Volcanic chemical gas speciation and atmospheric redistribution on terrestrial planets

Caroline Brachmann[1,2], Lena Noack[2], Frank Sohl[1]

[1]DLR, Institute of Planetary Research, Berlin, Germany,
[2]Freie Universität Berlin, Institute of Geological Sciences, Berlin, Germany

This work has been funded by the Deutsche Forschungsgemeinschaft (SFB-TRR 170, subproject C6)

Introduction

The internal constitution of rocky exoplanets can be inferred only indirectly via their atmospheric composition. To address this issue with confidence requires the coupling of interior and atmospheric models to each other. In the past, various atmospheric redistribution models were developed to determine the composition of exoplanetary atmospheres by varying element abundance, temperature and pressure. One example for such a model was published by Woitke et al., 2021, they used a simple stochiometric approach to calculate chemical equilibrium in the C-H-O-N system and proposed a classification of exoplanet atmospheres based on their 4 most abundant gases: type A atmospheres contain H_2O, CH_4, NH_3 and H_2 (A1) or N_2 (A2). Type B Atmospheres contain O_2, H_2O, CO_2 and N_2 and type C atmospheres contain H_2O, CO_2, CH_4 and N_2, these types are visualized in Fig. 1. However, this model as well as similar work neglect that present-day atmospheres were formed via volcanic degassing and, consequently, element abundances are limited by thermodynamic processes accompanying magma ascent and volatile release. Here we combine a volcanic outgassing with the model used by Woitke et al., 2021 to simulate the evolution of C-H-O-N atmospheres in thermal equilibrium below 650 K. For the present study, we built a basic model to calculate possible atmospheric compositions by varying oxygen fugacity, melt and surface temperature and volatile abundances. Furthermore, we consider the solubility of each phase, atmospheric processes such as water condensation, graphite precipitation, hydrogen escape and the effect an already existing atmosphere may have on further degassing.

