NUMBER DENSITIES OF INDIVIDUAL SPECIES

General Considerations

The steady-state vertical distribution of a minor gas species of number density n_i (m^{-3}) and molecular weight M_i (kg $kmol^{-1}$) is governed by the vertical component of the momentum equation for that gas (for example, Colegrove et al., 1965):

$$n_i v_i + D_i \left(\frac{dn_i}{dZ} + \frac{n_i(1 + \alpha_i)}{T} \cdot \frac{dT}{dZ} + \frac{n_i}{H_i} \right) + K \left(\frac{dn_i}{dZ} + \frac{n_i}{T} \cdot \frac{dT}{dZ} + \frac{n_i}{H_P} \right) = 0 \qquad (5)$$

where

v_i = the flow velocity (m s^{-1}) of the *ith* species,

D_i = height-dependent, species-dependent, molecular-diffusion coefficient (m^2 s^{-1}) for the *ith* minor species diffusing through the major background gas,

α_i = thermal diffusion factor (dimensionless) for the *ith* species (having a value of −0.4 for He, and zero for O, O_2, and Ar),

K = height-dependent, eddy-diffusion coefficient ($m^2 s^{-1}$).

The quantity H_P is the height-dependent pressure scale height (m) for air

$$H_P \equiv \frac{R^* T}{Mg} \qquad (5a)$$

while H_i is the related parameter for a particular gas species, that is,

$$H_i = \frac{R^* T}{M_i g} \qquad (5b)$$

where M_i is the molecular weight (kg $kmol^{-1}$) for the *ith* species and g is the height-dependent acceleration of gravity (m s^{-1}), which for 45°N, is closely approximated by

$$g = g_0 \; [r/(r + Z)]^2 \qquad (5c)$$

In this expression, r = 6356.766 km, as previously defined.

Molecular Nitrogen

Equation 5 is used to calculate the distribution of each gas except molecular nitrogen. Since N_2 is the major gas in the lower part of the thermosphere, a different scheme is used to describe its distribution. From the lower boundary altitude of 86 km up to about 100 km, the atmosphere is well mixed as the eddy processes dominate the molecular diffusion, while above about 100 km, molecular diffusion dominates. Also, because $M(N_2)$, the molecular weight of N_2, that is, 28.0134 kg $kmol^{-1}$, is quite close to the mean molecular weight of air, 28.9644 kg $kmol^{-1}$, the transition from a mixed to a diffusive distribution of atmospheric gases at heights below which dissociation and diffusion become important, has little effect on the height profile of molecular nitrogen. This allows the use of the following simplified version of equation 5 with the flow velocity (v_i), as well as the eddy-diffusion coefficient (K) and the thermal-diffusion factor (α_i), all set equal to zero. In addition, $n(N_2)$ replaces n_i to represent N_2 number density, and $1/H(N_2)$ replaces $1/H_i$ through which equation 5b is seen to equal $M(N_2) \cdot g/(R^* \cdot T)$:

$$\frac{dn(N_2)}{dZ} + \frac{n(N_2)}{T} \cdot \frac{dT}{dZ} + \frac{n(N_2) \cdot M(N_2) \cdot g}{R^* T} = 0 \tag{6}$$

Since g varies only slowly with height, it is apparent that temperature is the dominant parameter governing the height profile of molecular nitrogen. The solution of equation 6 for $n(N_2)$ yields

$$n(N_2) = n(N_2)_7 \cdot \exp\left[-\int_{Z_7}^{Z}\left(\frac{M(N_2)\cdot g}{R^* T} + \frac{1}{T}\cdot\frac{dT}{dZ}\right)dZ\right] \tag{7}$$

where $n(N_2)_7$ is the N_2 number density at level 7 which is 86 km.

The slight change in the height distribution of N_2 caused by the transition from a mixing regime below 100 km to a diffusive-separation regime above this height is accounted for by using the value of the mean molecular weight of air in place of that of $M(N_2)$ at heights below 100 km.

Atomic and Molecular Oxygen, Helium, and Argon

Ideally, equation 5 is solved in conjunction with the equation of continuity (Colegrove et al., 1965; Keneshea and Zimmerman, 1970)

$$\frac{d(n_i v_i)}{dZ} = \zeta(Z) \tag{8}$$

where ζ denotes chemical production and loss terms. For the purpose of the single-profile steady-state model being generated here, however, such a sophisticated and detailed calculation is considered inappropriate. Instead, the flux term, $n_i v_i$, is artificially adjusted† to match the fluxes resulting from the diurnally averaged, time-dependent calculations (Minzner et al., 1976) which account for the effects of photochemical production and loss, as well as for vertical transport, on the vertical distribution of atomic and molecular oxygen. For helium and argon, the flux term represents only the vertical flow.

†Huang, F. T., private communication, 1974.

Equation 5 is integrated directly to obtain the following exponential expression:

$$n_i = n_{i,7} \cdot \frac{T_7}{T} \cdot \exp\left\{ - \int_{Z_7}^{Z} \left[F(Z) + \left(\frac{v_i}{D_i + K} \right) \right] dZ \right\} \qquad (9)$$

where $n_{i,7}$ represents the number density at the lower-level boundary of Model II for any one of the minor species, O, O_2, Ar, and He. The values of $n_{i,7}$, one for each of these minor species as well as one for $n(N_2)_7$, were generated in a manner described in Minzner et al. (1976) and are given in table 2.

