

HELIUM AND HYDROGEN DISTRIBUTIONS IN THE UPPER ATMOSPHERE

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ABSTRACT : The physical processes involved in the computation of helium and hydrogen distributions are described for steady state conditions. A solution of the general transport equation is given to indicate the effects of molecular and eddy diffusion. The concept of maximum transport velocity is introduced in relation to the initial distribution prevailing at an altitude of about 100 km. The effect of eddy diffusion is particularly important for the helium distribution. Variations of a factor of 4 in the helium concentration at high altitude can be explained by a change of a factor of 10 for the eddy diffusion coefficient in the 100 km region.

1. - Introduction

The study of the upper atmosphere above 100 km has developed greatly since the first rocket soundings in 1945. It has been possible to show that the atmospheric density decreases less between 100 km and 200 km than between ground level and 100 km. The diffusion effect in the earth's gravity field was theoretically derived by Nicolet and Mange (1954), and has been confirmed by the observation of molecular oxygen up to an altitude of 180 km (Byram et al., 1957). Observations of the atomic hydrogen Lyman- α nightglow (Kupperian et al., 1958) indicated that atomic hydro-

gen can play a significant role above 100 km altitude. These results imply that there must be a change in the composition of the upper atmosphere (Mange, 1955; Nicolet, 1960; Mange, 1961).

Since 1957, considerable progress has been made concerning the density distribution deduced from satellite drag data. Even by using round figures, it is possible to show that the decrease in density at high altitude is completely different from the decrease observed between ground level and a height of 100 km. Within the first hundred kilometers, the density decreases roughly from $10^{-3} \text{ g cm}^{-3}$ to $10^{-9} \text{ g cm}^{-3}$, whereas between 150 km and 400 km, between 400 km and 700 km, and between 700 km and 1800 km, the decrease is successively of the order of a factor of 100.

A general understanding of this situation can be obtained from the hydrostatic equation and from the perfect gas law. These equations lead to the general relation:

$$\frac{d\varrho}{\varrho} + \frac{dT}{T} - \frac{dm}{m} = - \frac{dz}{kT/mg} \quad (1)$$

where ϱ , T and m respectively represent the density, the temperature and the mean molecular mass at a height z, where g is the gravity acceleration. Equation (1) shows that the slow decrease in the density is due to an increase in the atmospheric scale height H given by:

$$H = kT/mg \quad (2)$$

where k is Boltzmann's constant.

An increase in H with height can be due to two factors: an increase in the temperature T and/or a decrease in the mean molecular mass m. The temperature increase is directly related to solar ultraviolet heating and to heat transport. A decrease in the mean molecular mass can arise from a diffusive separation of the atmospheric constituents. At ground level, a mean molecular mass of 29 corresponds to an atmospheric compo-

sition of 21% O₂, 78% N₂ and 1% Ar. If diffusion prevails above a certain height, the mean molecular mass can a priori reach a value of 1 amu (atomic hydrogen) after passing through the values corresponding to atomic oxygen (16 amu) and to helium (4 amu). The helium mixing ratio is 5.24x10⁻⁶ (Gluckauf, 1946) at ground level, and can reach values of the order of 1 in the upper atmosphere.

The problem is even more complex for hydrogen, which does not exist in its atomic form at ground level. Below 100 km, atomic hydrogen is produced through photodissociation of water vapour and methane, as well as through oxidation reactions of excited O(¹D) atoms with CH₄, H₂ and H₂O (Nicolet, 1970). These minor constituents are subject to molecular and eddy diffusion below 100 km, and an atomic hydrogen concentration of 3x10⁷ cm⁻³ corresponds to a relative abundance of the order of 2x10⁻⁶ at 100 km altitude. At greater heights, this relative abundance also increases, and diffusive transport successively creates an atomic oxygen belt, a helium belt and an atomic hydrogen belt. In this paper, the physical processes responsible for the increase in the He and H relative abundances will be described under steady state conditions.

2 - Diffusion Equation

When an atmospheric component is transported by diffusion in the atmosphere, it is possible to express the flow $F = n_i w$ of particles 1 in the form:

$$F = F_D + F_E \quad (3)$$

where F_D represents the flux due to molecular diffusion, and F_E is the flux due to eddy diffusion.

