.

Perfect mixing distribution ($v_{iK} = 0$) and diffusive equilibrium distribution ($v_{iD} = 0$) are the two extreme cases. An inert constituent can switch from one case to the other depending on the values of the coefficients D_i and K. Such a situation is illustrated in Figures 4 and 5 which correspond to a gas having a mass smaller than the mean molecular mass and to a gas with a mass greater than the mean molecular mass. The region where $K \gg D_i$ is the homosphere characterized by perfect mixing for major constituents and inert minor constituents such as helium and argon. The region where $D_i \gg K$ is the heterosphere characterized by molecular diffusive separation. Figure
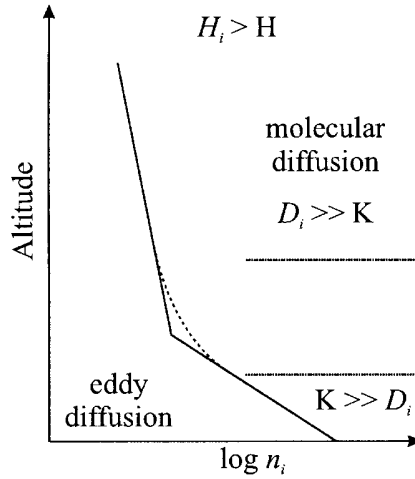
$H_i > H$

molecular
diffusion

$D_i \gg K$

eddy
diffusion

$K \gg D_i$

$\log n_i$

Altitude

Figure 4. Schematic vertical distribution of light constituent.

$H_i < H$

molecular
diffusion

$D_i \gg K$

eddy
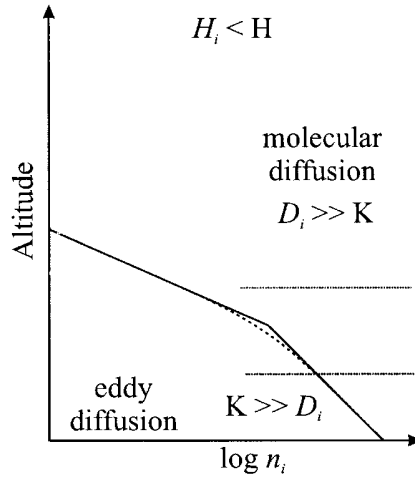diffusion

$K \gg D_i$

$\log n_i$

Altitude

Figure 5. Schematic vertical distribution of a heavy constituent.

4 corresponds to the case for helium since H_i is greater than the atmospheric scale height H. The abundance of helium decreases less in the heterosphere than in the homosphere. A reverse situation can be seen on Figure 4 which can be applied to argon.

If we assume in equation(19) that constituent i is in perfect mixing, i.e $\partial n_i/(n_i\partial z) = -(1/H) - (1/T)(\partial T/\partial z)$, the maximum molecular diffusion transport velocity is given by

$$v_{iDmax} = +\frac{D_i}{H}\left[1 - \frac{H}{H_i} - \frac{\alpha_i H}{T}\frac{\partial T}{\partial z}\right] \tag{23}$$

Similarly, if the constituent i is supposed to be in diffusion equilibrium i.e $\partial n_i/(n_i\partial z) = -(1/H_i) - [(1+\alpha)/T](\partial T/\partial z)$, then the maximum transport velocity resulting from turbulence can be obtained with equation (19)

$$v_{iKmax} = -\frac{K}{H}\left[1 - \frac{H}{H_i} - \frac{\alpha_i H}{T}\frac{\partial T}{\partial z}\right] \tag{24}$$