The function F(Z) in equation 9 is defined as

$$F(Z) = \frac{D_i}{H_i (D_i + K)} + \left(\frac{\alpha_i D_i}{D_i + K} \right) \frac{1}{T} \cdot \frac{dT}{dZ} + \frac{K}{H_p (D_i + K)} \qquad (10)$$

The height profile of the eddy-diffusion coefficient, K, used in the calculation of number density is defined in three segments:

1. For $86 \leqslant Z < 95$ km,

$$K = 1.2 \times 10^2 \ m^2 \ s^{-1} \qquad (11)$$

2. For $95 \leqslant Z \leqslant 115$ km,

$$K = 1.2 \times 10^2 \cdot \exp\left(1 - \frac{400}{[400 - (Z - 95)^2]} \right) \qquad (12)$$

3. For $Z > 115$ km,

$$K = 0.0 \qquad (13)$$

The height-dependent molecular-diffusion coefficients, D_i, for the various species are associated with diffusion through molecular nitrogen, and have the general form

$$D_i = \frac{a_i}{N} \left[\frac{T}{273.15} \right]^{b_i} \qquad (14)$$

where N is the total number density at height Z. The value of the coefficients a_i and b_i for various species, O, O_2, Ar, and He (Colegrove et al., 1966) are listed in table 4. With the appropriate values of these coefficients used in equation 14, the resulting value of the function D_i, the molecular-diffusion coefficient, for each of the four indicated species is found to be as plotted in figure 3 for the height interval 86 to 150 km.

Table 4
Values of Species-dependent Coefficients Used in the Expressions for Molecular-diffusion Coefficients

Gas	a_i (m^{-1} s^{-1})	b_i (dimensionless)
O	6.986 X 10^{20}	0.750
O_2	4.863 X 10^{20}	0.750
Ar	4.487 X 10^{20}	0.870
He	1.700 X 10^{21}	0.691

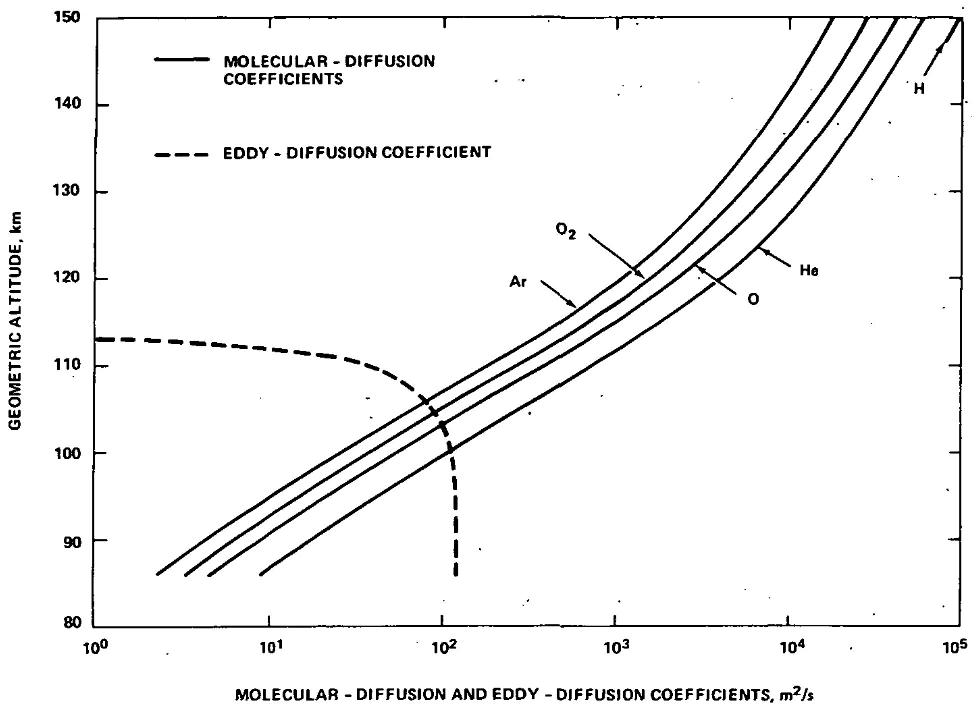

Figure 3. Molecular- and eddy-diffusion coefficients versus altitude, 86 to 150 km.

Figure 3 also shows the shape of the function K and the eddy-diffusion coefficient defined by equations 11, 12, and 13. The significance of K in the height distribution of the number densities of the several species is seen to decrease rapidly above 100 km and to vanish at 115 km. Thus, for $Z > 115$ km, F(Z) defined by equation 10 simplifies to

$$F(Z) = \frac{1}{H_i} + \frac{\alpha_i}{T}\frac{dT}{dZ} \qquad (15)$$

and it is obvious that values of D_i no longer enter into the calculation of F(Z), and, hence, not into the calculation of n_i for O, O_2, Ar, and He. Consequently, the height variation of D_i for each of these four species is plotted in figure 3 only for a limited height region, 86 to 150 km. In the calculation of the number density for atomic hydrogen H (see Appendix A), the values of D_i for H are significantly involved to heights far in excess of 150 km. Since n(H) is not calculated for heights below 150 km, however, the graph of D_i for H appears only as a short dash below the 150-km coordinate of figure 3.

