Chapter 3

Structure and Composition of the Middle and Upper Atmosphere

In this section we describe the neutral atmosphere in the altitude range between 10km and 120km, i.e., the atmosphere above the "weather zone". The upper boundary of the weather zone may vary between 10-15km, sometimes visualized by high cirrus clouds. The middle atmosphere ranges between 10-90km and includes the stratosphere and the mesosphere. The upper atmosphere starts at 90km and includes the ionosphere, which will be described in more detail in Chapter 4.

Let us first ask the question: Why is it important and interesting to study the upper atmosphere? Some answers may be apparent:

- Solar-terrestrial coupling. The atmosphere is coupled to the interplanetary space, and atmospheric physics is of crucial importance to the study of the sun's contribution to, for example, climatic variations on the earth.
- The upper atmosphere acts like a shield, which absorbs high-energy radiation from the sun and outer space. This radiation consists mainly of X-rays, ultraviolet rays and high-energy particles. The high-energy particles, which especially intrude into the atmosphere at high latitudes, are manifest in the northern lights.
- High-energy particles form plasma in the upper atmosphere. This ionized layer is called the ionosphere and is relevant for the propagation of radio waves, which can be reflected and absorbed within the layer. The ionosphere is of great importance for radio communication and navigation.
- The natural plasma in the upper atmosphere can in many situations be used as a laboratory where one can study phenomena that are difficult to simulate in a lab with physical boundaries.
- Finally, it is important to be aware of the fact that the upper atmosphere contains small amounts of highly reactive matter, which is significant for the heat balance and absorption of radiation. Examples of such matter are ozone [O_3], atomic oxygen [O], nitrogen oxide [NO], water vapor [H_2O] and carbon dioxide [CO_2].

3.1 Energy balance in the upper atmosphere along general lines

Today, many resources are being used to explore the complicated and vital processes that determine the energy transformation in the sun-earth system. The middle and the upper atmosphere are of great importance in these processes, as illustrated in figure 3.1. We now give a brief description of energy sources and loss processes.

3.1.1 Energy sources

The primary energy source is, of course, the sun. A major part of the energy is carried by electromagnetic waves in the visible part of the spectrum (300-700nm) that penetrates the atmosphere down to the earth's surface. The energy is absorbed in the lower part of the atmosphere, in the oceans, and in the surface layer of the earth, giving rise to air and ocean dynamics known as weather phenomena. Some of the energy in these weather phenomena will propagate upwards as gravity waves that break near the top of the middle atmosphere, and hence create an important contribution to the energy balance there.

X-and ultraviolet radiation are absorbed by air molecules and represent an efficient heat source in the middle and the upper atmosphere. Within the polar cap and the auroral zone, energetic particles from the sun and magnetospheric boundary layers (electrons, protons and alpha particles) precipitate down into the

