The Boltzmann Equation to Study the Escape of Light Atoms from Planetary Atmospheres

Viviane Pierrard

Chargée de Recherches FNRS, Belgian Institute for Space Aeronomy
3, Avenue Circulaire, B-1180 Brussels, Belgium

Abstract. The atmosphere is bound to a planet by the planetary gravitational field. At high altitudes, light atoms such as hydrogen and helium can attain speeds in excess of the escape speed of the planet. These particles escape provided they suffer no further collision. In exospheric models, it is assumed that the escape flux is contributed only by particles moving outwards with a speed greater than the escape speed. The exospheric theory has served as a useful model for comparison with satellite and ground-based measurements, but it presents limitations inherent to the collisionless approach. To study the transition region between the collision-dominated and the collisionless domains of the neutral planetary atmospheres, it is necessary to use a model based on the solution of the Boltzmann equation. Such a model is presented in the present work to study the escape of light atoms from the terrestrial atmosphere through a background of oxygen atoms. The escape of hydrogen atoms out of the atmosphere of Mars is also discussed. A spectral method, initially developed to study the polar wind, is used to solve the Boltzmann equation. The effects of the planetary curvature and the gravitational force are taken into account. Two boundary conditions are imposed: one at the bottom and one at the top of the transition region. With this model, the velocity distribution function of the light atoms can be calculated at different altitudes. The density, flux, bulk velocity, and temperature profiles are obtained by calculating the moments of the velocity distribution function. The escape flux is found to be reduced compared with purely exospheric Jeans’ flux. The results are compared with those of the exospheric models, as well as with previous collisional models based on Monte Carlo simulations or on the Boltzmann equation with different assumptions.

INTRODUCTION: THE EXOSPHERIC APPROACH

The exobase of a planetary atmosphere is defined as the altitude for which the mean free path of atmospheric constituents is equal to the density scale height i.e. where the Knudsen number is equal to 1 (Kn=1). Above this altitude, collisionless exospheric models have been developed assuming that the particles move on collision-free trajectories [1]. In these models, light atoms such as hydrogen and helium can escape at high altitude provided they have a velocity larger than the escape velocity, given by

\[ v_e = \left(\frac{2GM}{r}\right)^{1/2} \]

where \( G \) is the gravitational constant, \( M \) is the mass of the planet (\( M=5.9736 \times 10^{24} \ \text{kg for the Earth and} \ M=6.4219 \times 10^{23} \ \text{kg for Mars} \)) and \( r \) the radial distance. For instance, for the Earth, the escape velocity is \( v_e=10.8 \ \text{km/s} \) and for Mars, \( v_e=4.8 \ \text{km/s} \) at the exobase level, located respectively at an altitude of 500 km for the terrestrial neutral particles and around 250 km in the Martian atmosphere.

In these exospheric models, the velocity distribution function (VDF) of the particles is assumed to be truncated at the exobase, as shown on Figure 1. For \( v<v_e \), the VDF is symmetric because these particles have not enough energy to escape and come back to the planet. But for \( v>v_e \), the downward part of the VDF (with \( v_{\text{radial}}<0 \)) is assumed to be empty since no neutral particles come from the interplanetary space to the planet. In most exospheric models, a truncated Maxwellian distribution of particle velocities is assumed at the exobase. Lorentzian distributions have also been proposed in the case of space plasmas where the observed VDFs show large suprathermal tails [2].
The escape flux (also called Jeans’ flux [3]) is contributed only by particles moving outwards with a speed greater than the escape speed, that is:

\[
\bar{F}_j = \int_{v_e}^{\infty} \bar{v} \bar{d}v = \frac{n}{2\pi^{1/2}} \left( \frac{2kT}{m} \right)^{1/2} \left( 1 + \frac{mv_e^2}{2kT} \right) \exp \left( -\frac{mv_e^2}{2kT} \right)
\]  (2)

**FIGURE 1.** Truncated velocity distribution function assumed at the exobase in exospheric models. The flux is only contributed by particles with a velocity larger than the escape velocity.

