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The escape of Martian atmosphere

Team 444

Abstract

The most crucial mechanisms of atmospheric escape are discussed and referred to in the context of the planet Mars. In the considered scenario the atmospheric pressure on the Martian surface is increased to 0.2 bar by vaporising its subsurface ice and polar capes. The Jeans thermal escape of hydrogen is introduced as the dominant phenomenon responsible for the rarefaction of Martian atmosphere and its impact on value of atmospheric pressure is derived. Calculations led to an ordinary differential equation of type: $\frac{dX(t)}{dt} = -\alpha X(t)$. Then, the partial hydrogen pressure as a function of time is expressed as an exponential decay. The oxygen escape is assumed to be proportional to that of hydrogen. It is calculated that the net pressure decreases by half in $\tau = 464500$ s. Based on aforementioned the differential equation a numerical model was constructed and calculations were performed to further visualise and explain the model, as well as simulate changes induced by the models modification. This suggests, that such high pressure is not easily sustainable on a planet as light as Mars. Experimental data could be used to perfect presented models.

Contents

1	Mechanisms of atmospheric rarefaction	3
1.1	Thermal escape	3
1.2	Suprathermal escape	3
1.2.1	Photochemical escape	4
1.2.2	Solar wind sputtering	4
1.2.3	Impact erosion	4
2	Problem Interpretation	5
3	Theoretical analysis	6
3.1	Partial pressure of oxygen and hydrogen	6
3.2	Jeans escape of hydrogen	6
3.3	Barometric formula and molecular density	7
3.4	Surface pressure's time dependency derivation	7
4	Numerical analysis	9
4.1	Numerical model	10
4.2	Water vapor dissociation model	11
4.3	Hydrogen molecule dissociation	15
5	Conclusions	18

1 Mechanisms of atmospheric rarefaction

The atmosphere is an immensely complex system of gas bound by the gravity well of a massive body. In close proximity to the planet surface, the gas is relatively dense and its molecules interact frequently with each other. In the upper parts of the atmosphere this frequency decreases with altitude. The height of the exobase serves as a useful threshold, establishing an abstract boundary between the denser parts of the atmosphere and the exosphere, where it is assumed that particle collisions do not occur[1]. The exobase is defined as the height at which the average distance travelled by a molecule between collisions is comparable with atmospheric scale height. If an exospheric molecule achieves escape velocity, it is no longer considered as part of the atmosphere. A plethora of phenomena has been theorised and observed which describe different escape mechanisms of molecules. [2] [3]. Considering the origin of the sudden momentum change, the escape mechanisms are divided into the following categories:

1.1 Thermal escape

During general particle collisions the velocity distribution among participants is not uniform. For high enough variation, one should observe some particles achieving very high velocities, even exceeding escape velocity v_e . The more thermal energy in the system, the higher the average velocity of each particle, but in a stronger gravitational field more energy is required to fill the potential energy deficit and achieve infinite separation. These relations are illustrated by the Jeans parameter:

$$\lambda = \frac{|U(r)|}{kT} \quad (1)$$

where $U(r)$ is molecules gravitational energy at distance r , k is Boltzmann constant and T is the temperature.

Astrophysicists use the Jeans parameter to predict the relative magnitude of single-molecule escape flux (Jeans escape) and hydrodynamic escape of fluid-like bodies of gas expanding to outer space. This body of work will focus mainly on the Jeans escape mechanism.

1.2 Suprathermal escape

Sources of critical particle momentum change may originate from outside the atmosphere. The main source of energy for such processes is the local star.

These include, but are not limited to:

1.2.1 Photochemical escape

When a high-energy photon is absorbed by a near-exospheric molecule, it can dissociate with excess photon energy converted into kinetic energy of resulting particles, as dictated by momentum and energy conservation laws. Such kinetically excited molecules are candidates for atmospheric escape, should they not suffer further collisions.

1.2.2 Solar wind sputtering

Charged particles from solar winds such as protons, β or α particles produce electromagnetic field disturbance as they travel at high velocities. Through interactions with these disturbances, ionised particles from upper atmosphere can be swept up and carried away from the planet [4]. This effect is strongly suppressed for planets with strong magnetosphere which deflects the stream of charged interplanetary particles. In the case of planet Mars, the most contributing factor to Martian magnetic field is not its core but rather the subsurface deposits of magnetized material in the planet's crust. Moreover, MAVEN spacecraft data suggests that the solar wind ions induce planet-wide currents in the red planet's ionosphere which in turn create a so-called induced magnetosphere.[6]

1.2.3 Impact erosion

Causes of atmospheric escape are not restricted to the atomic scale. Larger objects appearing in the vicinity of planetary atmospheres can induce such events. Such asteroids or comets usually drag along smaller objects with much larger effective cross-section of impact than the parent space object, or even eject hot vapor plumes that impart sufficient kinetic energy to atmospheric molecules for them to escape the atmosphere [5].

