

NEUTRAL ATMOSPHERE MODELING

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1. Introduction

In this introductory paper, no attempt will be made to describe any particular model or to compare different models. Emphasis will be given to the physical phenomena occurring in the terrestrial upper atmosphere.

A perfect atmospheric model is actually a set of numbers which is intended to represent the physical properties of the atmosphere in the past, in the present and in the future. This is a very ambitious goal which is far from being reached. There are, however, essentially three types of atmospheric models used for our partial understanding of the upper atmosphere.

The theoretical models result from the solution of some equations with simplifying hypotheses. These models always require a knowledge of boundary conditions which should come out of experimental data. Most of these models are discussed by Blum *et al.* (1972).

The semi-empirical models are usually based on a certain amount of observational data combined with some theoretical background such as the diffusive equilibrium hypothesis. Among the most widely used models are those of Jacchia (1965, 1971) which are based on satellite drag data. These semi-empirical models were initially guided by the theoretical approach developed by Nicolet (1961a, b).

The purely experimental models are a direct representation of physical parameters measured *in situ* by satellites. Since these models are by definition limited in time and in space, they lead very often to semi-empirical models by extrapolation and interpolation processes. As an example, the OGO-6 model (Hedin *et al.*, 1974) gives a worldwide distribution of temperature and concentrations by a spherical harmonic analysis of measured data. The ESRO-4 data described by von Zahn (1975) will probably give the next experimental model of the upper atmosphere.

It is clear, however, that all these models can make a valuable contribution to the knowledge of the upper atmosphere, not only through their internal results, but also by their mutual interaction.

2. Application of the Conservation Equations

The general conservation equations (Chapman and Cowling, 1970; Landau and Lifshitz, 1959) are usually simplified for atmospheric applications but, unfortunately, the simplifying assumptions are not always clearly stated in the literature. This situation can lead to some confusion when different results are compared.

For each atmospheric species with concentration n_i , the general continuity equation is

$$(\partial n_i / \partial t) + \nabla \cdot n_i (\mathbf{v}_0 + \mathbf{V}_i) = P_i - L_i \quad (1)$$

where P_i and L_i are, respectively, the production and loss rates of the constituent i . \mathbf{V}_i is the diffusion velocity and \mathbf{v}_0 is the mass average velocity. In a gas mixture, the diffusion velocity is characterized by the relation

$$\sum n_i m_i \mathbf{V}_i = 0 \quad (2)$$

where m_i is the mass of the particle i . Using this relation, the total density ($\rho = \sum n_i m_i$) continuity equation is obtained from Equation (1) as

$$(\partial \rho / \partial t) + \nabla \cdot (\rho \mathbf{v}_0) = 0. \quad (3)$$

The term $\sum_i (P_i - L_i)$ vanishes, since the total mass of the system is conserved. It should be noted that the use of Equation (3) for a single constituent is incorrect unless the diffusion velocity \mathbf{V}_i and the production and loss terms are zero. Extensive use has been made of Equation (1) to solve the problem of atomic and molecular oxygen distributions in the lower thermosphere.

Although the molecular diffusion velocity is given by gas kinetic theory (Chapman and Cowling, 1970), the mass average velocity \mathbf{v}_0 , however, requires the solution of the momentum equation. Considering the viscosity μ as constant and neglecting the gradient of $\nabla \cdot \mathbf{v}_0$, the momentum equation for a gas mixture, can be written

$$\rho [(\partial \mathbf{v}_0 / \partial t) + \mathbf{v}_0 \cdot \nabla \mathbf{v}_0] + \nabla_p - \mu \nabla^2 \mathbf{v}_0 - \sum_i n_i \mathbf{X}_i = 0, \quad (4)$$

where the total pressure is the hydrostatic pressure and \mathbf{X}_i is any external force acting on the i -type particles. In a rotating frame of reference

