

The behavior of volatile species in the Early Earth's global magma ocean

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The amount of volatile elements stored in hidden reservoirs, particularly the lower mantle and iron-rich core, is currently uncertain, and estimates of the flux of volatiles between the surface and mantle are model-dependent. To improve our understanding of Earth's global volatile cycle, it is critical to characterize the forms in which volatile elements existed in the molten Early Earth. Thus, using atomic simulations (i.e., first-principles molecular dynamics), we have characterized the vaporization behavior of volatile elements, particularly carbon and hydrogen, in silicate melts representing the composition of the Bulk Silicate Earth as a function of pressure, temperature and oxidation state. We describe the speciation of all volatile species and quantify the amount of carbon and hydrogen in the vapor phase compared to the silicate melt to provide insight into their fate after the Moon-forming impact. We find that the concentration of carbon and the oxidation state of the melts dictate the speciation of the vaporized carbon species, but do not affect the overall volatility of carbon. The concentration of CO₂, a greenhouse gas, increases at the expense of CO as the density of the system decreases, which would have presumably contributed to the formation of a hot dense atmosphere during the cooling of Early Earth. At the very high temperatures of 5000-6000 K, we predict that bubbles in the magma ocean contained a significant fraction of silicate vapor in addition to CO and CO₂, affecting the transport and rheological properties of the magma ocean. Furthermore, we examine the formation and dissociation mechanisms of methane, both as a vapor species and dissolved in the highly-reduced silicate melt, tracing the fate of carbon and hydrogen upon decomposition, and describing the kinetic barriers to the formation of methane in the Early Earth.

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Mots-Clés : carbon; hydrogen; vaporization; Early Earth; magma ocean; giant impact