**COLLISIONAL MODEL**

But a discontinuous change at the exobase level between the thermosphere (dominated by collisions) and the exosphere (corresponding to the collisionless region), as assumed in exospheric models, is not very realistic. It is better to consider a gradual transition between the collision-dominated region at low altitude and the collisionless region at high altitude. A comprehensive treatment of the exosphere and of the transition region has to proceed from the Boltzmann equation:

\[
\frac{\partial f}{\partial t} + (\bar{v}, \bar{\nabla}_v) f + (\bar{a}, \bar{\nabla}_v) f = \int \int [f^* f^{*M} - ff^M] \bar{g} \bar{d} \Omega \bar{d} \bar{v}
\]  (3)

The right hand side of this equation describes the effects of collisions with the background constituent. This term is neglected in exospheric models. \(\sigma\) is the cross section for elastic collisions assumed to be energy independent, \(g\) is the relative velocity, \(\Omega\) is the scattering solid angle and the primes distinguish the velocities of particles entering a collision from the values after a collision [4]. The acceleration \(a\) corresponds to the gravitational attraction.

At the vicinity of the exobase level, the terrestrial atmosphere is mainly constituted by atomic oxygen, with hydrogen and helium as minor species. We consider thus collisions with heavy background oxygen particles assumed to have a (non displaced) maxwellian distribution with a temperature \(T_o\). We use a spherical geometry and take into account the curvature of the Earth.
The results of the collisional model of the transition region are based on the steady state solutions of the Boltzmann equation. To solve the integro-differential equation, we express it as a function of $r$ the radial distance, $v$ the velocity and $\mu$ the cosine of the angle between these two vectors.

We employ the transformation to dimensionless velocity:

$$y^2 = \frac{mv^2}{2kT}$$  \hspace{1cm} (4)

and to dimensionless altitude variable

$$z = - \int_{r_{wp}}^{r} n(r')dr'$$  \hspace{1cm} (5)

where $n$ is the density of the particles and $r_{wp}$ is the top of the transition region taken at one mean free path above the exobase.

A specialized spectral method developed by Shizgal and Blackmore [5] has been used to solve the partial differential equation and obtain steady state solutions for H and He velocity distribution functions. A similar method had been used in Pierrard and Lemaire (1998) [6] and Pierrard et al. (1999) [7] to solve the Fokker-Planck equation in the polar wind and the solar wind case respectively. This method is described in more details in these papers.

The solution is expanded in terms of orthogonal polynomials:

$$f(z, y, \mu) = \exp(-y^2) \sum_{i=0}^{m} \sum_{j=0}^{n} \sum_{k=0}^{p} P_i(\mu) S_j(y) P_k(z)$$  \hspace{1cm} (6)

where $P_i(\mu)$ are Legendre polynomials used for the dependence of the solution as a function of $\mu$, $S_j(y)$ are speed polynomials introduced by Shizgal [8] to expand the solution with respect to $y$ and $P_k(z)$ are Legendre polynomials for the interval $[-z_0, 0]$ used to expand the solution with respect to the dimensionless altitude $z$, which corresponds to the number of mean free paths.

When the VDF of the particles is found as a solution of the Boltzmann equation, the moments of the VDF (n the number density, F the escape flux, T the temperature) can easily be calculated by using the polynomial expansion and orthogonal properties of the polynomials [9].

**THE BOUNDARY CONDITIONS**

Boundary conditions are also imposed in the model. At the bottom boundary level ($-z_0$), it is assumed that the upward part of the distribution function ($\mu y = v_{\text{radial}} > 0$) is a Maxwellian with the same temperature as the background particles:

$$f(y, \mu > 0, -z_0) = \text{Maxwellian.}$$  \hspace{1cm} (7)

The bottom level has to be sufficiently low so that this assumption is valid.

At the upper boundary ($z = 0$), downward moving particles ($\mu y = v_{\text{radial}} < 0$) with speeds in excess of the escape speed are taken to be absent:

$$f(y > y_c, \mu < 0, 0) = 0.$$  \hspace{1cm} (8)

Downward moving particles with speeds lower than the escape speed are assumed to be the specular reflexion of the upward moving ones:

$$f(y < y_c, \mu < 0, 0) = f(y < y_c, \mu > 0, 0).$$  \hspace{1cm} (9)

These conditions come directly from exospheric considerations.
Figure 2 shows a typical velocity distribution function of light atoms (here hydrogen atoms) found with the collisional model at different altitudes in the transition region. At the lower boundary level, the upward part of the VDF ($v_{\parallel}>0$) is given by the boundary condition, but the downward part ($v_{\parallel}<0$) is found as a solution of the model. In this region dominated by collisions, the distribution is close to a Maxwellian but there are more upward particles than downward particles because the flux is different from zero and some particles are escaping.

At the top level ($z=0$), the velocity distribution function shows an increasing deviation from the isotropic Maxwellian distribution, due to the top boundary conditions. The flux is contributed by the asymmetry of the high energy part of the distribution function in the vertical direction.