The molecular diffusion flow tends to distribute the different species according to their own mass, whereas eddy diffusion tends to maintain a mixing distribution in which all atmospheric constituents are distributed according to the mean molecular mass. Chemical reactions, photodissociation and ionization processes can compete with diffusive transport. If

these processes are fast enough, a particular atmospheric constituent will have a vertical distribution independent of molecular or eddy diffusion effects. For example, in the daytime, mesosphere ozone is always in photoequilibrium, since photodissociation is rapid and only a time of the order of 100 sec is required to reach the photoequilibrium conditions. This means that the times necessary to reach molecular diffusion equilibrium or mixing conditions are too long compared to the photodissociation time, for diffusion to be important. This is not the case for helium and hydrogen in the thermosphere, however.

For a two-component gas, the relative molecular diffusion velocity ($w_1 - w_2$) can be written (Chapman and Cowling, 1939):

$$w_1 - w_2 = - D_{12} \left[\frac{n^2}{n_1 n_2} \frac{d(n_1/n)}{dz} + \frac{m_2 - m_1}{m} \frac{1}{p} \frac{dp}{dz} + \frac{\alpha}{T} \frac{dT}{dz} \right] \quad (4)$$

In this equation, the subscripts 1 and 2 refer to the component 1 and 2, respectively. D_{12} is the molecular diffusion coefficient, p is the total pressure, α is the thermal diffusion factor, and $n = n_1 + n_2$ is the total concentration. The other symbols have the same meaning as in equations (1) and (2). From equation (4) we can see that molecular diffusion arises from three different effects; namely, concentration, pressure and temperature gradients.

If it is assumed that there is no net flow through an elementary surface at a height z , i.e., if:

$$n_1 w_1 + n_2 w_2 = 0 \quad (5)$$

then, equation (4) can be transformed into:

$$w_1 = - D_{12} \left[\frac{1}{n_1} \frac{dn_1}{dz} - \frac{1}{n} \frac{dn}{dz} + \frac{(m_2 - m_1)}{mn} \frac{n_2}{p} \frac{dp}{dz} + \alpha \frac{n_2}{n} \frac{1}{T} \frac{dT}{dz} \right] \quad (6)$$

Using the hydrostatic equation and the perfect gas law, equation (6)

can be written:

$$w_1 = - D_{12} \left[\frac{1}{n_1} \frac{dn_1}{dz} + \frac{1}{H_1} + \left(1 + \alpha \frac{n_2}{n}\right) \frac{1}{T} \frac{dT}{dz} \right] \quad (7)$$

where $H_1 = kT/m_1 g$ is the pressure scale height of the constituent 1.

Since helium and hydrogen are minor constituents in the lower thermosphere, their concentration and density are negligible compared to the total concentration n and to the total density ρ . In this case, equation (7) becomes:

$$w_1 = - D_{12} \left[\frac{1}{n_1} \frac{dn_1}{dz} + \frac{1}{H_1} + (1 + \alpha) \frac{1}{T} \frac{dT}{dz} \right] \quad (8)$$

A binary diffusion equation is used here, since the minor constituent is assumed to diffuse through another component which is actually the sum of all the major atmospheric constituents (O , O_2 and N_2). The molecular diffusion coefficient is therefore given by:

$$D_{12} = D_{IM} = \frac{3\pi}{32Q} \left(1 + \frac{m_1}{m}\right)^{1/2} \left(\frac{8kT}{\pi m_1}\right)^{1/2} \frac{1}{n} \quad (9a)$$

where Q is a momentum transfer cross section, m is the mean molecular mass, variable with height, and n is the total concentration. For a momentum transfer cross section of $2.83 \times 10^{-15} \text{ cm}^2$, the molecular diffusion coefficient (9a) in $\text{cm}^2 \text{sec}^{-1}$ is given by:

$$D_{IM} = 1.96 \times 10^6 \left(\frac{1}{m_1} + \frac{1}{m}\right)^{1/2} \frac{T^{1/2}}{n} \quad (9b)$$

where the masses m_1 and m are expressed in g, n in cm^{-3} and T in $^{\circ}\text{K}$. Fig. 1 shows the vertical distribution of the molecular diffusion coefficient for helium between 85 km and 120 km. The total concentration is also re-

presented in the same figure which indicates the large increase in $D_{He,M}$ proportional to the decrease of $n = \sum n_i$.