2 Problem Interpretation

Our team assumes that the resulting martian atmosphere will consist primarily of water vapor (the small CO_2 content is neglected). Furthermore, the temperature on the planet is assumed to be uniform and constant (see *Theoretical analysis*). In the considered vapor-rich Martian atmosphere the UV radiation causes water molecules to break apart into H and O molecules. We assume that rate of water vapor dissociation is higher than outflow of atmosphere, so it is considered to be instantaneous. The gasses are treated as ideal. In the relatively cold upper atmosphere hydrogen atoms recombine into H_2 molecules [7]. For such molecules, the Jeans escape is the dominating mechanism of escape [9][1]. For the rest of the atmospheric composition, it is assumed that other gasses (O and H_2O) are significantly heavier than H_2 and do not acquire sufficient kinetic energy as a result of thermal collisions [8]. Instead, it has been shown [8] that Oxygen escapes Martian atmosphere in approx. 1:10 outward flux ratio to that of Hydrogen and is mainly due to solar wind erosion. During analysis of the problem we aimed to find a mathematical relation between pressure on the surface and outflow of molecules and obtain its time dependency.

3 Theoretical analysis

To simplify such complex system as Martian atmosphere we made a few assumptions. Water vapor is affected by UV radiation and water molecules dissociate producing H₂ and O molecules. Although this process is not instant and has a certain progression rate, we assumed that martian atmosphere contains only H₂ and O molecules. In Earth's exosphere, the dominant species of hydrogen is its atomic form, however on colder planets such as Mars, hydrogen occurs mostly as H₂ molecules.

3.1 Partial pressure of oxygen and hydrogen

When a gas under net pressure p is comprised of two gases one can express the net pressure as a sum of partial pressures of these gases:

$$p = p_1 + p_2 \quad (2)$$

The relation between a partial pressure and the net pressure is given by:

$$\frac{p_i}{p_{net}} = \frac{n_i}{n} \quad (3)$$

where n_i and n are number of moles of a specific gas and total number of moles respectively. Thus, when average pressure on the surface of Mars equals $p_n = 0.2$ bar then partial pressures of both hydrogen (H₂) and oxygen equal $p_H = p_O = 0.1$ bar. Partial pressure concept is crucial in following analysis and allows for the consideration of changes in atmospheric pressures of hydrogen and oxygen independently.

3.2 Jeans escape of hydrogen

The dominant effect that determines the escape of a hydrogen from exosphere is Jeans thermal escape. When a molecule experiencing thermal collisions attains velocity greater than the escape velocity at the exobase it will escape from planet's atmosphere. For a certain molecule density n at exobase one can obtain the average velocity of molecules by adapting Maxwell-Boltzmann velocity distribution. By comparing it to the escape velocity we obtain Jeans escape flux formula [9]:

$$\Phi = \frac{n}{2\sqrt{\pi}} v_s \left(1 + \frac{v_s^2}{v_e^2} \right) e^{-\frac{v_s^2}{v_e^2}} \quad (4)$$

where $v_s^2 = \frac{2kT}{m}$ is the most probable velocity in the Maxwell Boltzmann distribution, $v_e^2 = \frac{2GM}{h+R_M}$ is the escape velocity, h is the distance from surface to exobase, R_M and M are the Mars radius and its mass, T is the temperature at h and m is the molecular mass of H_2 . Equation (4) describes the flux of molecules escaping from exobase when their density equals n at height h .

3.3 Barometric formula and molecular density

Assuming that the temperature in the atmosphere is constant and independent of height one can derive the barometric formula which describes the relation between atmospheric pressure and height:

$$p(z) = p_0 e^{-\frac{z}{H}} \quad (5)$$

where p_0 is a pressure and H is a scale height ($H = \frac{kT}{mg}$). By combining barometric formula and ideal gas law $\rho = \frac{p}{RT}$ one can express molecular density as:

$$n(z) = \frac{p_0}{RTm} e^{-\frac{z}{H}} \quad (6)$$

3.4 Surface pressure's time dependency derivation

The discussion of the impact of Jeans escape flux on Martian atmosphere is based solely on the behavior of hydrogen, due to the fact that oxygen molecules are too massive to be accelerated to escape velocity by thermal collisions. In the following derivation, hydrogen partial pressure p_H and hydrogen density n_H will be used.