The value of the total number density to be used in equation 14 is obtained by sequential calculations, with N_2 providing the value of N for the calculation of the diffusion coefficients for atomic and molecular oxygen, and the sum of the number densities for N_2, O_2, and O providing the value of N for the calculation of argon and helium diffusion coefficients.

The flux term, $v_i/(D_i + K)$ in equation 9, is represented by the following expression†

$$\frac{v_i}{D_i + K} = Q_i\,(Z - U_i)^2 \cdot \exp[-W_i\,(Z - U_i)^3] + q_i(u_i - Z)^2 \cdot \exp[-w_i(u_i - Z)^3] \qquad (16)$$

The coefficients q_i, Q_i, u_i, U_i, w_i, and W_i, which are constant for a particular species, are each adjusted such that appropriate densities are obtained at 450 km for O and He, and at 150 km for O, O_2, He, and Ar. The constant, q_i, is zero for all species except atomic oxygen, and is also zero for atomic oxygen above 97 km; the extra term for atomic oxygen is needed below 97 km to generate a maximum in the density-height profile at the selected height of 97 km. This maximum results from the increased loss of atomic oxygen by recombination at lower altitudes. The flux terms for O and O_2 are based on, and lead (qualitatively) to, the same results as those derived from the much more detailed calculations by Colegrove et al. (1965) and Keneshea and Zimmerman (1970). Table 5 lists the values of the coefficients q_i, Q_i, u_i, U_i, w_i, and W_i, for each of the four minor species being considered, while the lower boundary-condition number-density values required in equation 5 are included in table 2.

Table 5

Values of Species-dependent Coefficients Applicable to the Empirical, Integrable Equation 16 Representing the Flux Term $v_i/(D_i + K)$

Gas	q_i (km^{-3})	Q_i (km^{-3})	u_i (km)	U_i (km)	w_i (km^{-3})	W_i (km^{-3})
O	-3.416248×10^{-3}	-5.809644×10^{-4}	97.0	56.90311	5.008765×10^{-4}	2.706246×10^{-5}
O_2	0	1.366312×10^{-4}	–	86.000	–	8.333333×10^{-5}
Ar	0	9.434079×10^{-5}	–	86.000	–	8.333333×10^{-5}
He	0	-2.457369×10^{-4}	–	86.000	–	6.666667×10^{-4}

†Huang, F. T., private communication, 1974.

Number densities versus height for each of N_2, O, O_2, Ar, and He were computed using equations 6 through 16. Graphs of these data for each species were prepared for each of two height regions, 86 to 150 km and 100 to 450 km. These graphs are presented in figures 4 through 13.

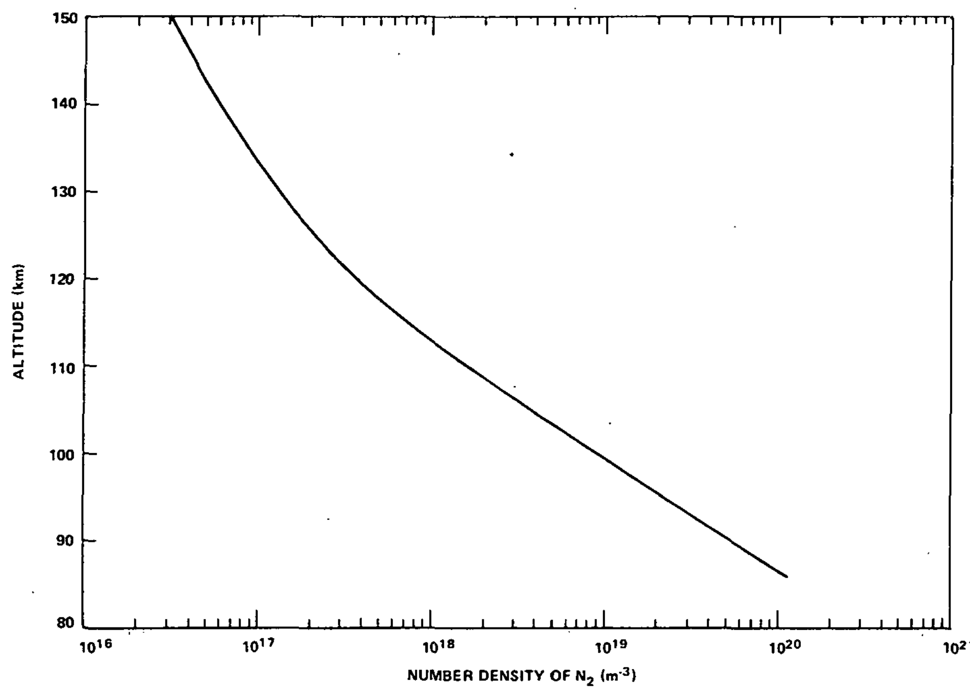

Figure 4. Number density of N_2 versus altitude, 86 to 150 km.