SOL

SOLVIND

ELEKTRONER, PROTONER

SYNLIG LYS

RØNTGEN

UV

HØYDE km

200

150

100

50

$\vec{J} = \tilde{\sigma} \vec{E}$

TURBULENT TRANSPORT

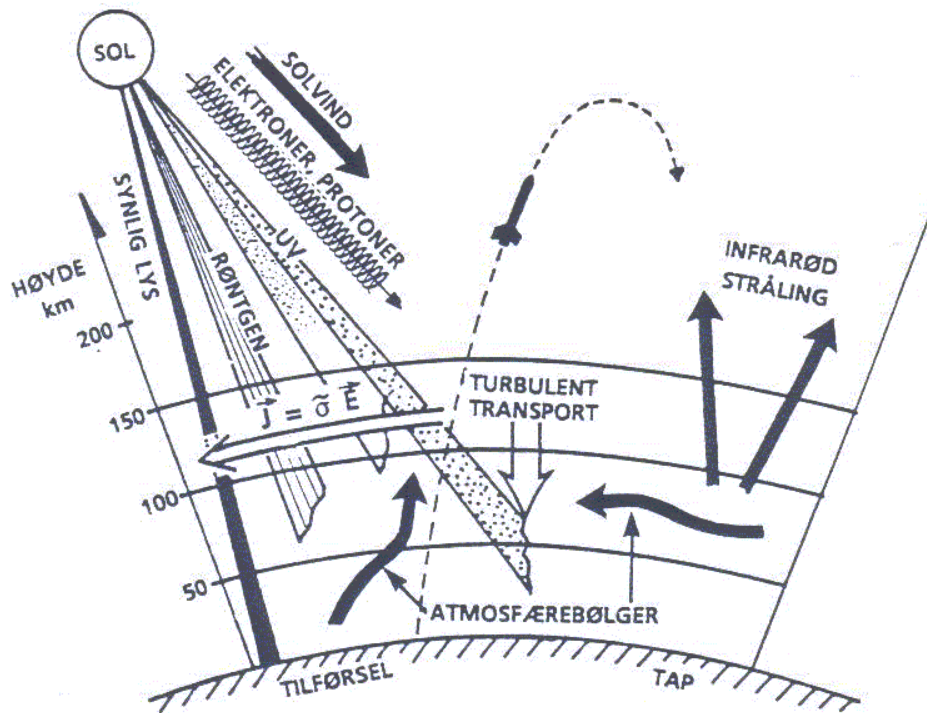INFRARØD STRÅLING

ATMOSFÆREBØLGER

TILFØRSEL

TAP

Figure 3.1.: Energy feeding and loss in the upper atmosphere

polar atmosphere and give rise to the aurora borealis and particle-impact ionization. Most of the energy related to particle fluxes is absorbed in the upper atmosphere above 100km, but in the case of solar storms and polar-cap absorption events, MeV particles may penetrate deep into the middle atmosphere and influence the ozone chemistry. As we will discuss further in Chapter 4, in the polar regions, strong electric fields give rise to frictional heating of the upper atmosphere (Joule heating).

3.1.2 Energy loss

The most important mechanisms of energy loss include
- Infrared radiation from the atmosphere into space is very important. Carbon dioxide is the gas that releases most radiation here.
- Further on, energy is lost through the transport of energy by wind and waves from one region to another.
- Finally, turbulent transport is an important factor, even though its importance is not yet determined quantitatively. Turbulence can probably both add and remove energy from a region in the atmosphere.

3.2 Structure of the upper atmosphere

The total air pressure and air density exhibit an exponential decrease with height, as demonstrated to the left in figure 3.2. At 100km height, for example, density has decreased to 1/10 000 000 of the air density at ground level. Despite the altitude, there are still 10^{12} molecules per cm^3.
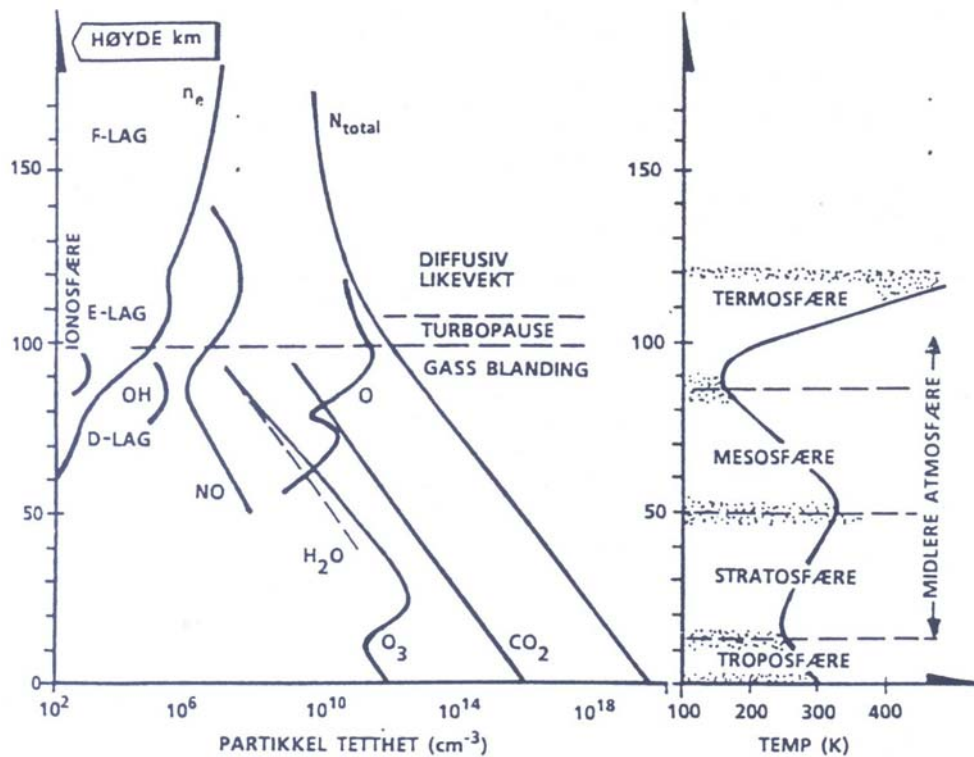
Figure 3.2.: Structure and composition of the atmosphere below 150 km. The height variation of some selected gasses are indicated

3.2.1 Division and temperature variation

Figure 3.2 gives an overview of the average composition and the neutral temperature as function of height from ground level up to 200km. Based on the temperature profile, the atmosphere is subdivided in regions, called *spheres*, intercepted by *pauses*. In the troposphere (0-12km), temperature decreases as one moves away from the warm surface of the earth. The temperature drops about 10 degrees per km to a minimum defined as the tropopause. Temperature in the stratosphere (12-50km) increases with height. The reason for this increase is the absorption of ultraviolet radiation by ozone. Temperature at the stratopause is approximately the same as on the ground, but in the mesosphere the temperature drops again until it reaches a well-defined minimum at the mesopause. The mesopause is the coldest place in the earth's atmosphere. Here, temperature can drop down to 120 K. Above 85km, in the thermosphere, temperature increases quickly until it reaches an approximately constant value of about 1500 K. Again, the increase in temperature is caused by absorption of UV radiation, but now with shorter wavelength than the radiation absorbed in the stratosphere. The middle atmosphere comprises the stratosphere, mesosphere and the lowest 10-15km of the thermosphere.