These two velocities have opposite signs and are equal in absolute value when $D_i = K$. As an example Figure 6 shows the maximum molecular diffusion velocity for atomic hydrogen and helium in the transition region between the homosphere and the heterosphere. The fact that these velocities
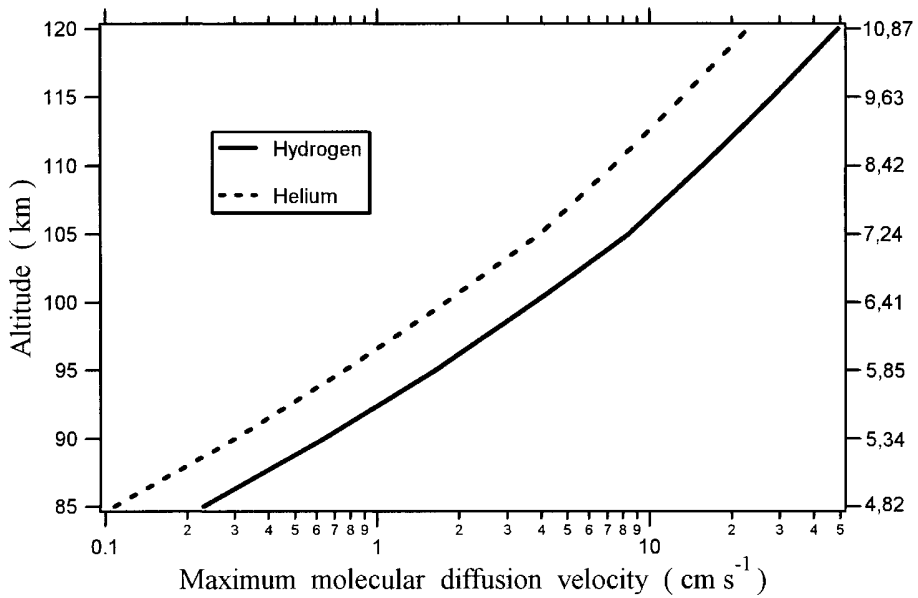
Figure 6. Maximum molecular diffusion velocity for He and H. Numbers on the righthand scale are the atmospheric scale heights in km corresponding to the altitudes of the lefthand scale.

are positive means that the transport occurs upwards. Furthermore, these velocities are usually much smaller then the global transport velocities. But their effect can be very important as it will be shown in section 6.

Instead of using the concept of maximum transport velocity, several authors [14] prefer to use the concept of limiting flow which is the maximum transport velocity times the corresponding concentration. The two approaches are equivalent. However, it should be noted that the maximum transport velocity depends on the nature of the constituent but not on its abundance, contrary to the limiting flow.

5. USEFUL APPROXIMATIONS

The full solution of equation (13) is not a trivial task. However, it is possible to develop useful approximations which usually are valid only over a specific altitude range.

- When the lefthand part of equation (13) is completely neglected, one gets a *photochemical equilibrium* situation for which production rates P_i are exactly balanced by loss rates $n_i L_i$. For each constituent, one has

$$P_i = n_i \times L_i \tag{25}$$

- When all transport phenomena are neglected, one obtains the *time evolution of the photochemical equilibrium*

$$\frac{\partial n_i}{\partial t} = P_i - n_i \times L_i \tag{26}$$
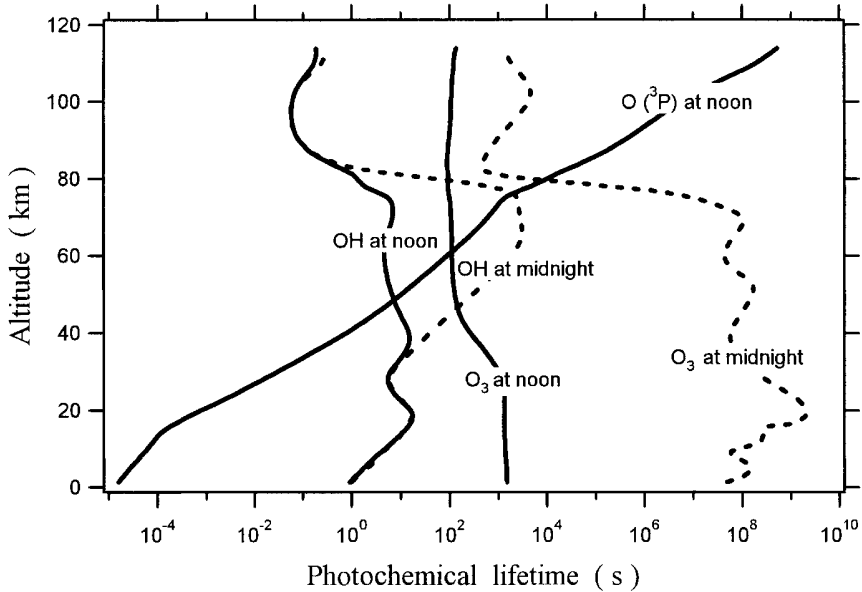
Figure 7. Chemical lifetimes for several constituents. Data used in this figure are kindly provided by Chabrillat [15].