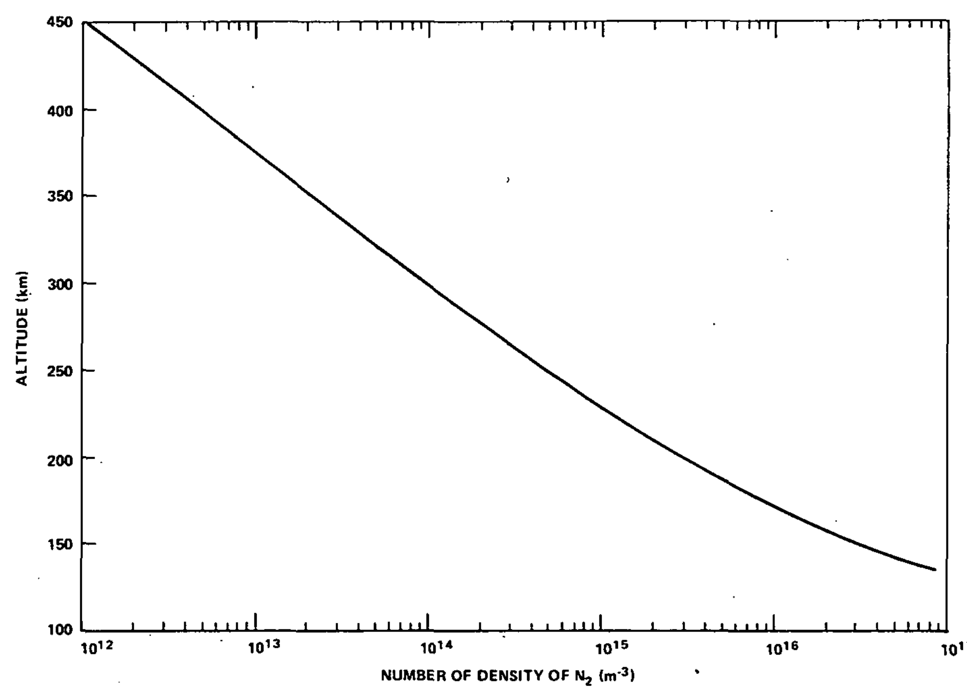

Figure 5. Number density of N_2 versus altitude, 100 to 450 km.

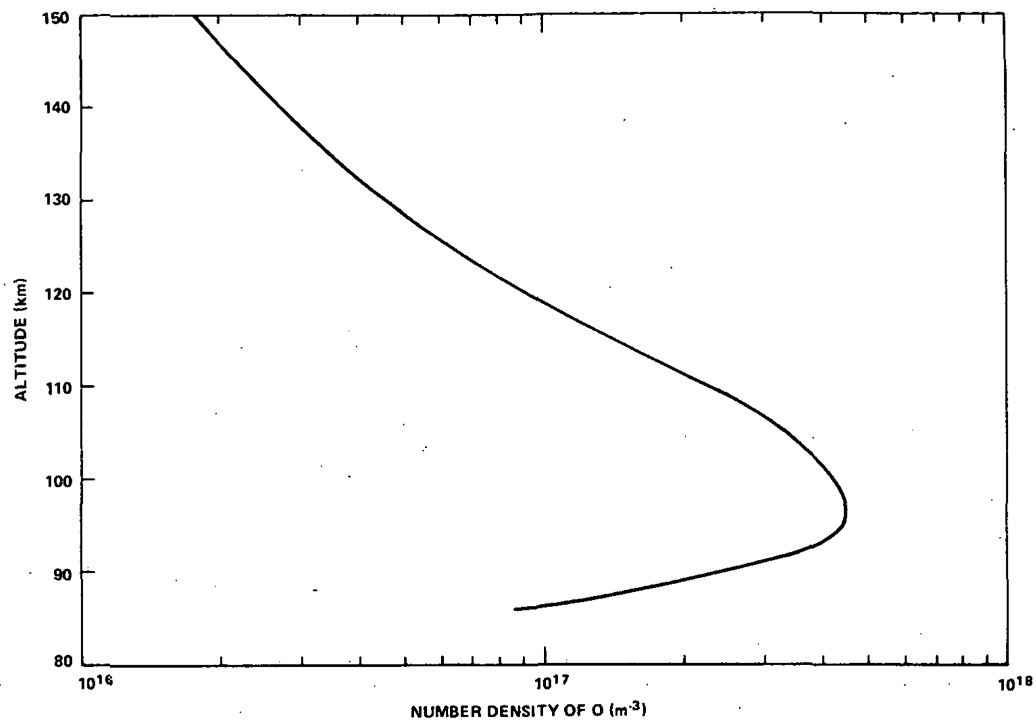

Figure 6. Number density of O versus altitude, 86 to 150 km.

