Source of Atomic Hydrogen in the Atmosphere of HD 209458b

Mao-Chang Liang, Christopher D. Parkinson, Anthony Y.-T. Lee, Yuk L. Yung

Division of Geological and Planetary Sciences, California Institute of Technology, 1201 E. California Blvd., Pasadena, CA 91125

mcl@gps.caltech.edu, cdp@gps.caltech.edu, ytl@gps.caltech.edu, yly@gps.caltech.edu

and

Sara Seager

Department of Terrestrial Magnetism, Carnegie Institution of Washington, 5241 Broad Branch Rd. NW Washington, D.C. 20015

seager@dtm.ciw.edu

ABSTRACT

Atomic hydrogen loss at the top of HD 209458b’s atmosphere has been recently detected (Vidal-Madjar et al. 2003). We have developed a 1-dimensional model to study the chemistry in the upper atmosphere of this extrasolar “hot jupiter”. The 3 most abundant elements (other than He), as well as 4 parent molecules are included in this model, viz., H, C, O, H₂, CO, H₂O, and CH₄. The higher temperatures (∼ 1000 K) and higher stellar irradiance (∼ 6 × 10⁵ W m⁻²) strongly enhance and modify the chemical reaction rates in this atmosphere. Our two main results are that (a) the production of atomic hydrogen in the atmosphere is mainly driven by H₂O photolysis and reaction of OH with H₂, and is not sensitive to the exact abundances of CO, H₂O, and CH₄, and (b) H₂O and CH₄ can be produced via the photolysis of CO followed by the reactions with H₂.

Subject headings: planetary systems—radiative transfer—stars: atmosphere—stars: individual (HD 209458)
1. INTRODUCTION

Since the discovery of the first extrasolar planet, 51 Peg b, in 1995 (Mayor & Queloz 1995), a total of 102 planets have so far been discovered (e.g., Butler et al. 2003; Udry et al. 2002, and references therein) and analyzed statistically in order to characterize the formation environment (Fischer et al. 2002; Santos et al. 2003). The formation of gas giants is thought to be complete in 10 Myr, before the disappearance of the gaseous stellar accretion disk, at distances > 5 AU from the parent star. They are then pulled to their present positions by tidal interaction between the gas disk and planet (e.g., Pollack et al. 1996; Ward 1997).

An edge-on planet provides a unique opportunity to investigate the planetary atmosphere. HD 209458b is such a planet, providing the first extrasolar planetary detection using the light curve obtained during a planetary transit of its parent star (Charbonneau et al. 2000; Henry et al. 2000). The orbital parameters were accurately determined by Charbonneau et al. (2000), Henry et al. (2000), and Mazeh et al. (2000). Strong absorption lines are required to make an atmospheric detection and Seager & Sasselov (2000) theoretically characterized the most prominent absorption features, viz., Na I and K I doublet resonance and He I $^{3}S-^{3}P$ triplets. Charbonneau et al. (2002) detected the Na I doublet at 589.3 nm in HD 209458b with $\sim 4\sigma$ confidence level. Following this, Vidal-Madjar et al. (2003) made the first observation of the extended upper atmosphere of HD 209458b with a $\sim 4\sigma$ detection of the H I atomic hydrogen absorption of the stellar Lyman-α line. They reported an absorption of $\sim 15 \pm 4\%$ and claimed this should be taking place beyond the Roche limit, thus implying hydrodynamic escape of hydrogen atoms from HD 209458b’s atmosphere.

The temperature and UV flux of close-in planets are high. This motivates us to study the chemistry that may be important in this ”hot jupiter”. In this paper, we consider a simple hydrocarbon/oxygen chemistry model to determine a source of atomic hydrogen in the atmosphere of HD 209458b and represents the first effort to investigate the UV enhanced chemical processes in ”hot jupiters”.

2. MODEL

Our model is based on the four parent molecules H$_2$, CO, H$_2$O, and CH$_4$ and is a derivative of the Caltech/JPL KINETICS model for the Jovian atmosphere. HD 209458b is orbiting at a distance of 0.05 AU. As HD 209458 is a G0 solar-type dwarf star, it is justified to use the solar spectrum. We expect the atmosphere to have a temperature, $\sim 1000$ K, and UV flux (< 1800 Å), $\sim 2 \times 10^{15}$ photons cm$^{-2}$ s$^{-1}$. By comparison the UV flux at Jupiter is a factor of $\sim 10^4$ lower.
Hydrocarbons The hydrocarbon photochemical scheme used here is a simplified version of the Jovian atmospheric model described in Strobel (1973) and Gladstone et al. (1996). The photodissociation of CH$_4$ and the subsequent reactions of the species with hydrogen produce all the other hydrocarbons present in a Jovian-type atmosphere. For lower temperatures and weaker stellar irradiation, the main source of H is from H$_2$ and CH$_4$ photodissociation and the main sink via C$_2$H$_2$, which acts as a catalyst in recombining H. HD 209458b receives much greater stellar irradiation and is therefore much hotter than Jupiter. In this case, the formation of H is greatly enhanced by photolysis of H$_2$O and reactions between O and OH radicals and H$_2$. The sink for H is more complex (see § 3.3).