![Figure 2](image)

**FIGURE 2.** Velocity distribution function of hydrogen atoms escaping from the Earth's atmosphere in a background temperature of 3570 K. The isocontours are given at different altitudes $z$ expressed in mean free paths ($z=0$ at the top boundary level).

**COMPARISON BETWEEN EXOSPHERIC AND COLLISIONAL RESULTS**

The model was applied to the escape of hydrogen and helium atoms from the terrestrial atmosphere. The background constituent is oxygen with a temperature equal to the temperature imposed to the minor atoms at the bottom boundary.

It is found that the actual velocity distribution function departs from a Maxwellian and the actual thermal escape flux in the real atmosphere is less than that predicted by Jeans. The flux ratio $F/F_J$ for the escape of hydrogen from the Earth is found to be around 0.6 at 2000 K with a slight decrease with the assumed background temperature.
We can compare these results with those of earlier models treating similar physical situations and reviewed in [1]. These models found factors for $F/F_j$ comprised between 0.3 and 0.8 for hydrogen escape at $T=2000$ K for instance. The different results depend on the assumptions made in the models and the different methods of solution: some models are based on Monte Carlo simulations, others are based on the Boltzmann equation with different kinds of approximations, especially for the collision term and the boundary conditions. Another difference is that the effect of planetary curvature and the gravitational term in the Boltzmann equation are taken into account in our model while they are neglected in most other models. The influence of these terms is limited to the second decimal in the flux ratio. A more detailed comparison can be found in [10].

Density and temperature profiles can also be determined with the model. The number density decreases a little bit faster than in a barometric model, obtained as a solution of the Boltzmann equation assuming a full Maxwellian at the top boundary level. But due to the top boundary condition (8), some particles are assumed to be missing in the VDF and the actual density decreases faster. The temperature of the escaping species decreases with the altitude. It is lower than the temperature of the background gas since a portion of the downward directed distribution is missing.

The model was also applied to study the escape of hydrogen atoms from other planets and especially Mars. The major constituent of the atmosphere of Mars is CO$_2$, and it was used as background particles in the earlier models [1]. But recent measurements in the Martian upper thermosphere have shown that O surpasses CO$_2$ at the altitudes $> 240$ km in solar maximum conditions and $215$ km at solar minimum conditions [11]. At the exobase level ($250$ km), oxygen atoms are dominant. Oxygen atoms were used as background particles in our model. In this case, the mass ratio between the minor escape gas (H) and the major background gas is 1/16. It is larger than the factor 1/44 used in earlier studies where the background particles were assumed to be CO$_2$. This leads to a flux ratio a little bit larger with oxygen background particles than with CO$_2$ background particles, but non-equilibrium effects are still large and the departure from Jeans' flux is quite important (around 57%).

Note that nonthermal processes, like charge exchange, dissociative recombination or interaction with the solar wind, were not considered in the present model but they provide an important escape mechanism for some particles and make even possible the escape of heavier species for which the thermal escape rate is very small. These processes could be taken into account by adding the appropriate terms in the Boltzmann equation.

**CONCLUSIONS**

To describe escape of neutral particles from planetary atmospheres, purely collisionless models have been developed. They proved to be very useful zero-order kinetic approximations but higher order kinetic approximations are necessary to take into account the effects of collisions. A model based on the solution of the Boltzmann equation is presented here and results compared to those of exospheric models.

This problem is quite similar to that presented in the same issue by Lemaire and Pierrard [12] except that the latest concerns the case of electrically charged atmospheric particles like the solar wind and the terrestrial polar wind. The major differences between the case of neutral particles presented in the present paper and the case of electrically charged particles are the following: (i) the collision terms are different: the Fokker-Planck collision term has to be used instead of the Boltzmann collision term since Coulomb collisions have to be simulated in the case of charged particles (ii) the Lorentz force due to the presence of the magnetic field has to be considered in the electrically charged case (iii) the electrostatic force has to be considered. The escape processes of neutral particles or charged particles from planetary atmospheres are thus quite different. For instance, the protons of the polar wind are accelerated outwards by the electrostatic potential while the neutral hydrogen atoms are on the contrary attracted to the planet by the gravitational force.

The collisional model can be used and adapted to study the escape of light atoms from other planets. The study of escape mechanisms from the planets is of considerable interest to understand the evolution and the present state of the atmosphere.
ACKNOWLEDGMENTS

V. Pierrard wishes to thank the Belgian FNRS for the grant FC 36556. She also thanks Prof. J. Lemaire and Prof. B. Shizgal for many discussions about this work.

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