Hydrogen escape occurs at temperature T and height h_e which corresponds to the altitude of the exobase. In our model we assume that these values will not change during the processes of polar caps vaporisation and subsequent atmospheric rarefaction. Eventually in calculations values equal $T = 250$ K and $h_e = 240$ km were used [9]. It is shown later that changes in these values do not significantly affect the final result, so this assumption is justified.

During outflow of hydrogen, pressure on the surface p_H varies with time, so density at height of exobase equals:

$$n(h_e) = \frac{p_H(t)}{RTm} e^{-\frac{h_e}{H}} \quad (7)$$

Therefore, Jeans escape flux is given as:

$$\Phi(t) = \frac{p_H(t) e^{-\frac{h_e}{H}}}{2\sqrt{\pi}RTm} v_s \left(1 + \frac{v_s^2}{v_e^2}\right) e^{\frac{v_s^2}{v_e^2}} \quad (8)$$

The particle escape flux is defined as:

$$\frac{dN}{dt} = \Phi(t)S \quad (9)$$

where S is the surface area through which the molecules are escaping and dN is amount of molecules lost. Consider a cylinder of height h_e and base surface S which is a fraction of Mars' atmosphere. The total amount of molecules in cylinder equals:

$$N_t = \int_0^{h_e} n(h)S dh = \frac{p_H(t)S}{RTm} (-H)e^{\frac{-h_e}{H}} \Big|_0^{h_e} = \frac{p_H(t)SH}{RTm} (1 - e^{\frac{-h_e}{H}}) \quad (10)$$

The escape flux of dN molecules in time dt through the upper bound of the cylinder can be expressed as a time derivative of N_t :

$$\Phi(t)S = -\frac{dN_t}{dt} = -\frac{dp_H(t)}{dt} \frac{SH}{RTm} (1 - e^{\frac{-h_e}{H}}) \quad (11)$$

Now we can use formula (8) for $\Phi(t)$ and obtain a differential equation with initial condition $p_H(0) = 0.1$ bar:

$$\frac{p_H(t)Se^{\frac{-h_e}{H}}}{2\sqrt{\pi}RTm} v_s \left(1 + \frac{v_s^2}{v_e^2}\right) e^{\frac{v_s^2}{v_e^2}} = -\frac{dp_H(t)}{dt} \frac{SH}{RTm} (1 - e^{\frac{-h_e}{H}}) \quad (12)$$

$$\frac{p_H(t)}{2\sqrt{\pi}H} \frac{1}{\left(e^{\frac{h_e}{H}} - 1\right)} v_s \left(1 + \frac{v_s^2}{v_e^2}\right) e^{\frac{v_s^2}{v_e^2}} = -\frac{dp_H(t)}{dt} \quad (13)$$

Defining all constants as A :

$$A = \frac{1}{2\sqrt{\pi}H} \frac{1}{\left(e^{\frac{h_e}{H}} - 1\right)} v_s \left(1 + \frac{v_s^2}{v_e^2}\right) e^{\frac{v_s^2}{v_e^2}} \quad (14)$$

results in differential equation for $p(t)$ in the form of:

$$\frac{dp_H(t)}{dt} + Ap_H(t) = 0 \quad (15)$$

And the solution is represented by:

$$p_H(t) = p_H(0)e^{-At} \quad (16)$$

It is estimated in Martian atmosphere models that outflow of oxygen is over 10 times lower and occurs mainly as a result of solar wind activity. Relation

between oxygen partial pressure and time is similar to equation (16). The constant A for oxygen (which is named \tilde{A}) is calculated in an analogous process as for hydrogen by changing the value of molar mass and scaling the outflow flux($\Phi_O(t) = \frac{\Phi_H(t)}{10}$). Eventually the net pressure time dependency is given by sum of partial pressures:

$$p_n(t) = p_H(0)e^{-At} + p_O(0)e^{-\tilde{A}t} \quad (17)$$

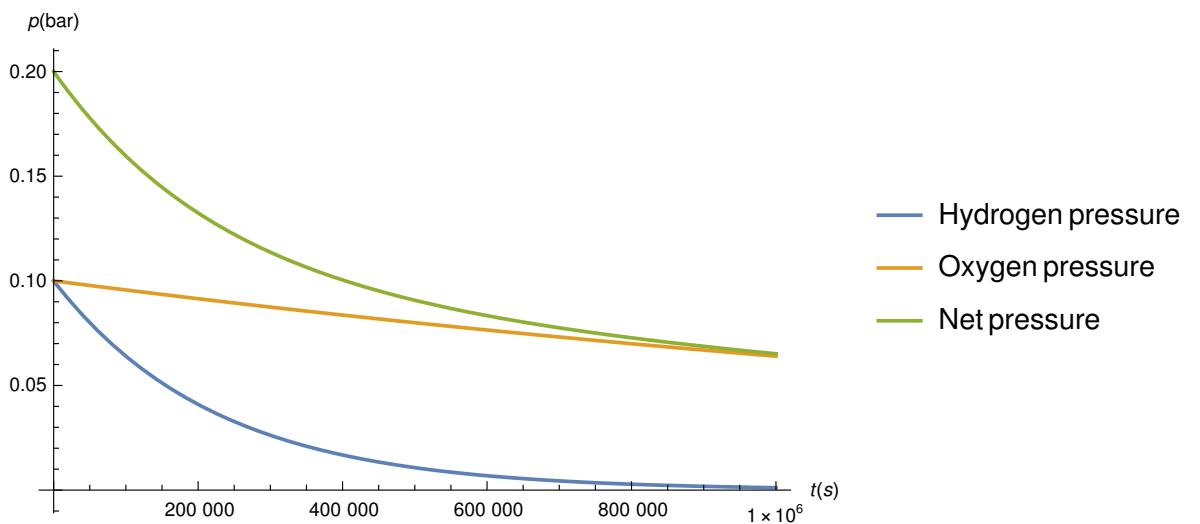


Figure 1: Net pressure ($p_n(t)$) and partial pressures of hydrogen ($p_H(t)$) and oxygen ($p_O(t)$) at surface level as a function of time.

While calculating values of A and \tilde{A} changes of T and h_e did not affect results significantly, so the assumption that the exobase's height and temperature are assumed correctly.

4 Numerical analysis

The result obtained is a product of many approximations, the most important of which is the assumption that all the water vapor molecules will dissociate in an instant. Furthermore, we only take into account the Jeans escape of H_2 molecules, which in reality also dissociate into single hydrogen molecules.

However, with the rate of said dissociations unknown, it is impossible to get a strict result with more advanced models that take them into account. One can only assume a rate of dissociation for either or both H_2O and H_2 .

molecules and then derive $p_n(t)$ either analytically or numerically from these more complicated models. Introducing unknown parameters to our equation doesn't help derive the sought value of τ , but becomes a useful tool, should one acquire experimental data (that could allow for the aforementioned dissociation parameters estimation).

4.1 Numerical model

In order to graph the changes in the atmosphere described by our basic model and to make further modifications to the model itself, we built a numerical model in Python. The model tracks the partial pressures of different molecules in the atmosphere and uses the A value to calculate the small changes in hydrogen pressure dp_H for a given time step dt . The partial pressure of oxygen changes in a previously explained correlation, proportionally to the \tilde{A} parameter. The formulas are directly derived from the differential equations used before (17).

The calculated relation $p_n(t)$ is shown on Figure 2.