3.2.2 Composition

The abundant gasses below 100km are molecular oxygen and nitrogen, whereas atomic oxygen is very important above ~120km. Figure 3.2 shows the height variation of important trace gasses. These trace gasses are shown as examples of photochemically active compounds, which exist in very small amounts, but are of great significance for heat and radiation balance. We earlier mentioned CO_2, which is an

important greenhouse gas, as being important for heat loss by infrared radiation. Water vapor (H_2O), nitrogen oxide (NO), hydroxyl (OH), and sodium (Na) (from meteor traces) are relevant as well for the complicated photochemical processes that determine the condition of the upper atmosphere. Notice that atomic oxygen becomes a major constituent at greater heights. The reason for this is that ultraviolet radiation decomposes the oxygen molecules. Atomic oxygen is a very reactive element. Last, but not least, we must mention the concentration of free electrons n_e. As we notice from figure 3.2, the concentration is significant above 50km. However, it is important to note that even where n_e is largest, i.e., where the ionosphere is most dense, the air is only weakly ionized. The n_e to N_T ratio in the middle atmosphere is less than 10^{-7}.

3.2.3 Dynamic processes in the upper atmosphere

The atmosphere above the tropopause is dynamically highly active, even though the air density is low. The complicated global air circulation that takes place here includes planetary waves, tide waves, and local winds and waves. Wind forces up to 200ms^{-1} are not unusual at an altitude of 80km. Above ~100km, electrodynamic processes in the plasma of the ionosphere are important for the movement of the air. An important boundary in the atmosphere occurs at around 100km. Beneath this altitude we have a domain where wind, waves and turbulence create an effective mixture of the atmospheric gasses so that the average molecule mass varies very little with height. Above 100km the viscosity of the air is so high that mixture processes no longer are effective. Here, we get a diffuse equilibrium where the light gasses float on top. The boundary between the two domains can be sharp and is called the turbopause.

3.3 The barometric equation

To give a quantitative description of the atmosphere we start with a very simple model. We study a static atmosphere in a gravity field and look at a column of air with a cross section 1 (for example 1m^2). An element of air at height z with density ρ and thickness dz will be balanced by pressure and gravitational pull.

$$dp = -\rho g dz = -n\overline{m}g\, dz \qquad (3.1)$$

where ρ is pressure and g is the acceleration of gravity. Mass density is given by

$$\rho = n \cdot \overline{m}$$

n is the number of molecules per volume unit and $\overline{m}$ is the average molecular mass. Combining eq. 3.1 with the ideal gas law

$$p = nkT$$

we get

$$\frac{1}{p}dp = -\frac{\overline{m}g}{kT}\, dz \qquad (3.2)$$

We then integrate this equation from the ground ($p = p_0$, $z = 0$) to an arbitrary height z, assuming that m, g and T are constants.

$$p + dp$$
$$p$$
$$dz$$
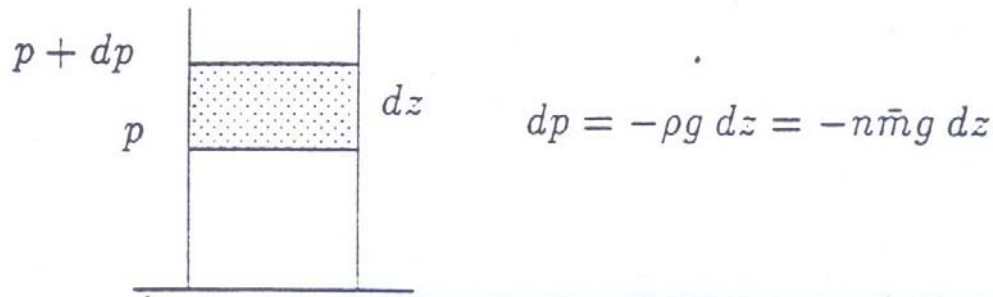
$$dp = -\rho g\, dz = -n\bar{m}g\, dz$$