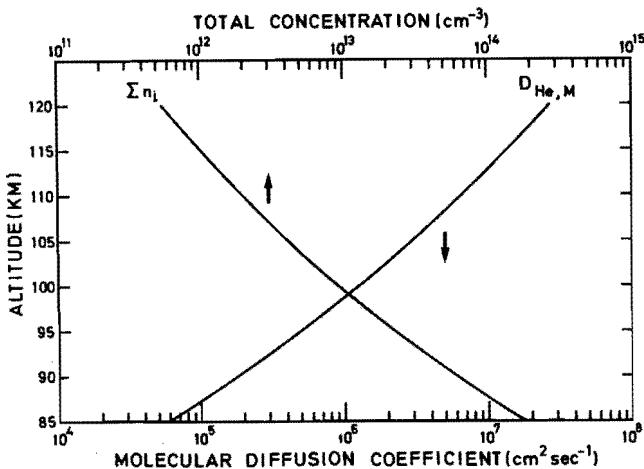


Fig.1 : Vertical distribution of the molecular diffusion coefficient for helium and of the total concentration.

The effect of thermal diffusion on the helium vertical distribution has been discussed by Kockarts (1963) and the thermal diffusion factor a can be taken as equal to -0.38 for helium and hydrogen. The thermal diffusion factor actually depends on the relative abundance of the diffusing component (Chapman and Cowling, 1952), but in the region where thermal diffusion is found to be important, helium and hydrogen are always minor constituents. Under these conditions, the interaction potential between the minor and the major component is not as important as when both constituents are of the same order of magnitude. The value -0.38 is then obtained for a rigid sphere interaction potential between the minor constituent (He or H) and molecular nitrogen which is the major component in the region where important temperature gradients exist.

Following Lettau (1951), the vertical eddy diffusion velocity w_e can be written as:

$$w_E = - K \frac{d(n_1/n)}{dz} / (n_1/n) \quad (10)$$

where K is the eddy diffusion coefficient.

Using the general relation:

$$\frac{dn}{n} = - \frac{dz}{H} - \frac{dT}{T} \quad (11a)$$

which arises from the hydrostatic equation:

$$\frac{dp}{dz} = - \rho g \quad (11b)$$

equation (10) becomes:

$$w_E = - K \left[\frac{1}{n_1} \frac{dn_1}{dz} + \frac{1}{H} + \frac{1}{T} \frac{dT}{dz} \right] \quad (12)$$

If we introduce a parameter $\Lambda = K/D$, equation (3) can be transformed into the following expression, by using (8) and (12):

$$\frac{dn_1}{dz} + \left[\frac{1}{1+\Lambda} \left(\frac{1}{H_1} + \frac{\Lambda}{H} \right) + \left(1 + \frac{a}{1+\Lambda} \right) \frac{1}{T} \frac{dT}{dz} \right] n_1 = - \frac{F}{D_{12}(1+\Lambda)} \quad (13)$$

This expression is similar to the form proposed by Colegrove et al., (1966) for a multicomponent system. The only difference results from the expression for the diffusion coefficient D_{12} . Colegrove et al., (1966) use an expression in which $D_{12}^{-1} = \sum_j D_{1j}^{-1}$, where D_{1j} are the binary diffusion coefficients. It is interesting to note, however, that for the atmospheric mo-

dels used in the present work, expression (9b) and the relation $D_{12}^{-1} = \sum_j D_{1j}^{-1}$ yield the same numerical results if a common momentum transfer cross section is used for all the binary diffusion coefficients. When $\Lambda=0$, i.e., when eddy diffusion is neglected, equation (13) reduces itself to the relationship used by Kockarts and Nicolet (1962, 1963) for the computation of atomic hydrogen distributions. It will be shown later that the introduction of an eddy diffusion coefficient is more important for helium than for atomic hydrogen.

A general solution of equation (13) can now be written in the following form:

$$n_1(z) = n_{eq} \left[1 - \int_{z_1}^z \frac{F}{D_{12}(1+\Lambda)n_{eq}} dz' \right] \quad (14)$$

where z_1 is the altitude at which the concentration n_1 is given and n_{eq} is the solution of equation (13) when the flow F is zero. The equilibrium distribution n_{eq} will be discussed later. A solution of the same type as (14) has been presented by Donahue (1969) in an analysis of deuterium in the upper atmospheres of Venus and Earth.