$$\mathbf{X}_i = [\mathbf{g} - 2\boldsymbol{\omega} \times \mathbf{v}_0 - \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r})] m_i + \mathbf{F}_i, \quad (5)$$

where the first three terms, respectively, represent the gravitational force, the Coriolis force and the centrifugal force at a geocentric distance \mathbf{r} when the angular velocity is $\boldsymbol{\omega}$. The external forces \mathbf{F}_i are the frictional forces such as ion drag. One sees that it is through these frictional forces that the ionosphere can interact with the neutral atmosphere. Applications of the momentum equation to the determination of winds in the upper atmosphere are described by Kohl (1975).

Any solution of the momentum equation requires a knowledge of the thermal structure given by the energy equation. When P and L are respectively, the heat production and loss, the energy equation is given by

$$\rho [(\partial c_v T / \partial t) + \mathbf{v}_0 \cdot \nabla (c_v T)] + p \nabla \cdot \mathbf{v}_0 + \nabla \cdot \mathbf{E} - \sum_i n_i \mathbf{F}_i \cdot \mathbf{V}_i = P - L, \quad (6)$$

where T is the temperature and c_v is the specific heat at constant volume for the gas mixture. The heat flow \mathbf{E} is given by

$$\mathbf{E} = -\lambda \nabla T + T \sum_i c_{pi} q_i \mathbf{V}_i, \quad (7)$$

where λ is the heat conductivity of the gas mixture and c_{pi} is the specific heat at constant pressure for the i -type particle.

With the addition of an expression for the diffusion velocity, the system of coupled Equations (3), (4), and (6) is complete and can in principle be solved. Up to now, simplifying assumptions have always been used. They are discussed by Banks and Kockarts (1973).

Solutions of the energy equation are usually based on the assumption that the atmospheric constituents are in diffusive equilibrium, i.e. $V_i = 0$. The diffusion terms are, therefore, omitted in Equations (6) and (7), with the consequence that the diffusion time should be small compared to the heat conduction time. On the other hand, such an assumption, mainly introduced to simplify the mathematical problem, is not necessarily correct. The diffusion time τ_D is usually defined as

$$\tau_D = H^2/D \quad (8)$$

where H is the atmospheric scale height and D is the molecular diffusion coefficient. The heat conduction time τ_H can be written

$$\tau_H = \rho c_v H^2 / \lambda, \quad (9)$$

where all the symbols have been previously defined.

The comparison between τ_D and τ_H is given in Figure 1 which is computed using the parameters of the mean COSPAR international reference atmosphere (Champion and Schweinfurth, 1972). The expression for the heat conductivity is taken from Banks and