Oxygen O is similar in abundance to C and represents a cosmic abundance of these species. The atmospheric H$_2$O abundance will be controlled mainly by the comparative richness of these two species. The amount of H$_2$O and CO governs the amount of atomic oxygen present and the related reactions are of great interest. The oxygen related reactions are taken from Moses et al. (2000).

Model atmosphere Three models are investigated in this paper. Our standard reference model using solar abundances is shown in Fig. 1 (Model A). We also consider 2 other cases, Model B and Model C, in which H$_2$O and CO abundances are 10 times lower, respectively. We have taken the 1 bar level to be "0" km, and all heights are referenced from this level. The temperature-pressure profile and chemical abundances are based on Seager et al. (2000). The temperature decreases from the bottom to the top of the atmosphere. The abundances of CO and H$_2$O are, 3.6 × 10$^{-4}$ and 4.5 × 10$^{-4}$, respectively. These values are similar to solar abundances. The CH$_4$ abundance is determined by the thermodynamic equilibrium chemistry in the deep atmosphere. We adopt the value 3.9 × 10$^{-8}$, which is the lower end of the model by Seager & Sasselov (2000). The temperature-pressure profiles are not certain, because global circulation and high temperature condensation (Seager & Sasselov 2000; Sudarsky et al. 2000) are not included in generating the model atmosphere. Nevertheless, the present standard reference model is accurate enough for a first order understanding of the chemistry and characterizes a source of H in the upper atmosphere. The eddy diffusion is proportional to n$^{-\alpha}$ (n is number density) where $\alpha$ is taken to be $\sim$ 0.6 – 0.7.

3. RESULTS

The principle results for our three models will be described in three sections. Section 3.1 deals with OH and O radicals, followed by CO$_2$ and CH$_4$ in section 3.2. The important question of hydrogen production in relation to H$_2$O is addressed in section 3.3.
Fig. 1.— Vertical profile of temperature, total density, and constituent number density.
3.1. OH and O radicals

Fig. 2 shows the OH and O radicals in our models. OH and O are the most important radicals as they drive most of the chemical reactions. O is the most important element in facilitating the formation of OH radicals in the water-poor atmosphere. These species are produced photochemically, for example,

$$CO + h\nu \rightarrow C + O,$$

$$H_2O + h\nu \rightarrow H + OH.$$  

CO photolysis is an important source of O and H$_2$O is the main source of OH. Though O($^1D$) is not as abundant as O ($\lesssim 10^{-5}$ [O]), it can react with H$_2$ to produce a similar amount of OH. O is increasing with altitude as a consequence of H$_2$O and CO photolysis. OH is increasing with altitude until it starts decreasing at $\sim 10$ nbar. The decline of OH above 10 nbar is due to OH photodissociation. We see the mixing ratio of OH radicals is not sensitive to the abundance of CO and H$_2$O. With an order of magnitude change in H$_2$O (Model B) or CO (Model C), OH is changed only by a factor of $\lesssim 3$. However, O is sensitive to both CO and H$_2$O concentrations and preferentially forms OH. From Fig. 2 we see that OH is not sensitive to H$_2$O abundance. The abundance of H$_2$O depends on the comparative richness of cosmic C and O. Under high stellar UV irradiation, a fraction of CO will be photodissociated. The resulting O will react with H$_2$ to form OH, which eventually forms H$_2$O by reacting with H$_2$. Therefore, the abundance of OH radicals is determined by the amount of O in the system. It does not matter whether O is in the CO or H$_2$O reservoir.

3.2. CO$_2$ and CH$_4$

CO$_2$ is formed via the reaction of CO and OH,

$$OH + CO \rightarrow CO_2 + H$$

Fig. 3 shows the vertical profiles of CO$_2$ for our three models. The CO$_2$ mixing ratio is enhanced in the upper atmosphere. At pressures of $\sim 10$ nbar for Model A, the CO$_2$ mixing ratio is only about 2 orders of magnitude less than its progenitor, CO. The CO$_2$ abundance in the model is rather insensitive to the abundance of H$_2$O. An order of magnitude decrease in H$_2$O results in only a factor of $\sim 3$ decrease in CO$_2$ abundance (cf. Models A and B in Fig. 3). However, CO$_2$ abundance varies approximately linearly with the abundance of CO (cf. Models A and C in Fig. 3).
Fig. 2.— Comparison of mixing ratios of OH and O radicals in Models A, B, and C.
The formation of CH$_4$ is initiated by the downward flux of C atoms produced in the photolysis of CO in the upper atmosphere. This obtains the following sequence of reactions:

\[
\begin{align*}
\text{CO} + h\nu & \rightarrow \text{C} + \text{O}, \\
\text{C} + \text{H}_2 + \text{M} & \rightarrow ^3\text{CH}_2 + \text{M}, \\
2 ^3\text{CH}_2 & \rightarrow \text{C}_2\text{H}_2 + 2\text{H}, \\
\text{C}_2\text{H}_2 + \text{H} + \text{M} & \rightarrow \text{C}_2\text{H}_3 + \text{M}, \\
\text{C}_2\text{H}_3 + \text{H}_2 & \rightarrow \text{C}_2\text{H}_4 + \text{H}, \\
\text{C}_2\text{H}_4 + \text{H} + \text{M} & \rightarrow \text{C}_2\text{H}_5 + \text{M}, \\
\text{C}_2\text{H}_5 + \text{H} & \rightarrow 2\text{CH}_3, \\
\text{CH}_3 + \text{H} + \text{M} & \rightarrow \text{CH}_4 + \text{M}.
\end{align*}
\]

Fig. 3 shows the vertical profiles of CH$_4$ in our models. We see that the CH$_4$ mixing ratio is increasing by a factor of 5-100 from the bottom to the 0.1 mbar level (cf. Fig. 3). Above this level, CH$_4$ rapidly decreases due to photodissociation. Some of the C is eventually converted to CO$_2$, whose mixing ratio increases while that of CH$_4$ decreases.

The CH$_4$ mixing ratio is increased by a factor $\sim 2$ when we lower the H$_2$O abundance by an order of magnitude (cf. Models A and B in Fig. 3). We suggest this increase is due to less UV shielding by water above. The CH$_4$ mixing ratio is decreased by an order of magnitude when we lower the CO abundance by an order of magnitude. The reason is that CO photolysis is the source of the C in CH$_4$.

### 3.3. H and H$_2$O

Fig. 3 shows the mixing ratios for H and H$_2$O. The most striking features are the production of H (all three models) and the production of H$_2$O (Model B). In our 1-D model, the production rate of atomic hydrogen is not sensitive to the exact abundances of CO and H$_2$O. With an order of magnitude change in the abundance of either CO or H$_2$O, the atomic hydrogen changes by only a small factor, $\sim 1 - 2$. This implies the production of H in three models is limited by the availability of UV photons. The H production is also not sensitive to the abundance of CH$_4$. CH$_4$ abundance has been increased to be as high as CO, and the H mixing ratio is only changed by a small factor. A more comprehensive discussion will be given in a separate paper (Liang et al. 2003, in preparation). The mixing ratio of H exceeds 10% at the top of atmosphere. At the top of the atmosphere ($< 1$ nbar), H$_2$ will
be photolyzed and is a source of H. This atomic hydrogen will fuel the hydrodynamic loss process, as observed by Vidal-Madjar et al. (2003) and is discussed in more detailed in the companion paper by Parkinson et al. (2003, in preparation).

In a water-poor atmosphere (e.g., Model B), CO will be driving the photochemical reactions to form H$_2$O:

\[
\begin{align*}
\text{CO} + h\nu &\rightarrow \text{C} + \text{O}, \\
\text{O} + \text{H}_2 &\rightarrow \text{OH} + \text{H}, \\
\text{OH} + \text{H}_2 &\rightarrow \text{H}_2\text{O} + \text{H}.
\end{align*}
\]

H$_2$O and H are the net products. The produced H$_2$O will be recycled and is an important source of OH radicals and H atoms. Near the top of atmosphere, a large fraction of H$_2$O is destroyed due to the high UV bombardment. However, CO is more stable.

Fig. 4 shows the production rate of H and the photolysis rate of H$_2$O. The rates are not sensitive to the abundance of CO, but are sensitive to the abundance of H$_2$O. By comparing the H$_2$O photolysis rate with H production rate, it is evident that production of H is mainly driven by H$_2$O photolysis and the reaction of OH with H$_2$. Below $\sim 1$ mbar, HCO plays a role in the removal of H via

\[
\begin{align*}
\text{CO} + \text{H} + \text{M} &\rightarrow \text{HCO} + \text{M}, \\
\text{HCO} + \text{H} &\rightarrow \text{CO} + \text{H}_2.
\end{align*}
\]