3 - Transport Velocities

From Equation (14), we can immediately see that any departure from an equilibrium solution is related to the importance of the transport flow F compared to $D_{12}(1+\Lambda)$. When a significant flow is present, the corresponding concentration distribution is always less than the equilibrium distribution. It is therefore necessary to investigate the transport velocities associated with equations (13) or (14).

We shall first consider the physical conditions prevailing in the lower boundary region, where there is a tendency to diffusive separation. It is always possible to express the concentration gradient of a minor constituent as a function of the total concentration gradient in a form such as:

$$\frac{1}{n_1} \cdot \frac{dn_1}{dz} = X(z) \frac{1}{n} \frac{dn}{dz} \quad (15)$$

where $X(z)$ is the vertical distribution factor that is height dependent. Using relation (11), equation (15) can be written as:

$$\frac{1}{n_1} \frac{dn_1}{dz} = - X(z) \left[\frac{1}{H} + \frac{1}{T} \frac{dT}{dz} \right] \quad (16)$$

With the preceding equation, the total transport velocity w can be obtained from equation (13):

$$w = \frac{D_{12}}{H} \left[X - \frac{H}{H_1} - \frac{H}{T} \frac{dT}{dz} (1 + \alpha - X) \right] + \frac{K}{H} [X - 1] \quad (17)$$

where the contributions due to molecular diffusion and to eddy diffusion are respectively represented by the terms proportional to D_{12} and to K .

When the minor constituent n is characterized by a mixing distribution, the vertical distribution factor is equal to 1 in the region where mixing prevails. Under this condition, the transport velocity arises from molecular diffusion alone and equation (17) is reduced to:

$$w = \frac{D_{12}}{H} \left[1 - \frac{H}{H_1} - \frac{\alpha H}{T} \frac{dT}{dz} \right] \quad (18)$$

Actually, equation (18) represents the maximum molecular diffusion transport velocity for a constituent which follows the distribution of the major components. When the mass m_1 of the minor constituent is less than the mean molecular mass m , equation (18) shows that w is positive, i.e., directed upwards. This is the case for helium and hydrogen. In the case of Ar however, $w < 0$, i.e., downwards, since $m_1 > m$. Table 1 gives the maximum transport velocities between 100 km and 120 km for hydrogen, helium and argon. It can be seen that the molecular diffusion velocities are always of the order of a few cm sec^{-1} around a 100 km altitude. A knowledge of the concentration at the lower boundary thus immediately gives

the maximum flow which can be transported by molecular diffusion into the upper atmosphere.

TABLE 1 - Maximum molecular diffusion transport velocities (cm sec^{-1})

$z(\text{km})$	$H(\text{km})$	$T(^{\circ}\text{K})$	w_H	w_{He}	w_{Ar}
100	6.41	209.2	3.76	1.78	- 0.36
105	7.24	230.9	8.35	3.94	- 0.84
110	8.42	261.9	15.6	7.35	- 1.72
115	9.63	293.0	28.1	13.3	- 3.31
120	10.87	324.0	48.8	23.0	- 6.11

Since the molecular diffusion velocity is proportional to D_{12} , it increases with height. Above a certain level however, the diffusion equation can no longer be applied, since collisions become less frequent. This is the beginning of the exosphere, where collisions are neglected. Actually, the term F/D_{12} in equation (13) becomes less important with increasing height and the diffusive flow is controlled by escape from the earth's gravitational field. If r represents the geocentric height of the critical level, i.e., the beginning of the exosphere, it is possible to show that, at this level, the effusion velocity is given by (see for example Nicolet, 1957):

$$v = (g/2\pi)^{1/2} r H_1^{-1/2} (1 + H_1/r) e^{-r/H_1} \quad (19)$$

Fig.2 shows the effusion velocity of atomic hydrogen as a function of the thermopause temperature. The two curves correspond to critical levels fixed at 500 km and 1000 km. The critical level is actually temperature dependent, but this is not important for the present discussion. It is clear from Fig.2 that v varies more strongly with temperature than with height. Fig.3 shows the same situation for deuterium and here the importance of