Figure 3.3.: Height variation of the pressure

$$\int_{p_0}^{p} \frac{1}{p}\, dp = -\frac{\bar{m}g}{kT} \int_{0}^{z} dz \qquad (3.3)$$

$$p = p_0 \cdot e^{-\frac{\bar{m}g}{kT} z} \qquad (3.4)$$

This is the barometric equation for an isothermic atmosphere. We introduce a new quantity H_p, referred to as the scale height, for variation in pressure

$$H_p = \frac{kT}{\bar{m}g} \qquad (3.5)$$

and get

$$p(z) = p_0 \cdot e^{-\frac{z}{H_p}} \qquad (3.6)$$

We see that the scale height is the height where the pressure has decreased to $p(H) = 1/e\, p_0$, and therefore it represents a measure for how fast the pressure varies with height. Using the definition of scale height, eq. 3.2 can be written as

$$\frac{1}{H_p} = -\frac{1}{p}\frac{dp}{dz} \qquad (3.7)$$

In differential form the ideal gas law can be written as

$$\frac{1}{p}\frac{dp}{dz} = \frac{1}{n}\frac{dn}{dz} + \frac{1}{T}\frac{dT}{dz} \qquad (3.8)$$

By introducing a scale height for density variation given as

$$\frac{1}{H_n} = -\frac{1}{n}\frac{dn}{dz}$$

we get

$$-\frac{1}{H_p} + \frac{1}{H_n} = \frac{1}{T}\frac{dT}{dz} \tag{3.9}$$

In the case of an isothermic atmosphere, $H_p = H_n$.
Equation 3.4 is the barometric equation, which shows that in an isothermic atmosphere pressure and mass density will decrease exponentially with height (and with the same rate as long as temperature and molecular mass are constant). In the earth's atmosphere, the scale height at ground is about 8km.

3.4 The adiabatic atmosphere

An adiabatic process occurs when a volume element in the atmosphere moves in altitude without any exchange of heat with the surrounding atmosphere. For an adiabatic process, the law

$$p\rho^{-\gamma} = A \tag{3.10}$$

is valid, where A is a constant and $\gamma = \frac{C_p}{C_v}$ is the adiabatic constant, the ratio of heat capacities at constant pressure and constant volume. For diatomic gasses $\gamma=1.4$. If we combine equation 3.10 with the ideal gas law on the form $p = \rho R T$ we get

$$p\left(\frac{RT}{p}\right)^{\gamma} = A \tag{3.11}$$

The temperature becomes

$$T = \frac{1}{R}A^{\frac{1}{\gamma}} \cdot p^{\frac{\gamma-1}{\gamma}} = A_1 \cdot p^{\frac{\gamma-1}{\gamma}} = A_1 \cdot p^{\frac{R}{C_p}} \tag{3.12}$$

$$P = P_0 + \Delta P$$
$$\rho = \rho_0 + \Delta \rho$$
$$z = z_0 + \Delta z$$

$$P' = P$$

$$P'_0 = P_0$$
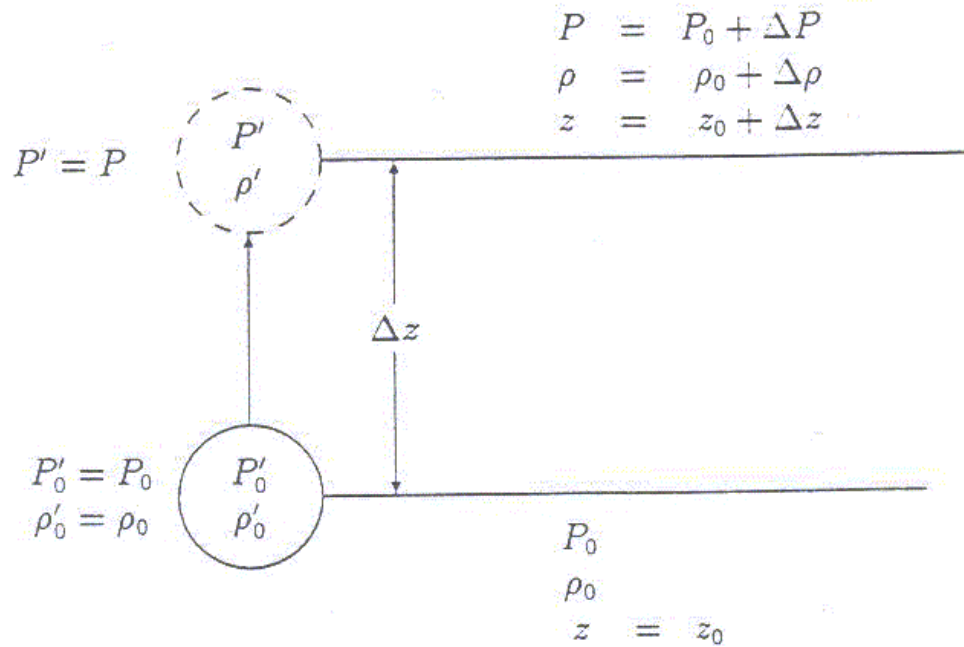$$\rho'_0 = \rho_0$$

$$P_0$$
$$\rho_0$$
$$z = z_0$$

Figure 3.4.: An air element is moved adiabatically from one starting point $z = z_0$ to a new height $z = z_0 + \Delta z$.