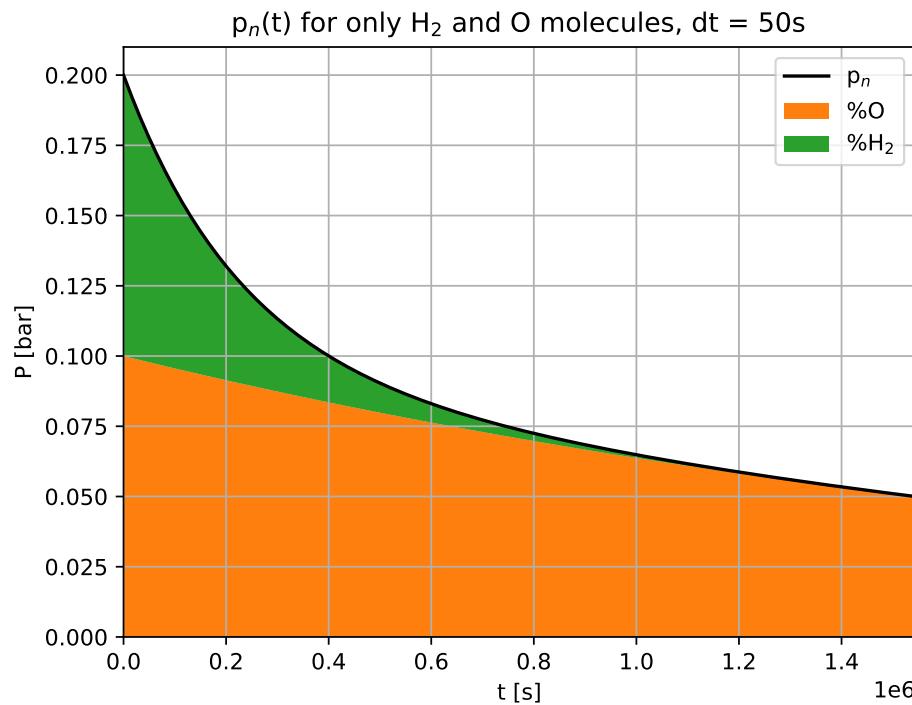


Figure 2: Numerical analysis of atmosphere's partial pressures, for time step $dt = 20\text{s}$. The black line represents the net pressure p_n and the colors underneath represent the partial pressures – for a given t , the color contents of the graph at t are proportional to the partial pressures. Because molecule density is proportional to partial pressure, one can think of the color composition of the area under a small fraction of the graph as of the atmosphere composition at that moment t . As seen on the graph, the percentage (molar) content of hydrogen and oxygen in the atmosphere begin at equal, but gradually the oxygen becomes the dominant component. In this model, τ is around $4 \cdot 10^5\text{s}$.

4.2 Water vapor dissociation model

The initial atmosphere composition is 100% water vapor and in time it dissociates to oxygen and hydrogen molecules – due to UV radiation. One can expect the rate at which it dissociates to be proportional to the density of water molecules exist in the atmosphere. Because the partial pressure of water molecules p_W is proportional to the density of molecules, one could

state:

$$\frac{dp_W}{dt} \sim p_W \quad (18)$$

Which gives:

$$p_W(t) = p_{initial} \cdot \exp(-2\beta t) \quad (19)$$

Where $p_{initial}$ is the initial partial pressure of water (because it is the only component of the atmosphere at $t = 0$), and β is an arbitrary positive parameter (the value 2 represents how dp_H distributes equally among $dp_H + dp_O$), describing the rate of dissociation. The equation (19) describes the most basic model of water vapor dissociation, which is not necessarily accurate. Nevertheless, one could use this simple model and see the changes it inflicts of the general atmosphere escape model.

A larger β value results in a lesser change to our model (compared to the instant dissociation model) – as seen on Figure 3, the value of τ only changes by 10^5 s compared to the model represented by Figure 2.

For medium β values, even more interesting patterns show. As seen on Figure 4, the hydrogen to oxygen proportions vary at first, but become more stable later. Still, the net pressure steadily decreases and tends to zero.

For smaller β values, the water vapor dissociation becomes a major retardant of net pressure decrease over time. As seen on Figure 5, both oxygen and hydrogen molecules escape the atmosphere more quickly than they are produced, leaving the atmosphere with almost constant, small partial pressures p_H and p_O , with the biggest contributor to net pressure being the partial pressure of water vapor (which is steadily decreasing).

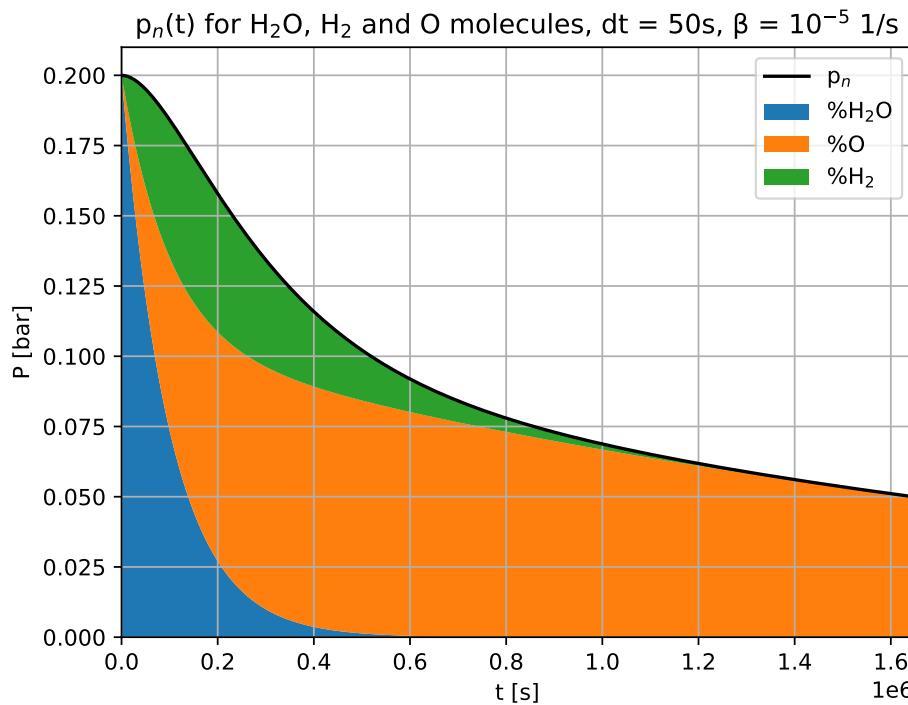


Figure 3: Numerical analysis of atmosphere's partial pressures, for time step $dt = 50$ s, taking into consideration gradual water vapor dissociation. The colors are kept in the same convention as on Figure 2, with blue representing the water content of the atmosphere. As can be seen on the Graph, for $\beta = 10^{-5}$ water dissociates more quickly than the hydrogen molecules escape, leading into an substantial increase of both hydrogen and oxygen contents of the atmosphere. The value τ is around $5 \cdot 10^5$ s. Later, the atmosphere becomes almost pure oxygen, and the net pressure gradually tends to 0.