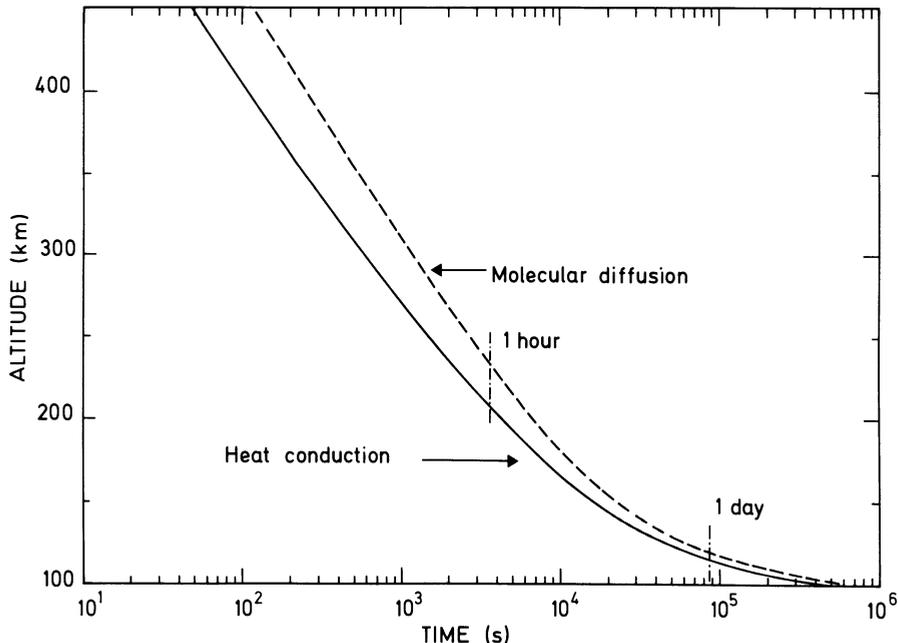


Fig. 1. Comparison between diffusion time and heat conduction time in the mean COSPAR international reference atmosphere.

Kockarts (1973). It can be seen from Figure 1 that the heat conduction time and the molecular diffusion time are of the same order of magnitude over the whole thermospheric height range. This means that the diffusion terms are not necessarily negligible in the energy equation, but further studies are required to clarify this point. Since the diffusion time is of the order of one day around 120 km, variations of the thermal structure will add to the difficulty for reaching diffusive equilibrium in that height region. Possible deviations from diffusive equilibrium have also been suggested (Stubbe, 1972) as a consequence of horizontal winds. There is, however, no general agreement for the magnitude of such an effect (Blum, 1974; Stubbe, 1974; Rishbeth *et al.*, 1974).

Up to now, almost all theoretical models were based on fixed boundary conditions at 120 km altitude. As a result of the variations observed in this height region, it seems better now to adopt boundary conditions at lower heights. In this case the transport effects of O and O₂ become more important and the energy equation must be solved simultaneously with the continuity and momentum equations. This procedure has been used by Chandra and Sinha (1974) in a one-dimensional case. These authors stressed, however, the importance of downward heat fluxes by eddy transport. Such a flux is to be added to the molecular conduction given in Equation (7). Hunten (1974) pointed out that the introduction of eddy conduction may result in an overestimate of the downward heat transfer since dissipative phenomena such as gravity waves may also contribute to the heating. This shows that lowering the boundary level results not only in more complicated mathematics, but introduces also complex physical problems which are not yet completely understood.

Even if the mathematical techniques were available to solve the three-dimensional time-dependent conservation equations, one has still to determine the different production and loss terms as well as the external forces acting on the system.

3. Energy Sources and Sinks

The terms involving the mass average velocity in the energy equation are sometimes considered as compressional heat sources during the night and expansive heat sinks during the day. Since the total contribution is zero over a 24 h period, these terms do not constitute a real global source or sink for the system. They must, however, be included in the energy equation, since they strongly influence the diurnal temperature distribution. When the momentum and energy equations are not solved simultaneously it is difficult to estimate the effect of the compression and expansion terms. It has been shown (Kockarts, 1973) how such an effect can be simulated in a one-dimensional calculation by introducing a very small heat source during the night and a compensating sink during the day. Although the absolute magnitude of these sources or sinks is negligible compared with the total UV absorbed energy, their effect is important since they play a role in a height region above 200 km where very little UV radiation is absorbed.

The major heat sources of the thermosphere are solar UV radiation, Joule dissipa-

tion from ion-neutral interactions and atmospheric waves such as gravity waves and tidal oscillations. Although the physical mechanisms are fairly well understood, there is still some uncertainty with regard to the amount of energy deposited in the upper atmosphere.