The last two equations can be used to define a chemical lifetime τ_c by $1/L_i$. Figure 7 shows the chemical lifetimes for several constituents in the homosphere and lower thermosphere These lifetimes are computed by Chabrillat [15] after the full equation (13) including transport is solved. They correspond to the equator. It should be noted from Figure 7 that a huge domain of values is possible from 10^{-4} to 10^9 s. If ozone can be considered nearly in photochemical equilibrium at noon above 40 km (lifetime < 100 s), this is not at all the case at midnight. In the mesosphere O (^{3}P) is never in photochemical equilibrium.

- When time variations are neglected the full equation leads to the *general steady state*

$$\operatorname{div}(n_i \, \boldsymbol{W}_i) = P_i - n_i \times L_i \tag{27}$$

- When a constituent is not produced or destroyed by chemical reactions, one gets the *transport time evolution*

$$\frac{\partial n_i}{\partial t} + \operatorname{div}(n_i \, \boldsymbol{W}_i) = 0 \tag{28}$$

This form is suitable for a study of inert gases such as helium or argon.

- In the heterosphere atomic hydrogen is characterized by a constant upward flux which is very close to the maximum molecular diffusion flux obtained from equation (23). In this case one can use the *steady state equation with constant flux*

$$\operatorname{div}(n_i \, \boldsymbol{W}_i) = 0 \quad \text{or} \quad n_i \, \boldsymbol{W}_i = \text{constant} \tag{29}$$

This equation can be integrated analytically (Banks and Kockarts [13], Kockarts [4]).

A schematic vertical distribution obtained from equation (29) is shown on Figure 8. An interesting effect can be seen in the heterosphere on this figure. The two dashed curves correspond to diffusive
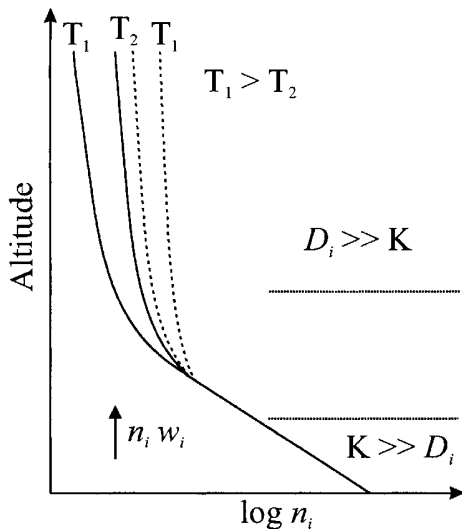
Figure 8. Schematic vertical distribution of light constituent with a constant upward flux.

equilibrium distributions characterized by two temperatures such that $T_1 > T_2$. The highest temperature leads to the highest concentration. But, when a constant upward flux exists and is close to the maximum diffusion flux, it is seen from the full line curves that a lower temperature leads to a higher concentration. This is the case for atomic hydrogen in the heterosphere.

6. HOMOSPHERE–HETEROSPHERE TRANSITION

Molecular diffusion and turbulent diffusion exist simultaneously at any height in a collisional dominated atmosphere. A competition occurs, however, between these two types of transport. Figure 9 shows vertical profiles of the molecular diffusion coefficient for molecular nitrogen (D_{N_2}) and turbulent diffusion coefficient (K), also called eddy diffusion coefficient. The two distributions of the turbulent diffusion coefficient reflect real variations and uncertainties. On sees that in the homosphere below 100 km altitude, the turbulent diffusion coefficient is always greater than the molecular diffusion coefficient. For this reason, all inert atmospheric components can be considered in perfect mixing. Their vertical profiles depend on the atmospheric scale height. In the heterosphere, molecular diffusion becomes progressively the most important transport process. The vertical decrease of individual constituents depends now on their own scale height H_i.