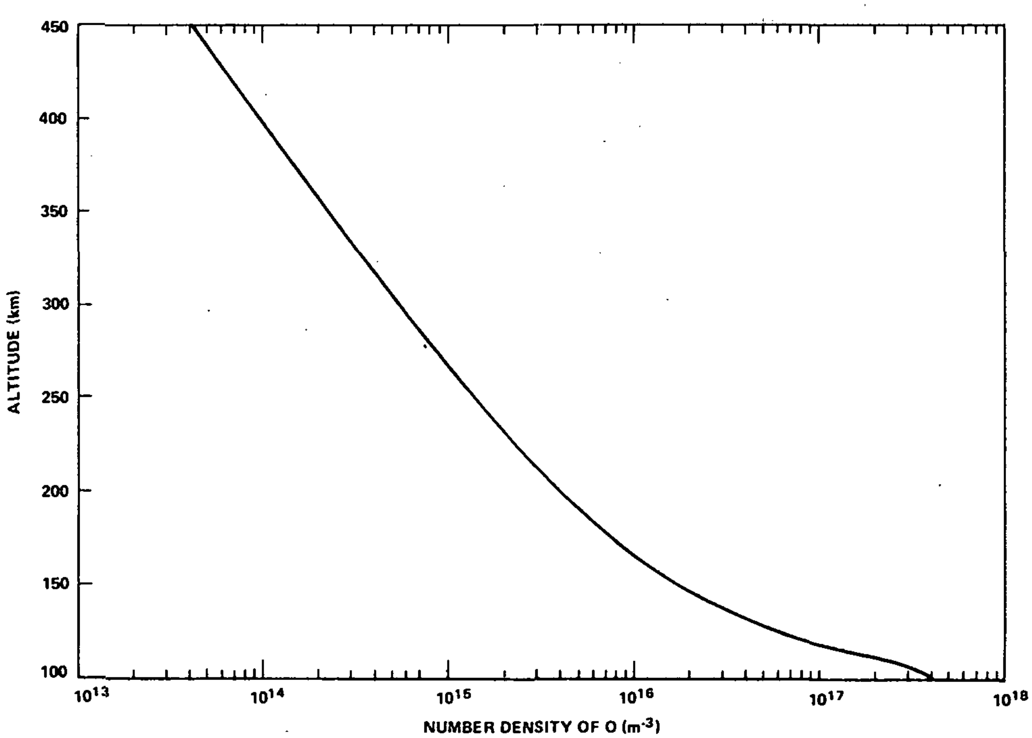

Figure 7. Number density of O versus altitude, 100 to 450 km.

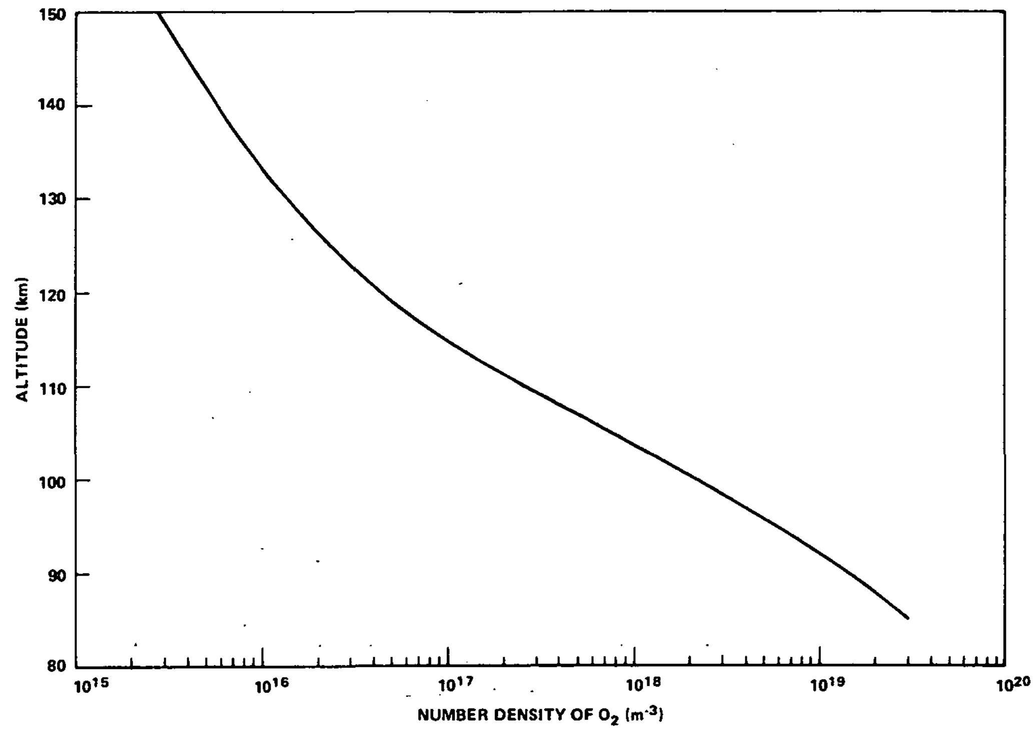

Figure 8. Number density of O_2 versus altitude, 86 to 150 km.