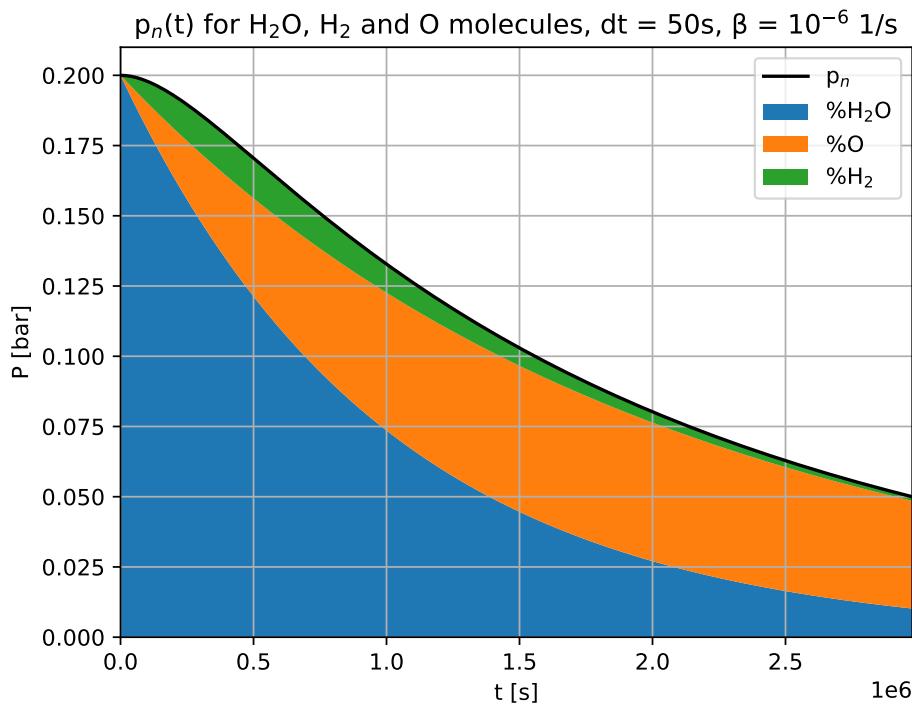


Figure 4: Numerical analysis of atmosphere's partial pressures, for time step $dt = 50$ s, taking into consideration gradual water vapor dissociation. For $\beta = 10^{-6}$, the net pressure decreases more slowly, and so the value τ increases to around $1.5 \cdot 10^6$ s. This shows how much τ relies on β . When net pressure drops by $3/4$ (which marks the end of the graph), there is still a non-negligible water content in the atmosphere.