Some important quantities:

$$C_p = C_v + R$$

$$A_1 = \frac{1}{R} A^{\frac{1}{\gamma}} = \text{constant}$$

$$R = \frac{\text{universal gas constant}}{\text{molweight}} = \frac{1}{m \, N_A} R^*$$

$$R^* = k N_A = 8.31432 \cdot 10^3 \left[\frac{Nm}{kmol \cdot K} \right]$$

$$k = \text{Boltzmann's constant}$$

$$N_A = \text{Avogadro's number}$$

We aim to find out how the temperature is varying with height in an adiabatic process. By differentiating Eq. 3.12 we get

$$\frac{1}{T} \frac{\partial T}{\partial z} = \frac{R}{C_p} \cdot \frac{1}{p} \frac{\partial p}{\partial z} \tag{3.13}$$

From Eq. 3.1 we have that $\dfrac{\partial p}{\partial z} = -\rho g$, and using the ideal gas law $p = \rho R T$ can write Eq. 3.13 in the following form

$$\frac{\partial T}{\partial z}\Big|_{ad} = -\frac{RT}{C_p} \cdot \frac{\rho g}{p} = -\frac{g}{C_p} = \alpha^* \qquad (3.14)$$

α^* is called the adiabatic lapse rate, and it depends only on the acceleration of gravity and the heat capacity of the gas, and is approximately constant with height. In the case of powerful circulation (turbulence), a gas will after a while get close to the adiabatic lapse rate, which is about -10° C per km. In average, this lapse rate is occurs in the troposphere. The temperature at 1000 meter altitude is therefore in average 10 degrees colder than at sea level.

We can as well derive an adiabatic density gradient by writing

$$p\rho^{-\gamma} = A_2 \qquad (3.15)$$

$$\frac{1}{p}\frac{\partial p}{\partial z} = \frac{\lambda}{\rho}\frac{\partial \rho}{\partial z} \qquad (3.16)$$

$$\frac{\partial \rho}{\partial z}\Big|_{ad} = \frac{\rho}{\gamma\, p}\frac{\partial p}{\partial z} = -\frac{\rho^2 g}{\gamma\, p} = -\frac{\rho g}{\gamma\, RT} \qquad (3.17)$$

3.5 Atmospheric stability

We know by experiment that air can be both stable and unstable. An unstable situation occurs when a layer of heavy air is situated above a layer of lighter air, which results in the temperature of the air decreasing more rapidly than the adiabatic lapse rate. Then, the gravitational force will give rise to a turnover of air masses, i.e., we will have convective instability. Let us consider the conditions for such instability by first using qualitative arguments.

3.5.1 Unstable and stable air masses

Let us imagine an air element in equilibrium at a height z (see figure 3.8) in an atmosphere where the density gradient $\dfrac{\partial \rho}{\partial z} > \dfrac{\partial \rho}{\partial z}\Big|_{ad}$. When the element is moved adiabatically to a new height (by an external force), the pressure will quickly adjust to the pressure at the new height, whereas the temperature and density will follow the laws

$$p\rho^{-\gamma} = \text{constant}$$

$$p \cdot T^{\left(\frac{\gamma}{1-\gamma}\right)} = \text{constant}$$

The element following the adiabatic temperature will be lighter than the surrounding air at the new height if it is moved upwards, and heavier if it is moved downwards. Buoyancy and gravity will therefore increase the perturbations, and hence we have instability.
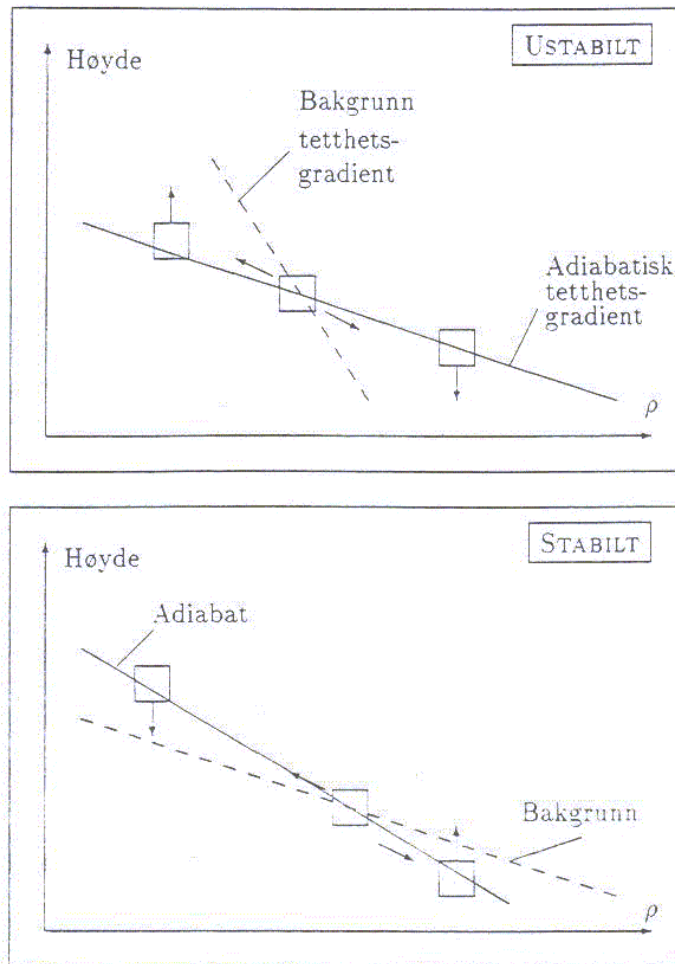
Figure 3.5.: Density variations in an unstable (at the top) and a stable atmosphere (at the bottom) during an adiabatic movement of an air element. The arrows ↑ and ↓ mark the buoyancy forces.