This simple view must be refined, since photochemical reactions can influence the vertical distributions. In particular this is true for molecular oxygen (O_2) which can be photodissociated leading to atomic oxygen (O). Let us consider the following two processes
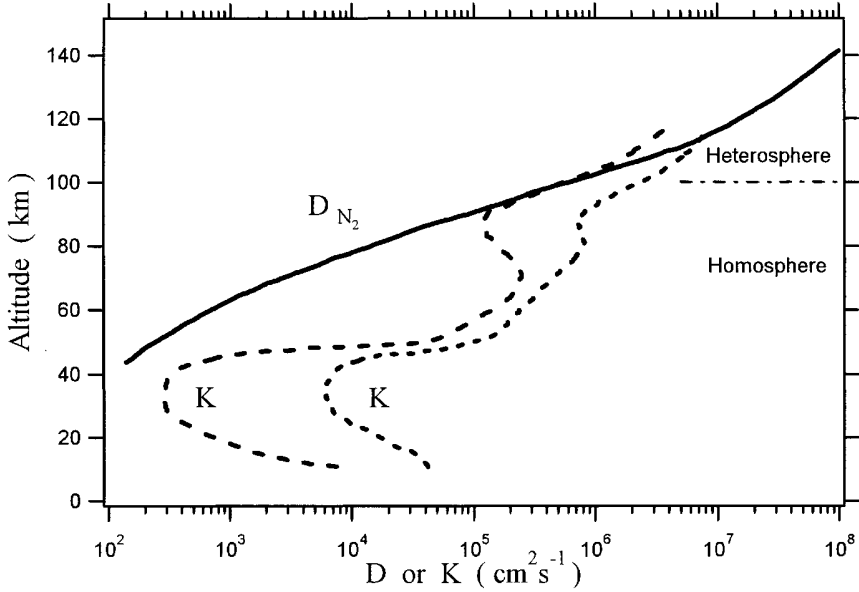
$$O_2 + h\nu \rightarrow O + O \tag{30}$$

where $h\nu$ is the photon energy leading to photodissociation with a coefficient J_2 in s^{-1}, and the three body recombination

$$O + O + M \rightarrow O_2 + M \tag{31}$$

with a rate coefficient k_0 in cm^6 s^{-1}. M is any third body.

Neglecting all transport processes, the time dependent evolution of atomic oxygen is given by

$$\frac{\partial n(O)}{\partial t} = 2 \times J_2 \times n(O_2) - 2 \times k_0 \times n(M) \times n^2(O) \tag{32}$$

Figure 9. Vertical distribution of the molecular nitrogen diffusion coefficient and two distributions of the turbulent diffusion coefficient.

This equation can be written

$$\frac{\partial n}{\partial t} + \alpha \times n^2 = P \tag{33}$$

where $n = n(O)$, $\alpha = 2 \times k_0 \times n(M)$ and $P = 2 \times J_2 \times n(O_2)$.

Integration of equation (33) leads to

$$n(t) = (P/\alpha)^{1/2} \times \frac{1 + C \exp\left[-2 \times t \times \sqrt{P \times \alpha}\right]}{1 - C \exp\left[-2 \times t \times \sqrt{P \times \alpha}\right]} \tag{34}$$

with $C = [n(t=0) - n_{eq}]/[n(t=0) + n_{eq}]$ and $n_{eq} = (P/\alpha)^{1/2}$.