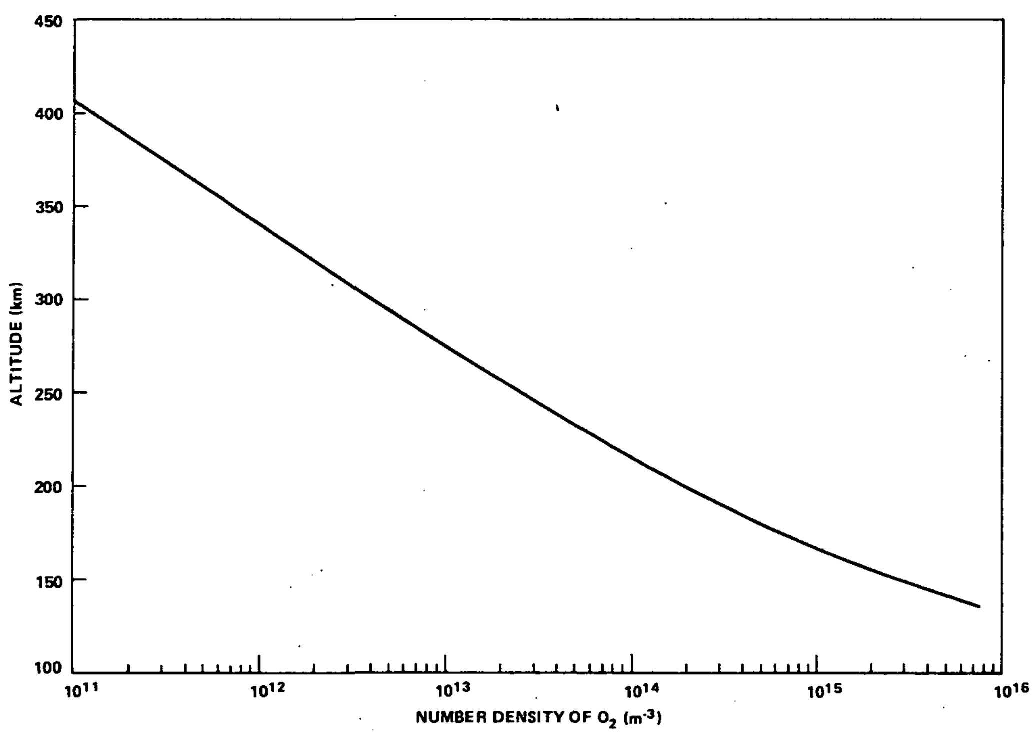

Figure 9. Number density of O_2 versus altitude, 100 to 450 km.

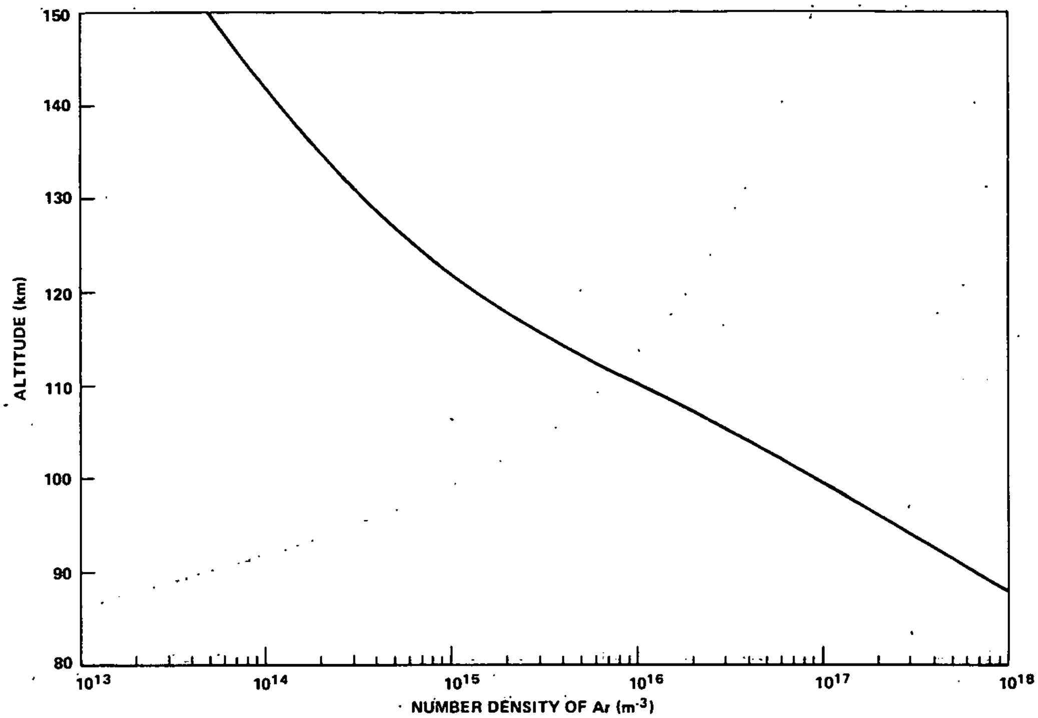

Figure 10. Number density of Ar versus altitude, 86 to 150 km.