In the upper atmosphere, H atom recombination and reactions with CH and $^3$CH$_2$ will drive the loss of H via

\[
\begin{align*}
2\text{H} + \text{M} &\rightarrow \text{H}_2 + \text{M}, \\
\text{H} + \text{CH} &\rightarrow \text{C} + \text{H}_2, \\
\text{H} + ^3\text{CH}_2 &\rightarrow \text{CH} + \text{H}_2, \\
\text{C} + \text{H}_2 + \text{M} &\rightarrow ^3\text{CH}_2 + \text{M}.
\end{align*}
\]

4. CONCLUSION

We have considered a series of possible chemical reactions using various models for a "hot jupiter". We have shown the mechanism for producing the atomic hydrogen. The production of H is not sensitive to the abundances of CO, H$_2$O, and CH$_4$. Lowering H$_2$O or CO an order of magnitude changes the concentration of H by only a factor of $\lesssim 2$. 
Fig. 3.— Comparison of mixing ratios of H, CH₄, H₂O, CO, and CO₂ in Models A, B, and C.
Fig. 4.— Production rate of H (dark lines) and photolysis rate of H$_2$O (gray lines) in Models A, B, and C.
However, the production rate of H is sensitive to the temperature profile. A 30% change in the temperature will result in $\sim 50\%$ change in the H concentration.

Our calculations show that the H mixing ratio at $\sim 1$ mbar is $\sim 10^{-3}$ and exceeds 10% in the top of the atmosphere. Being less gravitationally bound, the atomic hydrogen formed at the top of atmosphere can escape hydrodynamically as putatively suggested by observations of Vidal-Madjar et al. (2003). Since these close-in gas-rich giant planets are probably tidally locked, circulation may be important in transporting heat because the temperature gradient can be as high as 1000 K over the entire planet, which in turn implies wind speeds of a few km s$^{-1}$ (Showman & Guillot 2002; Cho et al. 2003). Therefore, it is of interest to simulate the differences in chemical processes between the day and night sides and the global transport of heat and mass as well.

We thank Dr. R. L. Shia and Dr. M. Gerstell for helpful comments and discussions. The support of NASA Grant NAG5-6263 to the California Institute of Technology is gratefully acknowledged. This work represents one phase of research carried out at the Jet Propulsion Laboratory, California Institute of Technology, under contract to the National Aeronautics and Space Administrations.

REFERENCES

Butler, R. P., Marcy, G. W., Vogt, S. S., Fischer, D. A., Henry, G. W., Laughlin, G., Wright, J. T. 2003, ApJ, 582, 455

Charbonneau, D., Brown, T. M., Latham, D. W., Mayor, M. 2000, ApJ, 529, L45

Charbonneau, D., Brown, T. M., Noyes, R. W., Gilliland, R. L. 2002, ApJ, 568, 377

Cho, J. Y.-K., Menou, K., Hansen, B. M. S.; Seager, S. 2003, ApJ, 587, L117

Fischer, D. A., Marcy, G. W., Butler, R. P., Laughlin, G., Vogt, S. S. 2002, ApJ, 564, 1028

Gladstone, G. R., Allen, M., Yung, Y. L. 1996, Icarus, 119, 1

Henry, G. W., Marcy, G. W., Butler, R. P., Vogt, S. S. 2000, ApJ, 529, L41

Mayor, M., & Queloz, D. 1995, Nature, 378, 355

Mazeh et al. 2000, ApJ, 532, L55
Moses, J. I., Lellouch, E., Bézard, B., Gladstone, G. R., Feuchtgruber, H., Allen, M. 2000, Icarus, 145, 166
Pollack, J. B., Hubickyj, O., Bodenheimer, P., Lissauer, J. J., Podolak, M., Greenzweig, Y. 1996, Icarus, 124, 62
Santos, N. C., Israeliian, G., Mayor, M., Rebolo, R., Udry, S. 2003, A&A, 398, 363
Seager, S., & Sasselov, D. D. 2000, ApJ, 537, 916
Seager, S., Whitney, B. A., Sasselov, D. D. 2000, ApJ, 540, 504
Showman, A. P., Guillot, T. 2002, A&A, 385, 166
Strobel, D. 1973, Journal of the Atmospheric Sciences, 30, 489
Sudarsky, D., Burrows, A., & Pinto, P. 2000, ApJ, 538, 885
Udry, S., Mayor, M., Naef, D., Pepe, F., Queloz, D., Santos, N. C., Burnet, M. 2002, A&A, 390, 267
Vidal-Madjar, A., des Etangs, A. Lecavelier, Desert, J.-M., Ballester, G. E., Ferlet, R., Hebrard, G., Mayor, M. 2003, Nature, 422, 143
Ward, W. R. 1997, Icarus, 126, 261

This preprint was prepared with the AAS LATEX macros v5.0.