It is now possible to define a characteristic time τ_{phot} to reach photoequilibrium

$$\tau_{phot} = 1/[2(P\alpha)^{1/2}] = 1/[4k_0 n(M) n_{eq}(O)] \tag{35}$$

with

$$n_{eq}^2(O) = J_2 n(O_2)/[k_0 n(M)] \tag{36}$$

Around 90 km, equation (35) leads to a characteristic time of the order of 10^6 seconds, i.e. more than 10 days. Such a long time should be compared to characteristic times for molecular and turbulent diffusion in order to know which phenomena are predominant.

A characteristic time can be defined as the ratio between a characteristic length and a characteristic velocity. The atmospheric scale height H is a typical characteristic length, since it represents the distance over which the concentration decreases by un factor e^{-1}. Equation(23) shows that D_i/H is a good characteristic velocity.

Therefore, the characteristic time for molecular diffusion transport can be written

$$\tau_D = H/(D_i/H) = H^2/D_i \tag{37}$$

Similarly the characteristic time for turbulent diffusion transport is given by

$$\tau_K = H/(K/H) = H^2/K \tag{38}$$

When equation (37) is applied around 90 km altitude, one finds that τ_D is of the order of 10^4 seconds, i.e. a time negligible compared to the characteristic time for photoequilibrium given by equation (35). As a consequence, at 90 km, molecular diffusion should influence the vertical distribution of atomic oxygen. These considerations provide the key for an understanding of Figure 10. When molecular
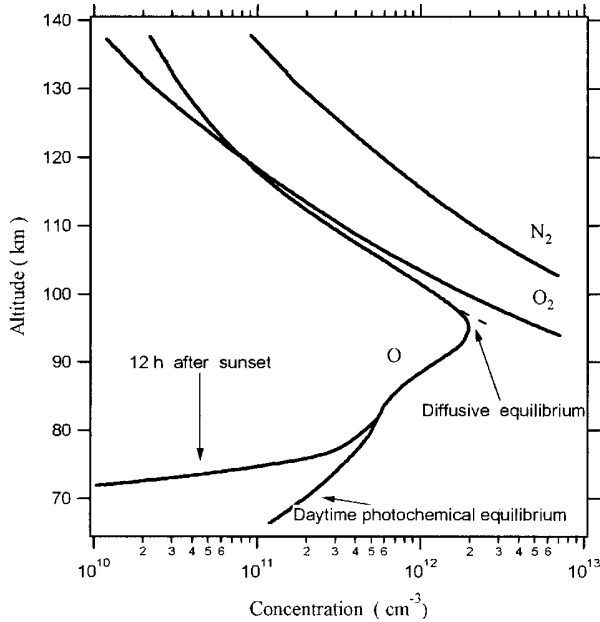

Figure 10. Transition from the homosphere to the heterosphere.

oxygen is photodissociated in the homosphere, several processes can influence the so produced oxygen atoms.

- Besides other reactions, atomic oxygen can recombine by a three body reaction. Since the third body M increases with decreasing altitude, atomic oxygen should decrease with decreasing altitude below a certain height as be seen on Figure . Furthermore, there is no more photodissociation after sunset, so that the decrease becomes even more important. The sink process by three body recombination leads to a downward transport of atomic oxygen, although its atomic mass (16 amu) is smaller than the atmospheric mean molecular mass (28.9). This means that chemistry can modify transport.

- Below 80 km one has always $\tau_K < \tau_D$ or $K > D_i$ implying that turbulent diffusion is the dominant vertical transport. Advection can also play a role. Between 80 km and 120 km, τ_K becomes comparable to τ_D and molecular diffusion transport becomes more and more important.