If, on the other hand, $\dfrac{\partial \rho}{\partial z} < \dfrac{\partial \rho}{\partial z}_{ad}$, the element will become heavier than the surrounding air when ascending, and lighter when descending. Gravity and buoyancy, therefore, force the element back towards the state of equilibrium, and we have a stable situation.

Let us describe the situation in more detail (see figure 3.8)
Suppose an atmosphere with pressure and density $p(z)$ and $\rho(z)$. At reference height $z = z_0$ we have $p(0) = p_0$ and $\rho(0) = \rho_0$. Suppose that an air element with pressure and density p'_0 and ρ'_0 is in equilibrium with its surrounding at $z = z_0$ so that $p'_0 = p_0$ and $\rho'_0 = \rho_0$. Let the element be moved a small altitude $\varDelta z$. The movement happens so slowly that the pressure in the element adjusts to its surrounding pressure $p'(z) = p(z)$, but fast enough so there is no heat exchange with the surrounding. The process is therefore adiabatic. As shown in figure 3.8, pressure and density in the new position will be $p' = p$ and $\rho' \approx \rho$. Force per mass unit acting on the element is then

$$\ddot{z} = \frac{g(\rho - \rho')}{\rho} \quad \text{(Sum of gravity and buoyancy)} \tag{3.18}$$

Further on we have

$$\rho = \rho_0 + \frac{\partial \rho}{\partial z} \cdot \Delta z \quad \text{(Surrounding)}$$

$$\rho' = \rho'_0 + \frac{\partial \rho}{\partial z_{ad}} \cdot \Delta z \quad \text{(Element)}$$

where, as shown earlier in equation 3.17

$$\frac{\partial \rho}{\partial z_{ad}} = -\frac{\rho g}{\gamma RT}$$

We therefore get

$$\frac{\rho - \rho'}{\rho} = \frac{1}{\rho}\left[\frac{\partial \rho}{\partial z} + \frac{\rho g}{\gamma RT}\right] \cdot \Delta z \tag{3.19}$$

and

$$\ddot{z} = \frac{g\Delta z}{\rho}\left[\frac{\partial \rho}{\partial z} + \frac{\rho g}{\gamma RT}\right] \tag{3.20}$$

We replace Δz with z and see that the equation has the same form as the one for an oscillator

$$\ddot{z} = \omega_B^2 z = 0 \tag{3.21}$$

where

$$\omega_B^2 = -g\left[\frac{1}{\rho}\frac{\partial \rho}{\partial z} + \frac{g}{\gamma RT}\right] \tag{3.22}$$