the mass involved in H_1 is evident. For helium, the effusion velocity is

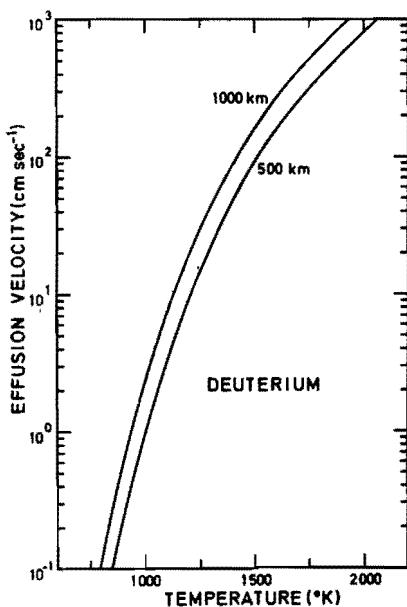


Fig.2 : Effusion velocity of atomic hydrogen as a function of the thermo-pause temperature for two critical levels, fixed at 500 km and 1000 km respectively.

always less than 1 cm sec^{-1} , even for temperatures as high as 2000°K . Fahr (1971) discussed some departures from expression (19), due to ballistic transport phenomena. Other processes can also lead to slight differences from equation (19) and the interested reader is referred to the paper by Brinkmann (1970). It should only be mentioned that corrections of the order of 10 to 20% in equation (19) do not modify the physical analysis presented here, since at the present time the concentration of atomic hydrogen is not known with an accuracy better than 20%.

Since the light particles are escaping from the earth's gravity field, it is possible to introduce the flow condition:

$$F = n_1(r) v(r) \quad (20)$$

at the critical level. Without loss or production in the upper atmosphere

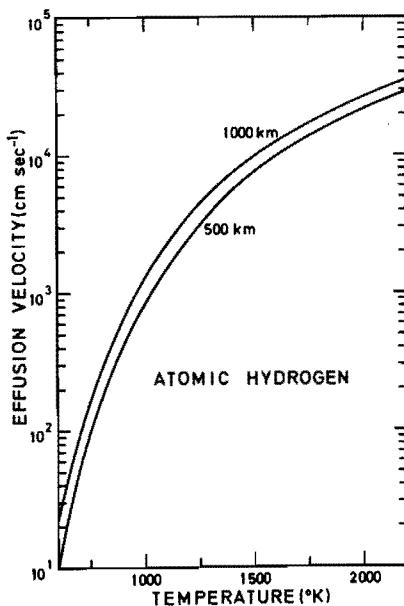


Fig.3 : Effusion velocity of deuterium as a function of the thermopause temperature for two critical levels, fixed at 500 km and 1000 km respectively.

where equation (13) is applied, the flux at two levels r_1 and r_2 must satisfy the condition

$$F_1 r_1^2 = F_2 r_2^2 \quad (21)$$

which arises from the equation of continuity. With equations (19), (20) and (21), it is then possible to compute the concentration distribution using (14).

4 - Vertical Distributions and eddy Diffusion

For a hydrogen concentration of the order of $4 \times 10^7 \text{ cm}^{-3}$ at 100 km, the maximum molecular diffusion flow is of the order of $1.5 \times 10^8 \text{ cm}^2 \text{ sec}^{-1}$, accord-

ing to Table 1. A hydrogen concentration of such an order of magnitude is required to explain the Lyman- α scattering observations (Donahue, 1966; Tinsley, 1969; Meier, 1970). Thus, the real upward flow through the lower thermosphere is practically identical to the maximum possible flow permitted by molecular diffusion. Solutions of equations (13) or (14) are presented in Fig. 4 for several thermopause temperatures. These vertical distributions of atomic hydrogen are similar to the results obtained by Kockarts and Nicolet (1962, 1963). In the numerical computation, eddy diffusion has been neglected ($\Lambda = 0$). This assumption is justified by the fact that between 100 km and 120 km the vertical distribution is almost identical to a mixing distribution, even though a molecular diffusion equation has been used. The physical reason for such a situation is the presence of a real flow which is nearly identical to the maximum molecular diffusion flow. For temperatures below 1000°K, the eddy diffusion can, however, affect the results, since upward transport fluxes are slightly reduced.