Most of the theoretical models are based on solar UV heating alone. For practical purposes the solar spectrum is often divided into two parts: the Schuman-Runge continuum below 1750 Å and the wavelength region below Ly- β (1026 Å) down to 80 Å. Longer and shorter wavelengths are not considered, since they are not significantly absorbed above 100 km altitude. The amount of energy available in the Schumann-Runge continuum is of the order of $15 \text{ erg cm}^{-2} \text{ s}^{-1}$ according to the tabulation presented by Ackerman (1971). Between 1026 Å and 80 Å the UV flux is more variable with solar activity and for medium solar activity the measured flux is of the order of $2.3 \text{ erg cm}^{-2} \text{ s}^{-1}$ (Hinteregger, 1970). The validity of Hinteregger's fluxes has been questioned several times in relation with the neutral and ionospheric heat balance. Recently, Prasad and Furman (1974) concluded that the arguments advanced for doubling the solar UV fluxes below 1300 Å are not compelling, since too many uncertain parameters are involved in such studies. The effects of changing solar UV fluxes from 1.7 to $4.5 \text{ erg cm}^{-2} \text{ s}^{-1}$ are indicated by Banks and Kockarts (1973) and by Kockarts (1973). New measured solar UV fluxes are now available below 1000 Å (Schmidtke *et al.*, 1974). Figure 2 shows a comparison between the fluxes measured onboard AEROS-A (Schmidtke *et al.*, 1974) on March 2, 1973, and the values given by Hinteregger (1970). With the exception of an Si_{II}, an Fe_{XV} line, and the 176–155 Å wavelength interval, Hinteregger's values are always smaller than the fluxes given by Schmidtke *et al.* (1974). The ratio of these measured values is presented in the lower part of Figure 2. The total flux below 1000 Å measured onboard AEROS-A is $3.8 \text{ erg cm}^{-2} \text{ s}^{-1}$. More data are, however, required before a definite conclusion can be reached with regard to the absolute UV fluxes. Furthermore, long term variations of the UV radiation emitted by the whole sun are not yet available, despite their fundamental importance in aeronomic studies.

Another important mechanism is the Joule heating resulting from ionospheric currents (Cole, 1971, 1972). Since Joule heating is proportional to the electron concentration and to the square of the electric field, its effect is predominant in the auroral region during disturbed conditions (see Wickwar, 1975). Joule dissipation is actually a linking mechanism between the neutral and the ionized atmospheres, as can be seen from the momentum and energy equations. Neutral winds related to the convection electric fields have been measured in the *E* region using the incoherent radar facility at Chatanika, Alaska. At nighttime, during storm conditions, neutral wind velocities up to 200 m s^{-1} are not uncommon (Brekke *et al.*, 1974). Horizontal winds as high as 1000 m s^{-1} have been deduced at 140 km (Chang *et al.*, 1974) from geomagnetic variations recorded at College, Alaska. As a result of the involved physical mechanism, Joule heating is strongly dependent on the latitude. A global estimation of the amount of heat available through this process requires simultaneous knowledge of the worldwide electric field and the electron concentration distributions. Using a global

from high altitude large scale wave generated in the auroral regions and traveling over large horizontal distances toward the equator. This means that atmospheric waves can introduce energy into the thermosphere from below and from above. Klostermeyer (1973) has shown that gravity waves generated in the auroral regions during geomagnetic disturbances can lead to temperature increases which are in agreement with the empirical relation deduced from satellite drag (Jacchia *et al.*, 1967).

The energy sources previously described, however can, not explain all the observational facts. Using observed temperatures, densities and winds, Barlier *et al.* (1974) have shown that a definite north-south asymmetry exists in the thermosphere. As an example, Figure 3 gives the ratio of the observed densities to Jacchia's 1971 model. It is seen that, even at the equinoxes, there is an asymmetry when the solar illumination is identical for both hemispheres. The total density is greater in the south. A similar

