Realistic Model of Hydrogen Constituents in the Lower Atmosphere and Escape Flux from the Upper Atmosphere

S. C. Liu and T. M. Donahue

The University of Pittsburgh, Pittsburgh, Pa. 15260

8 May 1974

ABSTRACT

A model for H_2O, CH_4, H_2 and odd hydrogen is developed that properly relates the measured mixing ratios in the stratosphere to escape of H in the form of Jeans flux, charge exchange and polar wind. The resulting model predicts a temperature-dependent Jeans flux in agreement with recent measurements.

1. Introduction

Recently we have published two papers (Liu and Donahue, 1974a, b) showing that the escape flux of hydrogen from earth must fall between 16 \times 10^7 and 31.1 \times 10^7 cm^{-2} sec^{-1} if the total hydrogen mixing ratio at the stratopause lies between 9 and 17.2 ppm by volume and the exospheric temperature is greater than 800K. This range of mixing ratios corresponds to the measured mixing ratio for H_2O of 4 to 7.6 ppm (Mastenbrook, 1968), for CH_4 of 0.25 ppm (Ehelt et al., 1972), and for H_2 of 0.5 ppm (Ehelt et al.). The measured Jeans escape flux is closer to 5 \times 10^7 cm^{-2} sec^{-1} at 1000K. This discrepancy has led us to adopt the suggestion of Cole (1966) and Tinsley (1973) that charge exchange between exospheric H and hot H^+ can lead to large hydrogen escape fluxes. The contribution of lateral flow of hydrogen to supply the polar wind can also be appreciable. In fact, we found that if the Jeans flux at 1000K is 5 \times 10^7 cm^{-2} sec^{-1} the hydrogen density in the exosphere will be such that the charge exchange flux would be 20 \times 10^7 cm^{-2} sec^{-1} and the average flux supporting the polar wind \( 1.8 \times 10^7 \) cm^{-2} sec^{-1}. The resulting total flux would be \( 26.8 \times 10^7 \) cm^{-2} sec^{-1} and the mixing ratio of total hydrogen in the lower atmosphere that would provoke such a flux would be 14.8 ppm (0.5 ppm H_2, 0.25 ppm CH_4 and 6.4 ppm H_2O, at 50 km), a value nicely within the range of measured concentrations.

Since the escape flux belonging to this mixing ratio will remain at \( 26.8 \times 10^7 \) cm^{-2} sec^{-1} independent of exospheric temperature above 800K although the charge exchange flux will decrease with increasing temperature, because of the decrease in the quantity of hydrogen above the critical level, it follows that the Jeans escape flux must increase with increasing temperature. In our second paper (Liu and Donahue, 1974b) we showed how \( \phi_J, \phi_E \) and \( \phi_P \), i.e., the Jeans, charge exchange and
at 500 km as a function of the average exospheric temperature. From these data it is simple to compute the average escape flux for a given average $T_e$. Bertaux (1974) from experiments conducted on OGO-5 has succeeded in measuring effectively the hydrogen density and temperature directly, thus allowing an evaluation of the Jeans flux. In Fig. 1 we compare the fluxes measured by these observers with the values we have computed for a total hydrogen mixing ratio of 14.8 ppm. All fluxes are corrected by a factor of 0.73 for departures polar wind fluxes, vary with the temperature at the critical level $T_c$.

2. Measured versus theoretical Jeans flux

In this note we wish to do two things. The first is to compare the predicted dependence of Jeans flux on temperature with two recently reported measurements of that flux. These measurements were made by Vidal-Madjar et al. (1974) and Bertaux (1974). The former authors, by means of an experiment carried on OSO-5, have determined the average daily hydrogen density at 1000K exospheric temperature. The total hydrogen mixing ratio is 14.8 ppm at the stratopause.

![Figure 1: Jeans escape fluxes plotted as functions of exospheric temperature. The dotted line is evaluated by Bertaux (1974) from experiments conducted on OGO-5. The dashed line is deduced from measurements made by Vidal-Madjar et al. (1974) on OSO-5. The solid line represents the calculated values.](image1)

![Figure 2a: Densities of H, OH, HO2 and H2O2 for 1000K exospheric temperature. The total hydrogen mixing ratio is 14.8 ppm at the stratopause.](image2)

![Figure 2b: Densities of H2O, H2 and CH4 under the same conditions as Fig. 2a.](image3)
Fig. 3. Fluxes of H, H$_2$O, H$_2$ and CH$_4$ under the same conditions as Fig. 2a. Solid lines indicate upward fluxes and dashed lines indicate downward fluxes.

from a Maxwell-Boltzmann distribution near the critical level. The agreement among the results seems to us to be rather good.

