

Volatile outgassing and chemical speciation of the C-O-H system in the Earth's Magma Ocean

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Abstract

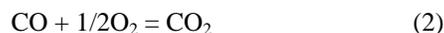
The aim of the research is to improve the present knowledge about the early phase of the Earth's evolution, subsequent to the formation of the Moon. In this period the Earth was probably characterized by the presence of a magma ocean or several magma ponds and the silicate melt was the main source of volatiles for the early atmosphere. Specifically, the volcanic degassing and the volatile chemical speciation were investigated through the use of numerical modelling of the outgassed species. We analysed the volatile transition from the mantle to the atmosphere of the C-O-H system by the usage of the equilibrium constants and mass balance method. Considering the oxygen fugacity (fO_2) as one of the main factors that affects the chemical speciation, we observed changes in the ratio of reduced (H_2 and CO) or oxidized (H_2O and CO_2) species with different fO_2 values. The results show an interesting aspect of the interaction between the solid/melt phase and the gas phase since the volatile final composition is directly related to the melt oxygen fugacity.

Introduction

During the early phase of its evolution the Earth was likely characterized by a magma ocean stage [1]. The planet was completely or partly molten and there was a strong interaction between the silicate melt phase and the atmosphere. The aim of the research is to better characterize the volcanic degassing of the magma ocean and the related development of the early Earth's atmosphere. The volatile speciation and transition from the mantle to the atmosphere was analysed throughout numerical model simulations. In particular, the gas chemical speciation of the C-O-H system and its relationship with the redox state of the magma ocean are investigated.

Methods

The magma ocean outgassing and the volatile chemical speciation of the C-O-H system are investigated with the "Equilibrium and mass balance method" [2, 3]. The following reactions are simulated at different thermodynamic conditions and redox ambient.



The equilibria (1, 2) are representative of the major volcanic volatile species of the C-O-H system. The composition of the gas phases are analysed with a fixed pressure of 1 bar and for a wide range of temperatures which are representative for the magma ocean context. The gas chemical speciation is influenced not only by the thermodynamic properties but, one of the most important aspects is the redox state of the melt during the outgassing process. The redox ambient of the magma ocean is represented by the level of oxygen fugacity of the melt silicate phase. In order to investigate the oxidation state of the melt, and therefore of the magma ocean, the oxygen fugacity is calculated using the well-known parametrizations for the most used petrological mineral buffers [4] and several meteoritic compositions [3]. To simulate the oxidizing ambient were selected the nickel-nickel oxide ($NiNiO$) and the quartz fayalite magnetite (QFM) buffers. In addition, to reproduce reducing conditions we selected the quartz-iron-fayalite (QIF) and iron wüstite (IW) buffers. Moreover, the calculated oxygen fugacity of undifferentiated chondritic meteorites (CI, CV, H and EH) and of differentiated eucritic composition were considered in combination with the mineral buffers. This method connects the redox state of the melt to the outgassed volatile

species, since the calculated oxygen fugacity is employed in the numerical modelling of the gas phase equilibria.

Results

In the figure 1 we show the calculated oxygen fugacity using the parametrization from [3, 4].

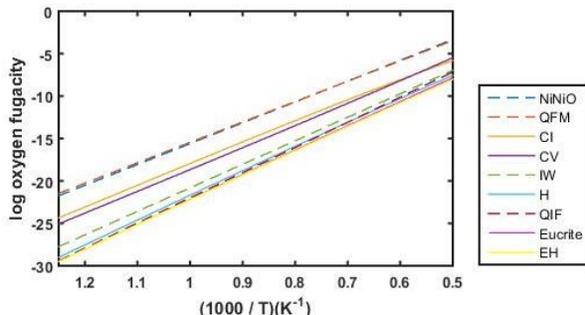


Figure 1. Calculation of oxygen fugacity of some of the most used petrological mineral buffers and meteoritic compositions.

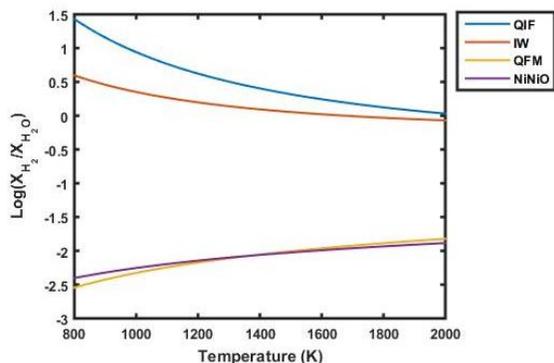


Figure 2. The diagram shows the ratio of H_2/H_2O for different oxygen fugacity over temperature ($P=1$ bar).

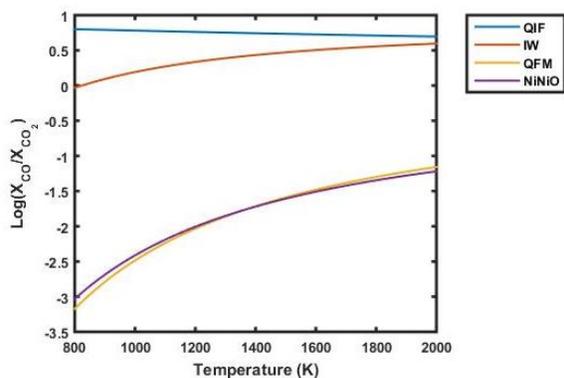


Figure 3. CO/CO_2 ratio related to different redox conditions as function of temperature ($P=1$ bar).

In the graphs we show the strong variations of oxygen fugacity for reducing or oxidizing ambient. The strong variation of oxygen fugacity deeply influences the gas chemical speciation. In figures 2 and 3 are plotted the ratio of H_2/H_2O and CO/CO_2 related to the redox conditions over an interval of temperatures and with a pressure of 1 bar. In the plots there is a strong change in the volatile composition connected to the redox state and to the temperature. For low temperatures and low oxygen fugacity (QIF and IW buffers) the main chemical species are CO and H_2 . On the other hand in an oxidizing ambient (NiNiO and QFM buffers) the volatile composition is substantially H_2O and CO_2 .

Discussion and conclusions

The main objective of our research was to shed light on the volatile outgassing during the Earth magma ocean stage and to the related composition of the early atmosphere. For this purpose, we simulated the volcanic outgassing and the speciation of the gas phases as a function of: pressure, temperature and redox state. As first step we calculated the oxygen fugacity for the most used petrological mineral buffers and for some meteoritic compositions. Subsequently, we estimated the outgassed volatile composition at different redox conditions. We observed that the redox state of the melt affects the gas phase composition. The main gas species under reducing conditions (QIF and IW mineral buffers) are H_2 and CO but for oxidizing conditions (NiNiO and QFM) H_2O and CO_2 are the dominant volatiles. In conclusion, this method permits to directly link the silicate melt to the outgassed species. The results show that the oxygen fugacity has a strong control on the volatile speciation and therefore, on the composition and evolution of the early Earth atmosphere.

Acknowledgements

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References

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