- Above 120 km, turbulent diffusion becomes negligible and molecular diffusion is the major transport mechanism. this explains why atomic oxygen becomes more important than molecular oxygen

Finally in the heterosphere, molecular diffusion is so important that minor constituent in the homosphere can become major in the heterosphere. Figure 11 shows the altitude, where the following
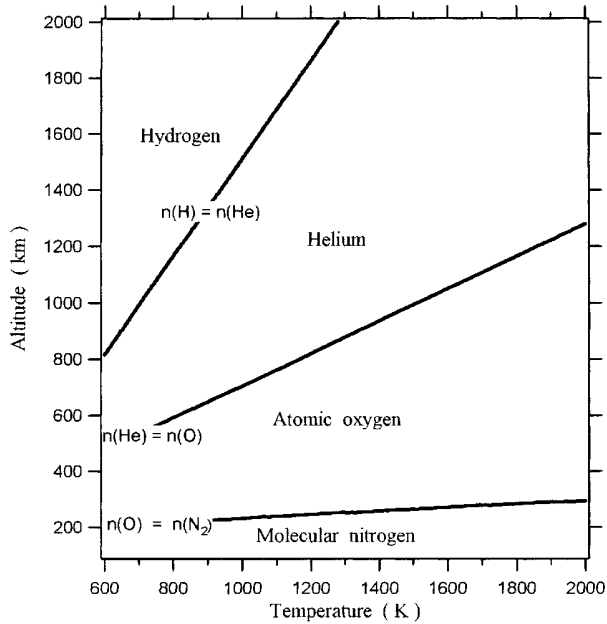
Figure 11. Schematic view of the different belts in the heterosphere as a function of the thermopause temperature.

relations between concentrations occur $n(O) = n(N_2)$, $n(He) = n(O)$ and $n(H) = n(He)$. These altitudes depend on the thermopause temperature which enter in the individual scale height of these constituents.

The transition from the homosphere to the heterosphere is, therefore, explained by the competition between photochemistry, turbulent diffusion transport and molecular diffusion transport.

7. HETEROSPHERE–EXOSPHERE TRANSITION

In the heterosphere, the concentrations of N_2, O, O_2, He and H decrease exponentially so that one could imagine that they tend asymptotically to zero. Reality is more complicated.

All particles in the heterosphere can characterized by a Maxwellian velocity distribution function with a given kinetic temperature. This implies a collision frequency and a mean free path between collisions. At ground level, this mean free path is of the order of 10^{-6} cm. Gas kinetic theory permits to compute the mean free path as a function of altitude as shown in Figure 12. Above 300 km altitude, the mean free path reaches values of several hundreds or even thousands kilometers. The triangles in Figure 12 indicate the altitude where the mean free path is equal to the local atmospheric scale height. This altitude is usually called the *critical level* or *exobase* which is the beginning of the exosphere. In a collisionless medium, several types of particles can be considered according to their trajectories. Four types of particles crossing a volume element are shown on Figure 13.

- The *ballistic* particles φ_1 which are launched from one point of the exobase and come back to an other point.

- The *satellite* particles φ_2 which orbit around the Earth.

- The *hyperbolic* particles φ_3 which leave or reach the critical with a velocity equal or greater than the escape velocity (11 km s^{-1}).
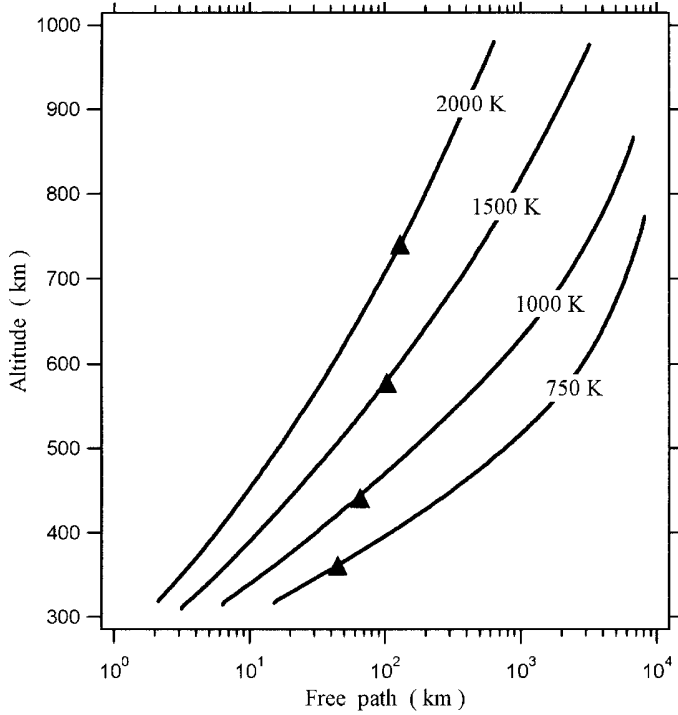
Figure 12. Mean free path as a function of height for several thermopause temperatures.
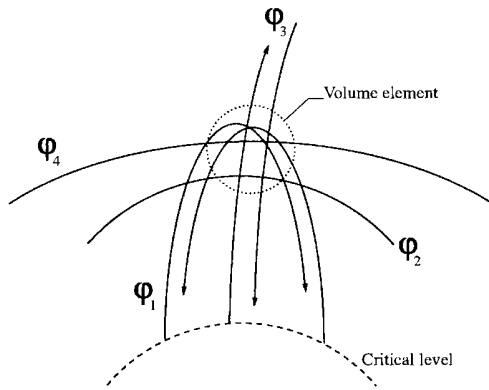