Table 1. Chemical reactions.*

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Rate Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>H + O$_2$ + M → HO$_2$ + M</td>
</tr>
<tr>
<td>R2</td>
<td>H + O$_2$ → OH + O$_2$</td>
</tr>
<tr>
<td>R3</td>
<td>OH + O → O$_2$ + H</td>
</tr>
<tr>
<td>R4</td>
<td>OH + O$_2$ → HO$_2$ + O$_2$</td>
</tr>
<tr>
<td>R5</td>
<td>HO$_2$ + O → OH + O$_3$</td>
</tr>
<tr>
<td>R6</td>
<td>OH + OH → H$_2$O + O</td>
</tr>
<tr>
<td>R7</td>
<td>OH + HO$_2$ → H$_2$O + O</td>
</tr>
<tr>
<td>R8</td>
<td>OH + H$_2$ → H$_2$O + H</td>
</tr>
<tr>
<td>R9</td>
<td>H + H$_2$O → H$_2$ + OH</td>
</tr>
<tr>
<td>R10</td>
<td>H$_2$ + O$_2$ → OH + H$_2$O</td>
</tr>
<tr>
<td>R11</td>
<td>HO$_2$ + H$_2$O → H$_2$O$_2$ + O$_2$</td>
</tr>
<tr>
<td>R12</td>
<td>OH + CH$_4$ → H$_2$O + CH$_3$</td>
</tr>
<tr>
<td>R13</td>
<td>O + CH$_2$ → OH + CH$_3$</td>
</tr>
<tr>
<td>R14</td>
<td>O$^+$ + O$_2$ → O + OH</td>
</tr>
<tr>
<td>R15</td>
<td>O$^+$ + H$_2$O → O + H$_2$ + O</td>
</tr>
<tr>
<td>R16</td>
<td>O$^+$ + H$_2$ → O + H$_3$</td>
</tr>
<tr>
<td>R17</td>
<td>O$^+$ + H$_2$ → O + H$_3$</td>
</tr>
<tr>
<td>R18</td>
<td>O$^+$ + H$_2$ → O + H$_3$</td>
</tr>
</tbody>
</table>

*Reaction rates with references can be found in Liu and Donahue (1974a).

3. Lower atmosphere model

Second, we wish to publish the distribution of species, fluxes, production and loss rates for this model with a mixing ratio of 14.8 ppm. These are shown in Figs. 2a, 2b, 3 and 4. The maximum atomic hydrogen density is 9×10$^7$ cm$^{-3}$ at 86.5 km. The densities at 100 km are 1.8×10$^7$ cm$^{-3}$ for H, 5.2×10$^6$ cm$^{-3}$ for H$_2$ and 1.02×10$^6$ cm$^{-3}$ for H$_2$O. The fluxes at 100 km are 3.2×10$^7$ cm$^{-3}$

Fig. 4. Principal reactions for production and loss of HO, H$_2$O and H$_2$ under the same conditions as Fig. 2a. The numbers on the figures correspond to the reactions listed in Table 1. Reaction rates rather than production and loss rates are plotted except that Σp and Σl are total production and loss rates for the species indicated. Solid lines indicate production reactions and dashed lines indicate loss reactions.
Fig. 5. Atomic hydrogen variations between 100 and 500 km that are needed to give the Jeans flux and total flux required in the model for exospheric temperatures between 900 and 1900K. Also plotted for comparison is the atomic hydrogen distribution for 1000K exospheric temperature when all escape flux \(2.68 \times 10^7 \text{ cm}^{-3} \text{ sec}^{-1}\) is Jeans flux and no \(H_2\) flux above 100 km.

\[
\begin{align*}
\text{sec}^{-1} \text{ in the form of } H, \quad 23.2 \times 10^7 \text{ cm}^{-2} \text{ sec}^{-1} \text{ for twice the } H_2 \text{ flux, and } 0.34 \times 10^7 \text{ cm}^{-2} \text{ sec}^{-1} \text{ for twice the } H_2O \text{ flux. } H_2 \text{ is the dominant form of hydrogen between 133 and 74 km. }
\end{align*}
\]

In Fig. 5 we also show the atomic hydrogen density variation between 100 and 500 km that is needed to give the Jeans flux and total flux required in the model for exospheric temperatures between 900 and 19000K.

Because of the large hydrogen concentrations the density of OH in the model tends to be large, especially if very low values are used for the rate constants of the reactions

\[
\begin{align*}
\text{OH} + \text{HO}_2 & \rightarrow H_2O + \text{O}_3 \\
\text{H} + \text{HO}_2 & \rightarrow \text{H}_2 + \text{O}_3
\end{align*}
\]

In Fig. 6 we compare the predicted integral values (column densities) of OH with the measurements of Anderson (1971). A rate constant \(k_{12}\) considerably greater than \(2 \times 10^{-10} \text{ cm}^3 \text{ sec}^{-1}\) (Kaufman, 1969) but not necessarily as large as \(2 \times 10^{-10} \text{ cm}^3 \text{ sec}^{-1}\)

Fig. 6. Comparison of computed and observed OH column densities. Observations by Anderson (1971) are indicated by \(\rightarrow\).
(Hochanadel et al., 1972) seems to be required for the best accord between observations and the model. We believe that the model for terrestrial hydrogen presented here very probably corresponds to the real average state of affairs and that the dominant escape flux mechanism is charge exchange rather than Jeans evaporation or the polar wind. In closing it is appropriate to remark that in his thesis Bertaux has recognized the contradiction between Hunten's principle and a temperature-dependent Jeans flux that would result unless there were some other important loss mechanisms. He also identified the polar wind and charge exchange as likely candidates but did not present a quantitative model.

Acknowledgments. This work was supported, in part, by the National Science Foundation, Atmospheric Sciences Section, under Grant GA-37744. We are grateful to Dr. Jean-Loup Bertaux for the opportunity to use his results before their publication.

REFERENCES