If we assume a harmonic solution

$$z = A \cdot e^{i\omega_B t} + B \cdot e^{-i\omega_B t} \tag{3.23}$$

ω_B can be interpreted as a frequency $\omega_B = 2\pi f_B$. We see that $\omega_B^2 > 0$ if $\frac{\partial \rho}{\partial z} \leq -\frac{\rho g}{\gamma RT}$. We will have real values for ω_B in this case, and the height of our air element oscillates. ω_B called Brunt-Vaisala frequency, and $\omega_B^2 > 0$ are the criteria for a stable atmosphere. ω_B is the natural resonance frequency that occurs when an element is moved away from one equilibrium position and then is released. ω_B is imaginary in the
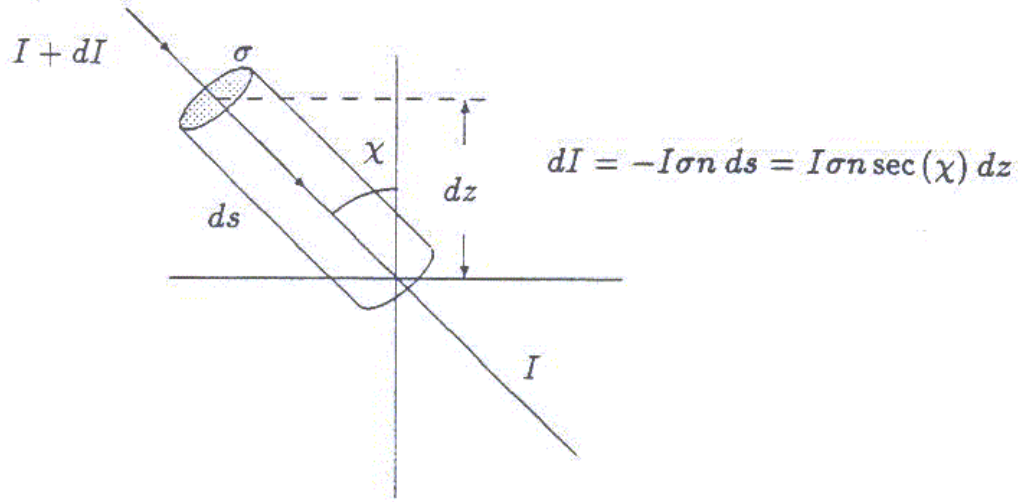
Figure 3.6.: Absorption of radiation in the atmosphere. σ is the absorption intersection and n is the number of molecules/atoms per volume unit.

case when $\frac{\partial \rho}{\partial z} \geq -\frac{\rho g}{\gamma RT}$. This corresponds to a convective unstable situation with no physical solution to the wave equation. This situation is illustrated in figure 3.9 by looking at a density gradient in a stable and unstable situation.

3.6 Absorption of radiation in the atmosphere

Before going into the Chapman theory, it is important to imagine that the altitude profile of ion production rate will have a peak at some altitude, as the ionization depends on both the neutral density (which decreases with height) and the incoming solar-radiation intensity (which increases with height).

Let us assume that atmosphere is exponential, planar, and horizontally stratified. As demonstrated in Figure 3.6, the line-of-sight path of monochromatic light of intensity I makes an angle χ with the zenith direction (zenith angle). The solar radiation intensity is I_∞ at the top of the atmosphere. At an altitude z, the intensity is I photons per unit of area per second. The radiation absorbed along a path element of length ds is given as

$$dI = -I\sigma \, n \, ds = I\sigma \, n \, \sec(\chi)dz \qquad (3.24)$$

where σ is the absorption cross section (square meters) and n is the number of absorbing molecules/atoms per unit volume. The height element dz is then given by $dz = \dfrac{1}{\sec(\chi)}ds$. The integral from $z = \infty$ down to z can be expressed as

$$\int_{I_\infty}^{I} \frac{1}{I}dI = \sec(\chi)\int_{\infty}^{z} \sigma n \, dz = -\tau \sec(\chi) \qquad (3.25)$$

where we have defined the optical depth of the atmosphere down to an altitude z

$$\tau \equiv -\int_{\infty}^{z} \sigma n \, dz$$

For the radiation intensity at altitude z we get

$$I = I_{\infty} e^{-\tau \, \sec(\chi)} \tag{3.26}$$

If the sun is in zenith $\chi = 0$, the radiation intensity has dropped to $I = \dfrac{1}{e} I_{\infty}$ when

$$\tau = -\int_{\infty}^{z} \sigma n \, dz = 1$$

Let us assume that σ is constant and that the density

$$n = n_0 \cdot e^{-\frac{z}{H_n}} \tag{3.27}$$

has an exponential variation with constant scalar height H_z. We then get

$$\tau = -\int_{\infty}^{z} \sigma \, n_0 \cdot e^{-\frac{z}{H_n}} \, dz = \sigma \, n \, H_n \tag{3.28}$$

The optical depth is therefore the number of absorbed particles (molecules/atoms) in a cylinder with cross section σ and height H_z. At a given density $n = \dfrac{l}{(\sigma \, H_n)}$, $\tau = 1$. To find the energy loss per unit height per second we use equations 3.24 and 3.26. Energy loss per unit height then becomes

$$\frac{dI}{dz} = I_{\infty} \sigma \, n \, \sec(\chi) \cdot e^{-\tau \, \sec(\chi)} \tag{3.29}$$

and energy loss per unit volume

$$\frac{1}{\sec(\chi)} \frac{dI}{dz} = I_{\infty} \sigma n \cdot e^{-\tau \, \sec(\chi)} \tag{3.30}$$

This equation forms the basis for calculating absorption of radiation as well as ionization and excitation resulting from absorption.