In the case of helium, the physical situation changes since the real flux of the order of $2 \times 10^6 \text{ cm}^{-2} \text{ sec}^{-1}$ is small compared to the maximum molecular diffusion flow which is about $10^8 \text{ cm}^{-2} \text{ sec}^{-1}$ at 100 km. When eddy diffusion is neglected, it is important to fix a level for the beginning of diffusive equilibrium. Kockarts and Nicolet (1962) have shown that an increase of 5 km for the beginning of the molecular diffusion leads to a decrease by a factor of two in the helium concentration at greater heights. Actually, there is a gradual change from mixing conditions to diffusion equilibrium. In order to analyze such a transition, it is worthwhile to develop the equilibrium solution n_{eq} used in equation (14). The integration of equation (13) knowing F/D_{12} gives the expression:

$$n_{eq}(z)/n_1(z_0) = (T_0/T) \exp \left\{ - \left[\int_{z_0}^z \left(\frac{1}{H_1} + \frac{\Lambda}{H} \right) (1+\Lambda)^{-1} dz' + \int_{z_0}^z \alpha (1+\Lambda)^{-1} \frac{dT}{T} \right] \right\}$$

(22)

where $n_i(z_0)$ is the concentration at a height z_0 , characterized by a temperature T_0 . If $\Lambda = 0$, equation (22) reduces to the usual equation for com-

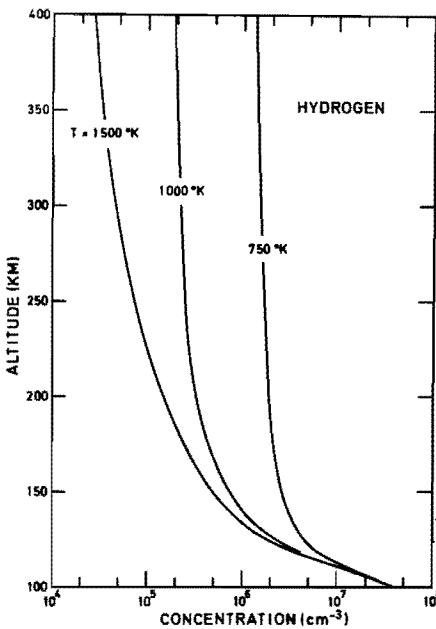


Fig.4 : Vertical distributions of atomic hydrogen for 750°K , 1000°K and 1500°K thermopause temperatures. The concentration at 100 km is $4 \times 10^7 \text{ cm}^{-3}$.

puting concentration in diffusive equilibrium.

The eddy diffusion coefficients are not well known at the present time. Therefore, the vertical distributions for helium, shown in Fig.5, are computed for several height-independent eddy diffusion coefficients. Since the molecular diffusion coefficient is $2.7 \times 10^7 \text{ cm}^2 \text{ sec}^{-1}$ at 120 km, the ratio $\Lambda = K/D$ varies between 3.7×10^{-1} and 3.7×10^{-2} , when K changes from $10^7 \text{ cm}^2 \text{ sec}^{-1}$ to $10^6 \text{ cm}^2 \text{ sec}^{-1}$ at 120 km altitude. Such a variation of K produces a change by a factor of 4 in the helium concentration. It should be noted that the introduction of an eddy diffusion coefficient leads to steeper helium concentration gradients between 100 km and 120 km altitude. These gradients are not produced by a transport flow, since equation (22)

implies a zero flow condition. Fig.6 shows how the helium concentration varies at 120 km as a function of the eddy diffusion coefficient. For a fixed thermopause temperature, it is therefore possible to explain variations in the helium concentration at greater heights by a change in the eddy diffusion coefficient in the 100 km region. However, for all the K values considered here, helium is in diffusive equilibrium above 120 km altitude. When an atmospheric model is calculated with $n(\text{He}) = (2 \pm 1) \times 10^7 \text{ cm}^{-3}$ at 120 km, this implies that below 120 km the eddy diffusion coefficient ranges between 10^6 and $5 \times 10^6 \text{ cm}^2 \text{ sec}^{-1}$.

In order to emphasize the importance of a study of the minor constituents H and He, Fig.7 shows how those components become major constituents above a height of 500 km. The difference in the extent of the helium belt in this figure compared to a similar figure given by Kockarts and Nicolet (1963) is due to an increase by a factor of 4 in the atomic hydrogen concentration. Fig.7 actually indicates the importance of diffusion in the upper atmosphere where successively an atomic oxygen belt, a helium belt and an atomic hydrogen belt are established by diffusive separation.