Figure 13. Possible types of particles in the exosphere.

- The *external hyperbolic* particles φ_4 which are deflected by the Earth's gravitational field.

If the velocity distribution in the exosphere is Maxwellian, i.e. is a solution of Boltzmann's equation without collisions, then

$$\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4 = 1 \tag{39}$$

Analytical expressions can be derived for each type of particles [13] either from Boltzmann's equation without collisions or from Liouville's theorem. If all types of particles are present, equation (39) leads to a hydrostatic distribution for a given constituent.

Simple physical considerations show that this is not the case. For the ballistic particles, the heterosphere should be perfectly symmetrical, although diurnal and seasonal variations exist. For satellite particles, there should be no external action capable to modify the orbit. Actually, these particles are subject to ionization and the resulting ions are deflected by the geomagnetic field. Furthermore, solar radiation pressure can distort the orbit. Hyperbolic particles are possible if, at the exobase, they have an upward velocity greater than the escape velocity. Hyperbolic particles coming from outside and crossing the critical level can be neglected, since there would be no net escape flux. Therefore, one considers only $\varphi_3/2$. External hyperbolic particles are also neglected since they are not of terrestrial origin.

The effect of these particles on exospheric concentration is shown on Figure 14. Hydrostatic
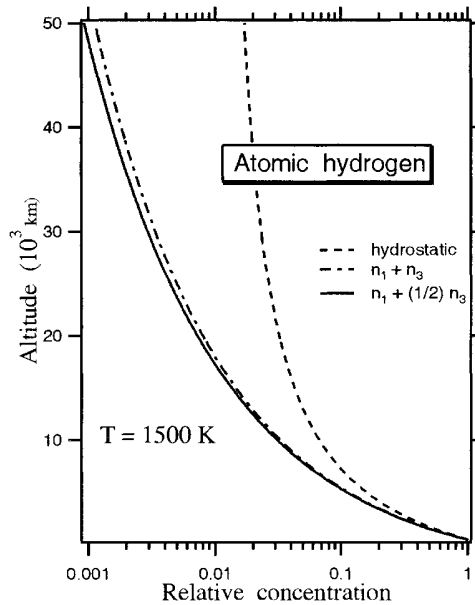

Figure 14. Exospheric vertical distributions of atomic hydrogen for a thermopause temperature of 1500 K.

distribution which would be correct when all types of particles are present, are given by the dashed lines. The full line correspond to $n_1 + n_3/2$, i.e. ballistic particles and half of hyperbolic particles. The dotted dashed line for hydrogen correspond to ballistic particles plus all hyperbolic particles. It should be noted that the difference between exospheric distributions and hydrostatic distributions is more important for hydrogen than for helium.

Since up going hyperbolic particles are lost from the atmosphere, a permanent upwards flux exists in the exosphere. This flux is called *escape flux* and results from particles with kinetic energy greater than gravitational potential energy. This condition leads to

$$v_c > (2 \times g_c \times r_c)^{1/2} \tag{40}$$

where v_c is the escape velocity and g_c is the gravity acceleration at geocentric distance r_c.