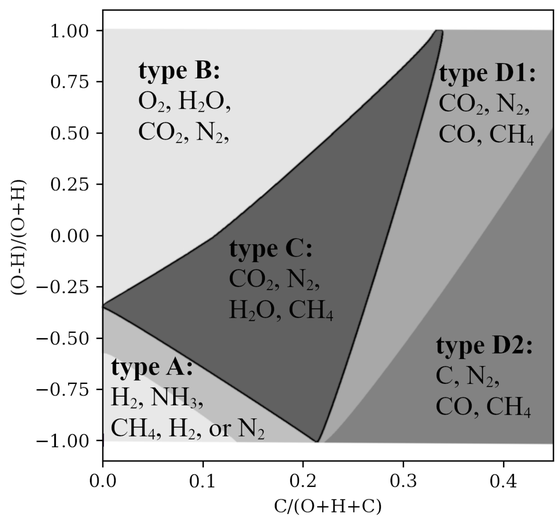


Figure 1: *Fig. 1.*

Methods

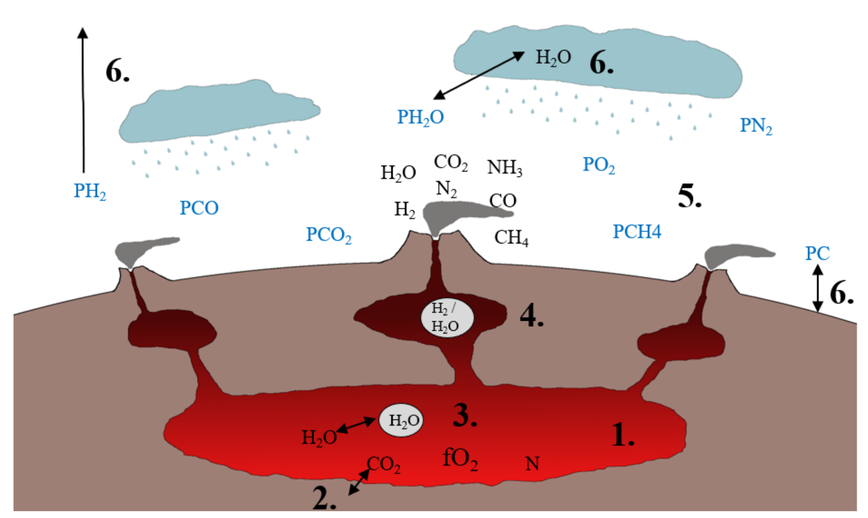
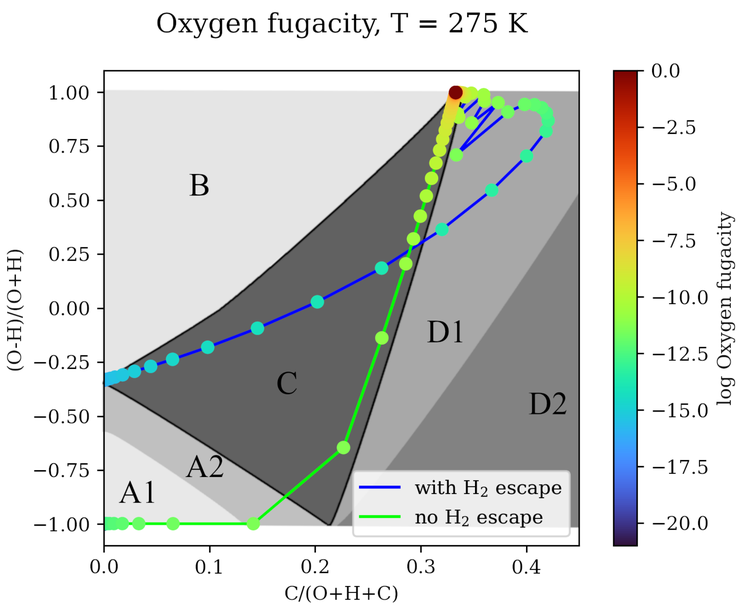
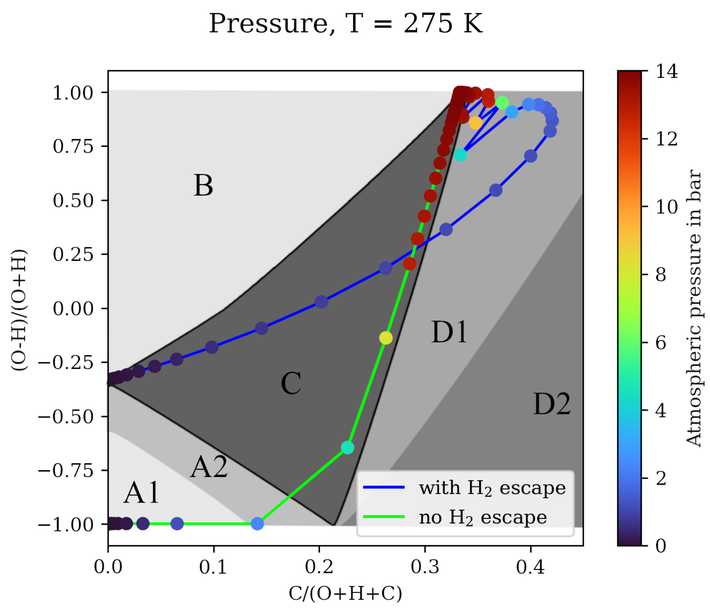


Figure 2 shows a simple sketch of the steps that are executed in the routine: First a basaltic melt is produced with set initial volatile content, oxygen fugacity, temperature and pressure (1). The CO_2 content of the melt is limited by the oxygen fugacity since Carbonate does not partition into the melt at low fO_2, hence the initial CO_2 is updated (2). To estimate how much of each volatile species will outgas the solubilty (3) as well as the speciation (4) of the gases is calculated based on our speciation code. The gases degas into the atmosphere and atmospheric pressure and weight are computed. Based on the stochiometric approach published by Woitke et al., 2021 the gases are redistributed reaching chemical equilibrium at set atmospheric temperature and calculated pressure (5). Lastly, H_2O condenses, C precipitates and H_2 escapes (6). The updated partial pressure of each species influences its solubility in the next degassing step. To simulate atmospheric build up over a long period of time, the routine is repeated 100 times equaling a melt production the weight of 4 times of Earth' crust