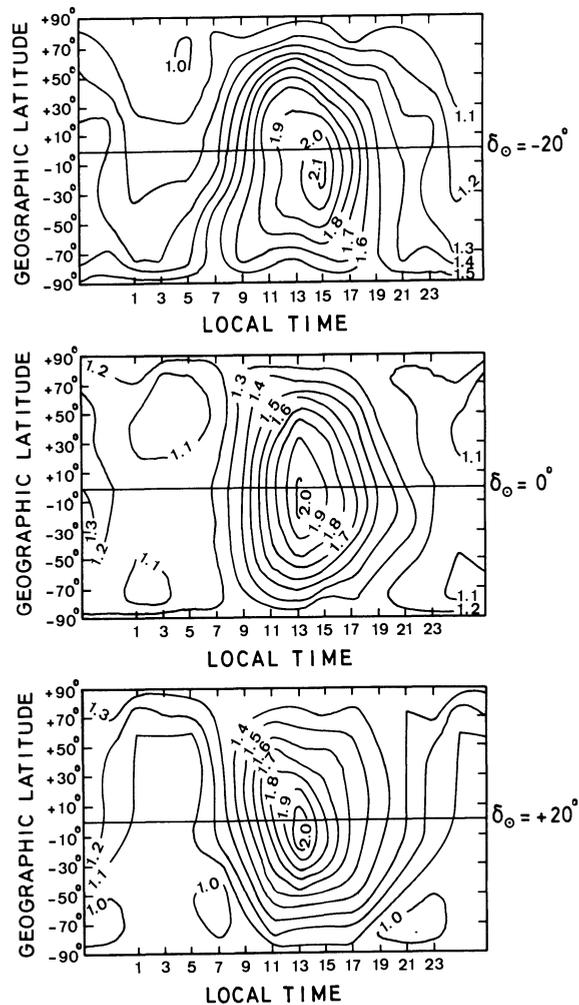


Fig. 3. Ratio at 280 km between observed densities and the nighttime minimum density of Jacchia (1971) as a function of local solar time and latitude. The solar declination is respectively -20° , 0° and $+20^{\circ}$.

asymmetry has also been observed in the global temperature distribution. From the large volume of data accumulated during the last solar cycle maximum, Barlier *et al.* (1974) conclude that the temperature is, on the average, higher in the southern thermosphere. These authors suggest that this fact could be related to the geomagnetic field asymmetry and to the tidal wave dissipation which is linked to the asymmetrical worldwide O₃ distribution in the stratosphere and mesosphere.

Since the construction of the first atmospheric models, heat sources other than the solar UV radiation have been discovered. Up to now, no thermospheric model has been published taking into account all these sources. The former problem of the lack of sufficient sources of energy is now perhaps replaced by the problem of how to lose sufficient energy to avoid high temperatures which are not observed. Besides the downward heat conduction mechanism, the IR emission of O at 63 μm is the sole loss process usually introduced in thermospheric models. It has been shown (Kockarts and Peetermans, 1970) that, below 150 km, radiative transfer strongly reduces the 63 μm volume emission rate and, therefore, decreases the cooling rate resulting from O. At 100 km altitude the 63 μm cooling rate is negligible. Molecular heat conduction can then lead to large temperature gradients in the 100 to 120 km region. Such a situation can, however, be avoided if other loss processes are introduced.

Some experimental results seem to indicate that other IR emissions could play a role in the upper atmosphere heat budget. Very high IR emission in the 3 to 8 μm spectral region has been observed at altitudes above 150 km (Markov, 1969) but no complete physical explanation has been given. Recently the IR emission of O₃ at 9.6 μm and of CO₂ at 15 μm has been observed in the mesosphere and lower thermosphere (Stair *et al.*, 1974). According to these data, the 15 μm CO₂ emission at 120 km and 100 km corresponds, respectively, to 1 and 10 $\text{erg cm}^{-2} \text{s}^{-1}$. It is, therefore, not excluded that CO₂ could be the cooling agent in the 100 to 120 km height range.

4. Conclusion

It appears from the above discussion that there is a need for more investigations designed to develop the numerical techniques used for the solution of the three-dimensional conservation equations. Furthermore, longterm observations are still needed. A better understanding of the time and space evolution of all heat sources and sinks which are the fundamental input parameters of any atmospheric model is necessary.

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