It is rather easy to compute the thermal escape flux F_c by integrating a Maxwellian velocity distribution function multiplied by the vertical component of the velocity between v_c and ∞. The result is given by

$$F_e = \frac{1}{2} n_c \left(\frac{2 k T}{\pi m}\right)^{1/2} \left(1 + \frac{m v_c^2}{2 k T}\right) \exp\left(-\frac{m v_c^2}{2 k T}\right) \tag{41}$$

where n_c is the particle concentration with mass m at the critical level. It should be noted that the escape flux depends exponentially of the mass of the particles.

The *effusion velocity* v_e defined by $v_e = F_c/n_c$ is shown on Figure 15. The effusion velocity for
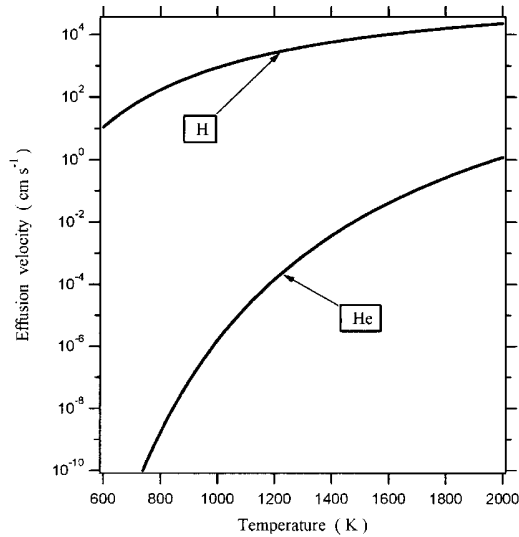
Figure 15. Effusion velocity for helium and hydrogen at 500 km as a function of the thermopause temperature.

helium is several orders of magnitude smaller the for hydrogen Therefore, the thermal escape flux for helium cannot eliminate the degassing flux of the order of 10^6 cm^{-2} s^{-1} coming from the crust and the mantle of the Earth. But we know that helium does not accumulate in the atmosphere. Other escaping mechanisms, such as the polar wind for helium ions, must be invoked (see [16]).

For hydrogen, the thermal escape flux is sufficient to explain the abundance of this constituent which results essentially from photodissociation of water vapor and methane in the mesosphere and lower thermosphere. Other escaping mechanisms, such as charge exchange with energetic protons also contribute to the hydrogen budget. Considering that a flux of the order of 10^8 cm^{-2} s^{-1} comes from H_2O, the Earth loses 84 tons of atomic hydrogen corresponding to 1500 tons of water in 24 hours. Total amount of water on Earth is of the order of 1460×10^{15} tons, so it is not tomorrow that the Earth will be completely dry. However, this escaping mechanism is responsible for the low abundance of water on planets like Mars or Venus.

8. CONCLUSION

Transport phenomena affect the atmospheric structure at any altitude from ground level to interplanetary space.

The nature of the effects depend essentially on external forces acting on the atmospheric components. Forces resulting from gravitational field and from Earth's rotation have the same action on all constituents. Other forces can be specific to a particular constituents. This is the case for ion drag and atmospheric drag which indicates that above 100 km interaction between the neutral atmosphere and the ionosphere is a dominant mechanism. Since ion and electron movements are influenced by the geomagnetic field and eventually by external electric fields, another complexity arises.

Even photochemistry can play a role and compete with molecular and turbulent diffusion. These three processes are necessary to explain the transition between the homosphere and the heterosphere where the constituents diffuse according to their own mass.

Due to the exponential decrease of the total concentration the mean free path increases with height such that the collisions frequency between particles becomes negligible. Even in the collisionless exosphere transport of particles occurs, leading to an escape flux by which the Earth loses definitely an amount of matter.

Transport phenomena are an essential ingredient to understand many atmospheric processes. A rigorous treatment is practically impossible and one should always be aware of underlying hypotheses when applying a numerical technique to solve a specific problem.

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