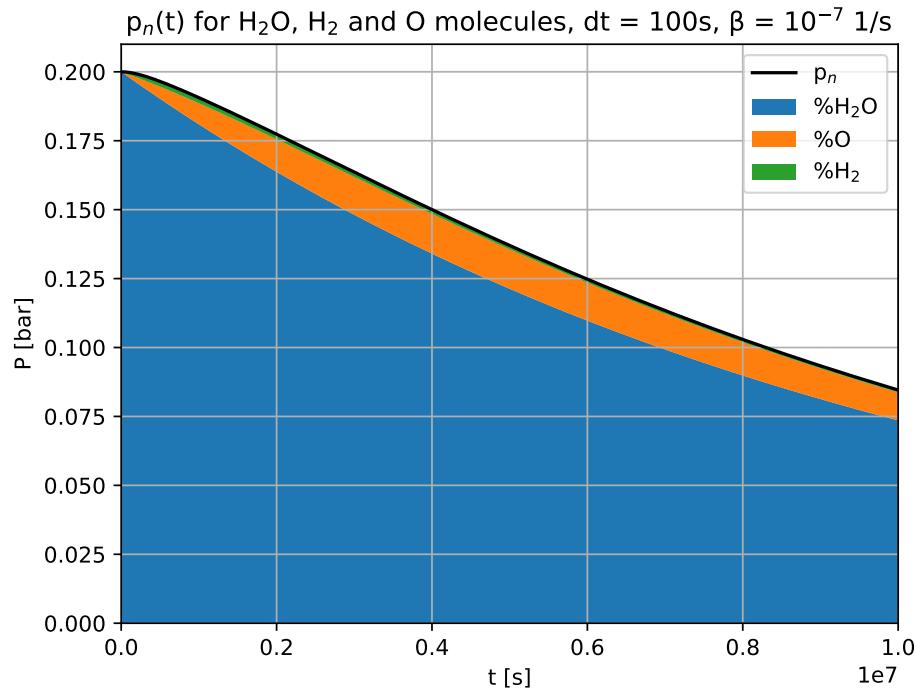


Figure 5: Numerical analysis of atmosphere's partial pressures, for time step $dt = 100$ s, taking into consideration a slow gradual water vapor dissociation, with $\beta = 10^{-7}$ 1/s. Hydrogen molecules escape the atmosphere much more quickly than they are being produced, thus the green area of the graph is barely visible. The net pressure decreases slowly due to the small β , which results in τ being equal around $8.3 \cdot 10^6$ s.

4.3 Hydrogen molecule dissociation

The most complex model of the Martian atmosphere we can derive from our general assumptions is one that takes into account both H_2O and H_2 molecule dissociation. We can also reinstate the presence of CO_2 in the atmosphere, as the approximation that it's partial pressure was negligible is no longer helpful.

This model, while still not being fully accurate, might give a better view of how complex the problem is and what one could expect to happen – rather than yielding practical numerical results or allowing to calculate parameters by fitting curves to experimental data.

We modify our numerical model, adding a hydrogen dissociation mechanism similar to that of water vapor dissociation. Let us rename partial

pressure of H_2 molecules to p_{H_2} and introduce partial pressure of single hydrogen atoms as p_H . Again, we think of small increases of partial pressures – this is the formula for a small change in p_{H_2} :

$$dp_{\text{H}_2} = (\beta p_W - Ap_{\text{H}_2} - \eta p_{\text{H}_2})dt \quad (20)$$

in which the consecutive summands are: the change resulting from H_2O dissociation, atmospheric thermal escape and the dissociation of H_2 molecules. Similarly, the small change in $dp_H = (\eta p_{\text{H}_2} - A'p_H)dt$ – where A' is similar to A , but calculated with the mass of a single hydrogen atom. The equations for calculating tiny changes in partial pressure from O and H_2O remain the same as in the previous subsection. The CO_2 partial pressure is approximated to be constant and it's implementation serves the purpose of better visualising the limit of p_n as t approaches infinity.

We then choose parameters β, η such that our graph is clear and shows a possible evolution of the net pressure and its partial components as a function of time. If one had experimental data of said partial pressures, they could match the parameters (and possibly entire functions, to better approximate dissociation) so that the curves best fit the data. We can see one example of the result of aforementioned simulation on Figure 6.