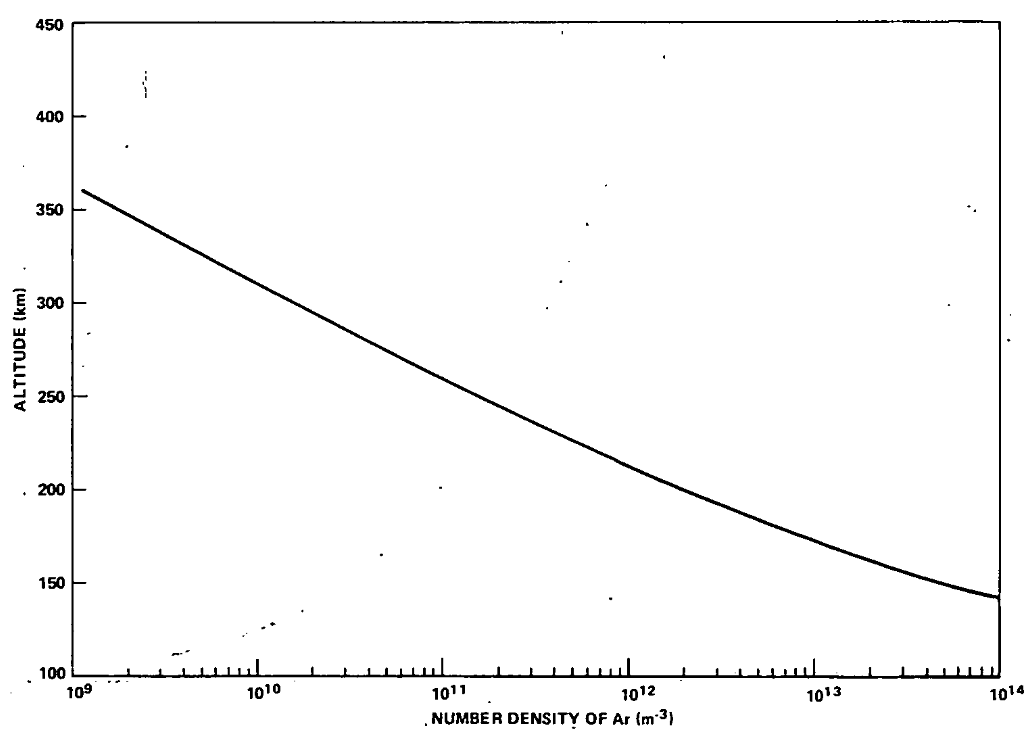

Figure 11. Number density of Ar versus altitude, 100 to 450 km.

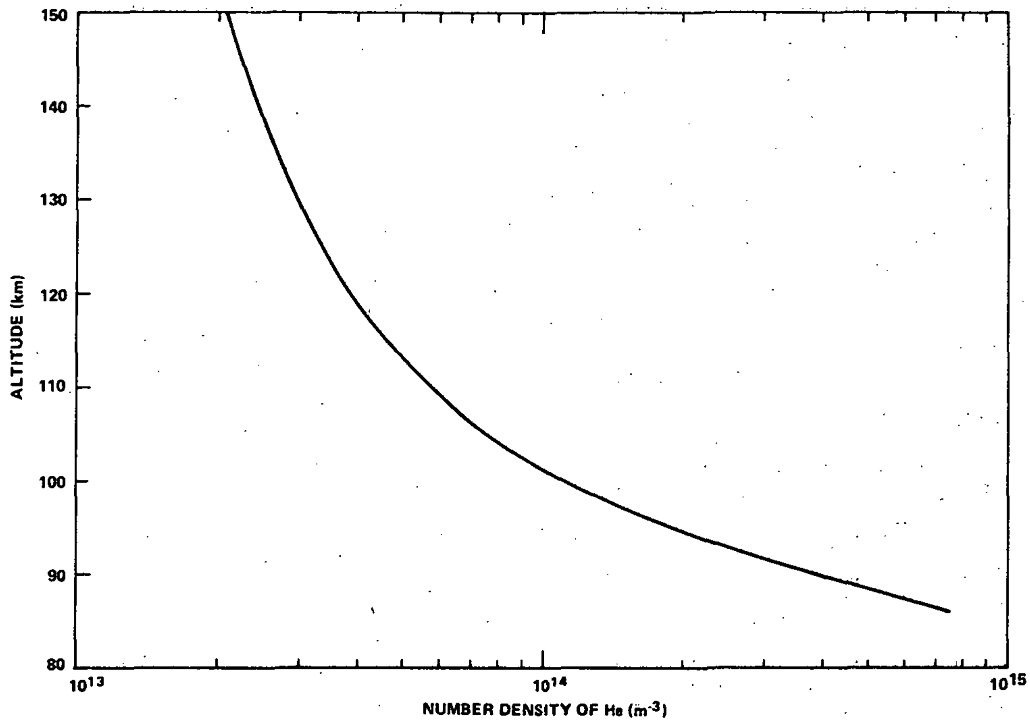

Figure 12. Number density of He versus altitude, 86 to 150 km.