5 - Conclusion

The analysis of the general diffusion equation indicates the importance of transport processes in the earth's heterosphere. The structure of the upper thermosphere depends strongly on the behaviour of minor light constituents such as H and He in the lower thermosphere. Since the atomic hydrogen vertical flow leads to an important term in the diffusion equation, the vertical distribution of atomic hydrogen is completely different from the vertical distributions of the other constituents which are in diffusive equilibrium. The atomic hydrogen concentration, at any given level in the upper atmosphere, decreases with increasing temperature. It has also been shown that eddy diffusion is not as important for atomic hydrogen as for helium. This fact is justified by the greater transport flow for atomic hydrogen. It appears that important variations of the helium concentration at 120 km can be accounted for by

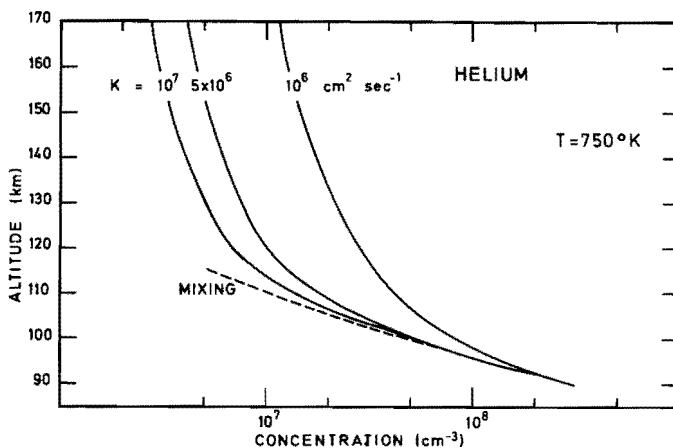


Fig.5 : Vertical distribution of helium in the transition region for eddy diffusion coefficients of $10^7 \text{ cm}^2 \text{ sec}^{-1}$, $5 \times 10^6 \text{ cm}^2 \text{ sec}^{-1}$ and $10^6 \text{ cm}^2 \text{ sec}^{-1}$, respectively. A complete mixing distribution is shown for comparison.

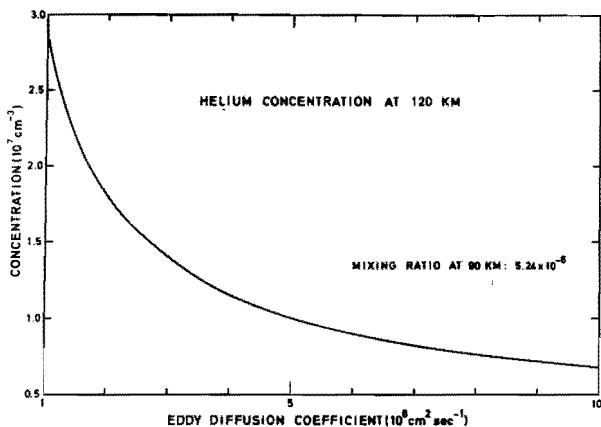


Fig.6 : Helium concentration at 120 km as a function of the eddy diffusion coefficient adopted above 90 km.

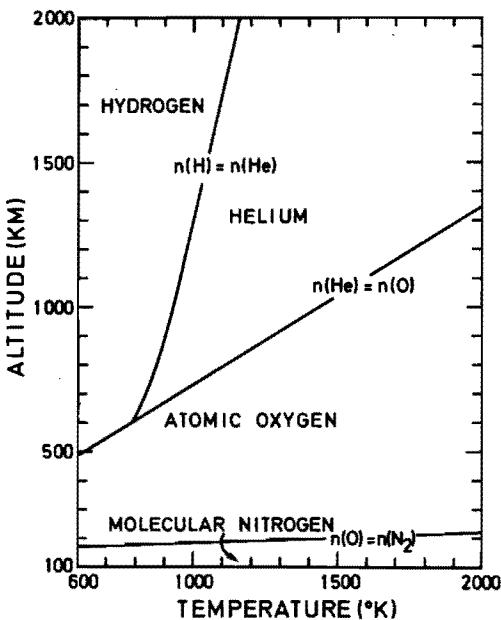


Fig. 7 : Atomic oxygen, helium and hydrogen belts as a function of the thermopause temperature. The curves give the altitude where the respective concentrations become equal.

changes in the eddy diffusion coefficient in the neighbourhood of 100 km.

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