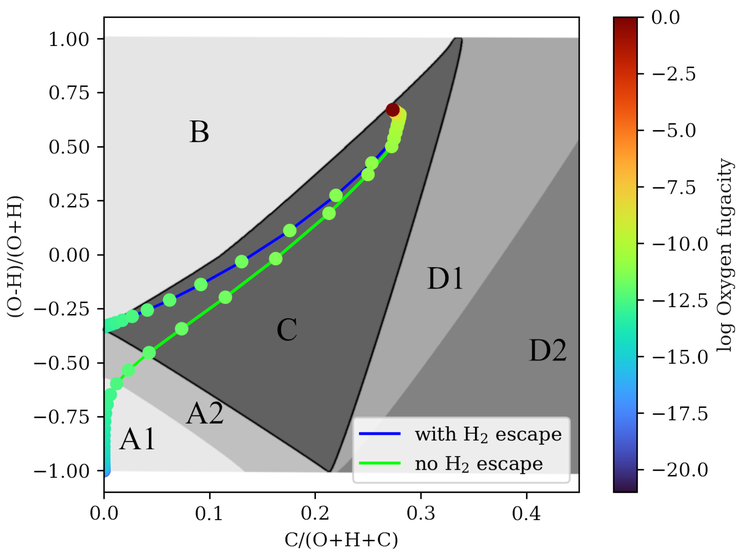
Results and Discussion



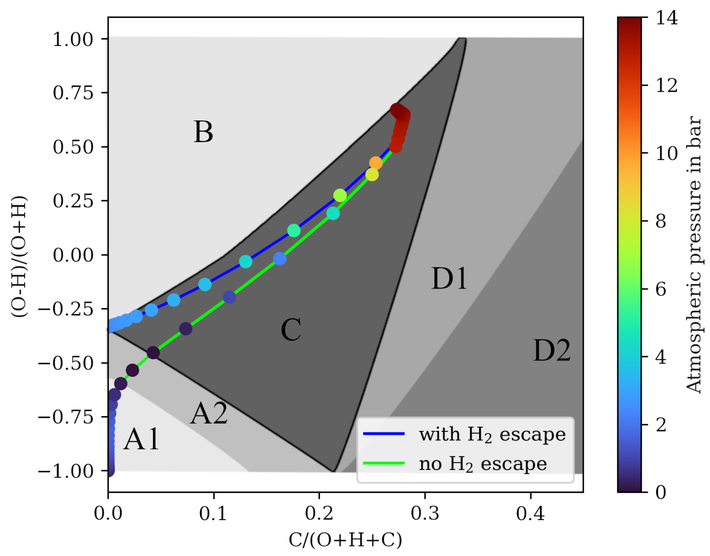
3a.



3b.



4a.



4b.

Figure 3 and 4 show the composition the atmosphere reaches after running the code for 100 steps at 275 K (3) surface temperature and 600 K (4) respectively for different initial oxygen fugacities. The color coded dots in 3a and 4a show the mantle fugacity varying from IW -8 to IW +12. The dots in 2b and 3b show the resulting atmospheric pressures of the same runs seen in 3b and 4b. The dots connected by the blue line show the composition if all H_2 escapes the atmosphere, the dots connected by the light green line represent the atmospheric composition if no H_2 is lost. Melts with low oxygen fugacities produce H_2-NH_3 dominated atmospheres with very low atmospheric pressures and only minor amounts of Carbon species, because carbonate is not dissolved in the melt at these conditions. With increasing oxygen fugacities the atmospheric pressure increases and more Carbon species (commonly CO_2 and CH_4) appear in the atmosphere as well as H_2O and N_2. Super oxidized magmas produce CO_2, N_2 and depending on surface temperature also H_2O dominated atmospheres with high atmospheric pressures. Varying the initial volatile abundance generally just leads o a shift along the lines but not to a significantly different atmospheric composition. The most common atmospheric type are type C atmospheres. Reduced mantles can lead to a formation of A1 or A2 atmospheres. O_2 dominated Type B atmospheres are never produced via degassing since O_2 does not degas by itself but always as CO_2, CO or H_2O, hence there is always enough hydrogen or carbon in the atmospheres to form other molecules. Intriguingly we see another atmospheric type not described by Woitke et al., 2021 which is referred to as D1. These atmospheres form at intermediate oxygen fugacities around the Iron Wustite buffer at low surface temperatures and hence condensation of all water steam and H_2 escape, leading to such high amounts of excess Carbon in the atmosphere that CO appears along CO_2, CH_4 and N_2. However, in this case we are reaching the limitations of the atmospheric redistribution model and more work is needed to confirm this. Woitke et al., 2021 mentioned in their work a theoretical Carbon dominated atmosphere in which graphite clouds occur (referred to as D2), but graphite was never formed in our calculations, because such a composition would need high amounts of Carbon and low amounts of Oxygen which are two prerequisites contradicting each other.

Summary and Conclusions

We have developed a model which allows us to calculate the influence of volcanic degassing on the evolution of atmospheres on terrestrial planets in the C-H-O-N system below 650 K.

- mantle and therefor melt redox state have a significant influence on the composition of planetary atmospheres
- the most common atmospheres that are to be expected on exoplanets are type C atmospheres dominated by CO_2, H_2O, CH_4 and N_2
- type A1, A2 and D1 atmospheres can form under the right conditions
- type B and type D2 atmospheres are never formed in our calculations, since O_2 and graphite never occur

Outlook:

- compare our results to other equilibrium chemistry codes eg. Stock et al., 2022 and include sulfur gases as well as higher temperatures

References

Stock, J. W., Kitzmann, D., & Patzer, A. B. C. (2022). Fastchem 2: An improved computer program to determine the gas-phase chemical equilibrium composition for arbitrary element distributions. *Monthly Notices of the Royal Astronomical Society*, *517*(3), 4070–4080. https://doi.org/10.1093/mnras/stac2623

Woitke, P., Herbort, O., Helling, C., Stüeken, E., Dominik, M., Barth, P., & Samra, D. (2021). Coexistence of ch 4 , co 2 , and h 2 o in exoplanet atmospheres. *Astronomy & Astrophysics*, *646*, A43. https://doi.org/10.1051/0004-6361/202038870