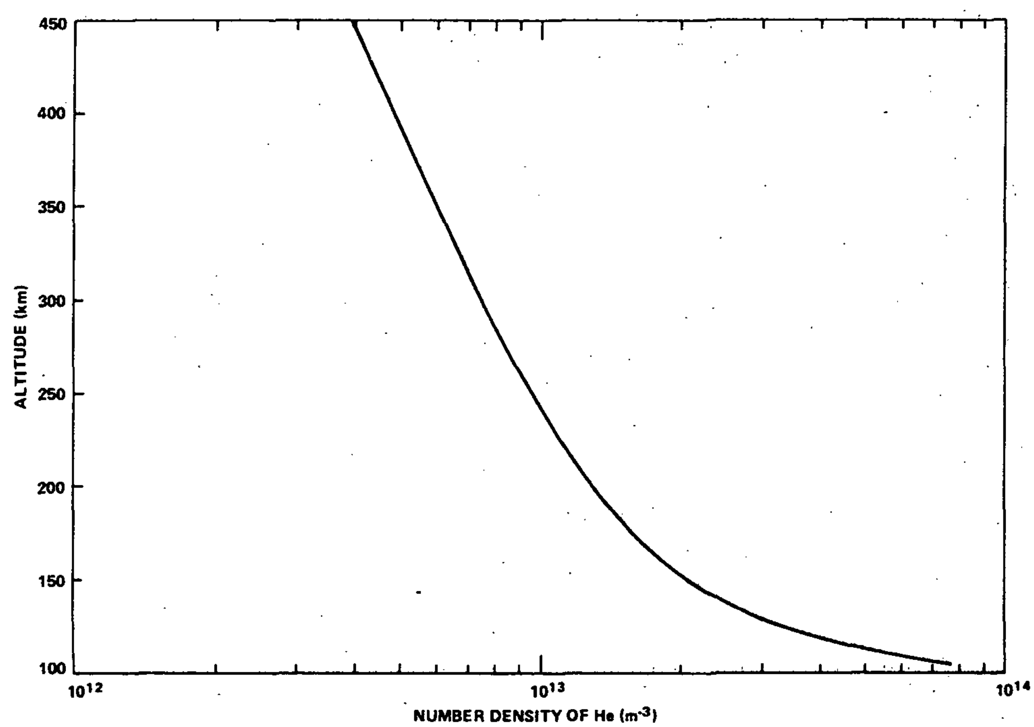

Figure 13. Number density of He versus altitude, 100 to 450 km.

Atomic Hydrogen

A set of calculated atomic-hydrogen number densities versus height, originally prepared for Task Group III for heights from 150 to 1000 km, were supplied to Task Group II by Forbes, in punch-card form. The method for calculating these values is given in Appendix A. The atomic-hydrogen height profile generated from the supplied values is shown in figure 14 for heights between 150 and 450 km, and has a value of 3.7541×10^{11} at 150 km. This value represents about one part in 100,000 of the N_2 number density (3.1221×10^{16}) at that height. Consequently, at heights below 150 km, for which height region no atomic-hydrogen number densities were given, these values would provide a negligible contribution to the four-significant-figure value of total number density N, and need not be considered in its calculation at these heights.

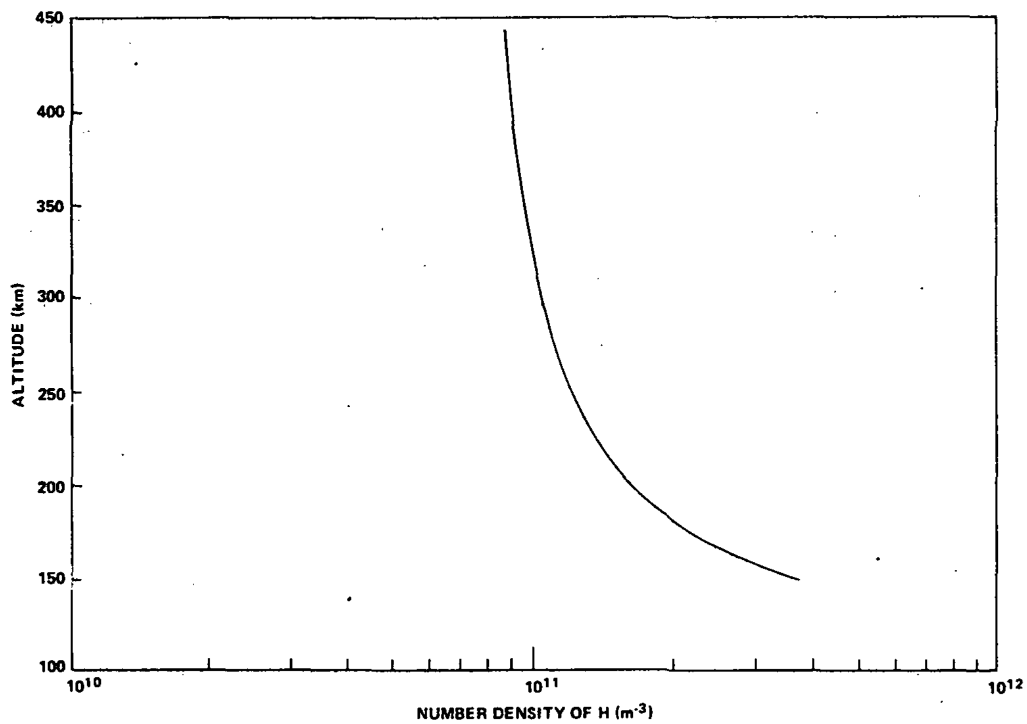

Figure 14. Number density of H versus altitude, 150 to 450 km.