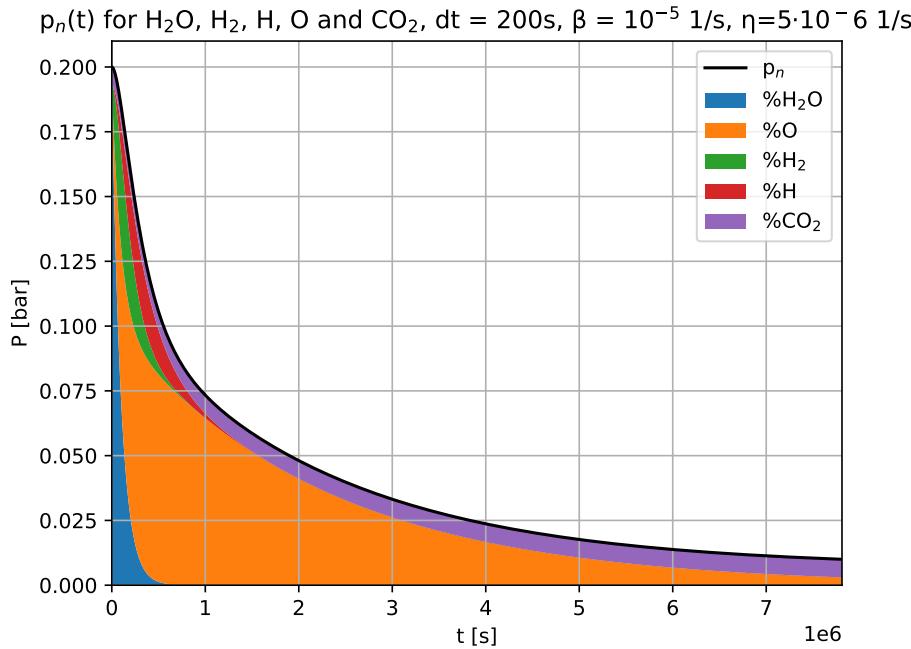


Figure 6: Graphical representation of our most complex numerical model of the Martian atmosphere. The time step $dt = 200$ s, parameters are: $\beta = 10^{-5}$ 1/s and $\eta = 5 \cdot 10^{-6}$ 1/s. The colors under the graph represent the ratios of partial pressures of molecules at a given time, and thus their relative ratios within the composition of the atmosphere. As can be seen on the Graph, the sequence of events can be roughly described as: First, H_2O dissociates into O and H_2 . Then, partial pressures of O , H_2 and H (which is created by dissociation of H_2) drop rapidly. We are then left with an atmosphere mostly composed of O and CO_2 , which steadily (but exponentially) tends to a constant net pressure of 0.007 bar, resulting only from CO_2 's partial pressure.

From all aforementioned models, this most complex one describes the mechanisms modifying Martian atmosphere's composition the most thoroughly. Neither does it explain the more complex phenomena of different atmospheric escape mechanisms, nor does it yield any numerical values that can be described as the sought value τ (which represents the time after which the net pressure drops by half). However, it is a useful visual representation and could be used as a tool to test the accuracy of made assumptions, should one have experimental data available.

This numerical analysis can provide the following conclusions: the true

of value τ should increase in respect to the one calculated with our analytical model. Depending on different parameters, which are difficult or even impossible to determine without experimental data, true τ could be even one order of magnitude bigger than our result (although for parameters as such the entire model is probably inaccurate).

5 Conclusions

The main goal of this body of work was to determine the time τ of the net pressure drop by half. The pressure function of time was derived. Calculations based on simplified atmosphere model described in *Problem Interpretation* and *Theoretical analysis* sections. Eventually we obtained pressure time dependency given by:

$$p_n(t) = p_H(0)e^{-At} + p_O(0)e^{-\tilde{A}t} \quad (21)$$

where A and \tilde{A} are constant values described by equation 14. It has been calculated that pressure at the surface will drop by half starting with value $p_n(0) = 0.2$ bar in time:

$$\tau = 464500 \text{ s} \quad (22)$$

In order to obtain an analytical solution to the problem, the complex system of a planetary atmosphere has undergone several simplifying assumptions. The authors of this body of work consider the model sufficient to predict the general tendency of water-vapor based martian atmosphere to dissipate over time. However in order to calculate the exact time τ , due to lack of available experimental data, approximations have been made that could prove inaccurate:

The invariability of temperature and exobase height as well as adoption of the ideal gas model was necessary to evaluate the exact thermal escape rates. The assumed proportionality of oxygen to hydrogen escape flux was an extrapolation of experimental data from existing publications that allowed the approximation of how many oxygen molecules escape the atmosphere. It was assumed that H_2O dissociates almost instantly and that H_2 does not dissociate at all (due to low temperature)– because the exact rates of dissociation could not be determined. It was also assumed that means of atmospheric escape that were not taken into account were insignificant in comparison to those discussed.

It was checked that changes in temperature or exobase height did not alter the results in a significant manner. The extrapolation of oxygen to

hydrogen escape ratio was possibly the most bold assumption, that could effectively prolong the time τ calculated. The assumption of instant dissociation of H_2O meant a decrease in the τ calculated and the negligence of H_2 dissociation increased the τ value (both by unknown margins). Because the calculations were performed in such a rough manner, neglecting less impactful mechanisms was justified.

To better visualise and understand the problem, we constructed a numerical model of the Martian atmosphere. By varying the complexity of our model, we managed to: confirm our theoretical analysis of the most basic model (Figure 2), see how the results would change if we assumed a non-instant dissociation of H_2O at different rates (Figures 3 - 5) and finally, visualise how the composition of the atmosphere would progress, if we assumed the most complex model derived from earlier analysis (Figure 6).

The result $\tau = 464500$ s is equal to about 129 hours or over 5 days. What this means (assuming calculations are correct), is that such a high pressure of hydrogen and oxygen is not easily sustainable. However, due to implied differences in hydrogen and oxygen escape, one could expect that for a time much longer than τ there will be non-negligible oxygen content in the atmosphere, apart from the existing (although neglected during calculations) carbon dioxide content. This could possibly be an indicator, that one could release controlled amounts of water vapor into the Martian atmosphere to introduce oxygen to the atmosphere and possibly even keep it at a constant, non-negligible level. One could perform adequate calculations and determine how this would affect the Martian climate, especially the temperature. Given some experimental data one could also describe the rates at which different molecules dissociate more accurately and further perfect the results of this body of work.

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