The optical depth is a useful term. Large values of τ mean that the radiation is heavily absorbed. The height z where $\tau = 1$ is often used as a measure for how fast a type of radiation is absorbed. Figure 3.7 shows the height z where $\tau=1$ as a function of wavelength for radiation with $\lambda < 300nm$. We see that light in the visible spectrum penetrates down to the ground, whereas radiation in the region of 200-300nm is absorbed in the stratosphere. For $\lambda > 200nm$, an essential part of the solar radiation is absorbed in the ionosphere.
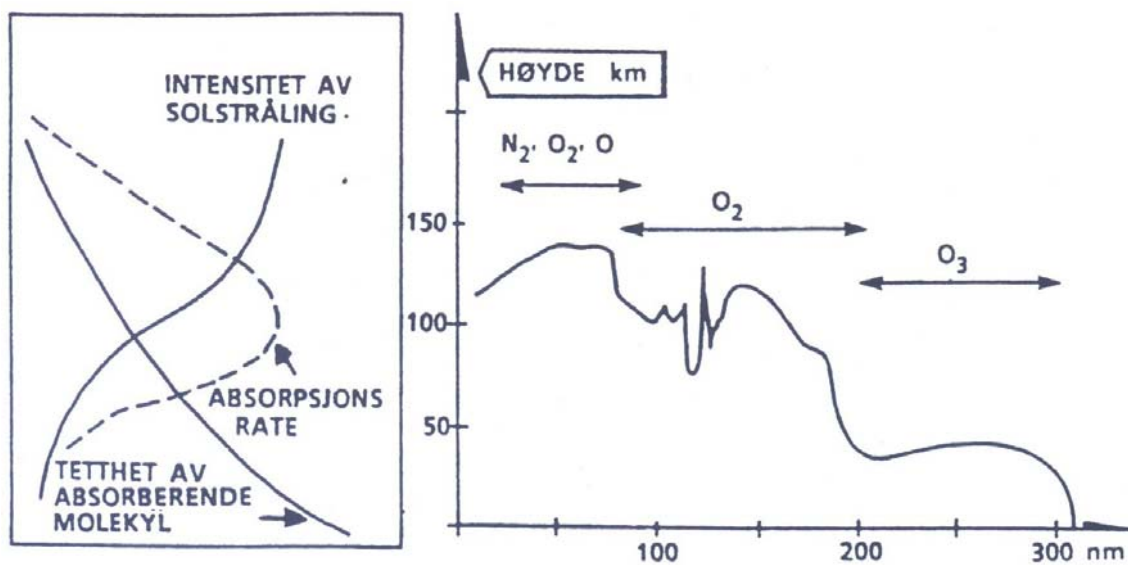
Figure 3.7.: The left part of figure 3.7 shows schematically how radiation is absorbed in the atmosphere. The right hand side shows a height where $\tau = 1$ as a function of the incoming radiations wavelength. The arrows indicate the atmospheric gasses which absorb in the different wavelength regions.

3.7 Ozone

Ozone [O_3] is a photochemically important component of the middle atmosphere. Height distribution of ozone shows a maximum at around 20km, but the amounts are rather small. If all the ozone in the atmosphere were to be compressed into a layer with one atmospheric pressure, the thickness of this layer would be about 4mm. We will in the following discussion briefly describe how ozone is formed and destroyed. The primary source of ozone is the dissociation of O_2 by ultraviolet light with wavelengths in the region of 200-300nm:

$$O_2 + hv \rightarrow O + O$$
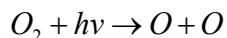
Atomic oxygen recombines quickly with molecular oxygen. Ozone is made in a three-particle collision, where the third molecule M is necessary to satisfy the conservation of impulse and energy in the process.

$$O_2 + O + M \rightarrow O_3 + M$$
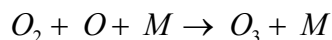
The decay of ozone can happen through several processes. The most important natural process is dissociation by ultraviolet light:

$$O_3 + hv \rightarrow O + O_2$$
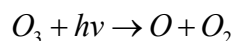
Further on, trace elements like OH, NO and ClO occur in catalytic reactions like

$$OH + O_3 \quad \rightarrow \quad HO_2 + O_2$$
$$HO_2 + O \quad \rightarrow \quad OH + O_2$$
$$\text{Netto } = O + O_3 \quad \rightarrow \quad 2O_2$$
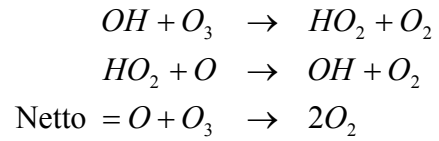
We see that the decay component is reproduced, and can be part of new reactions. Nitrogen oxide [NO] is formed by powerful precipitation of protons in the atmosphere, in connection with certain types of sun outbursts. ClO can be formed by photolysis of freon gasses, and is assumed to be an important source for anthropogenic changes in the ozone layer in the stratosphere. Dynamic processes are very important for the transport of ozone, and the entire ozone balance is very complicated.