Partitioning of H, C, N and S on a growing Earth estimated by empirical thermodynamic modelling

MURASE YUTARO[1], Hiroaki Saito[1], *Kiyoshi Kuramoto[1]

1. Department of Cosmosciences, Graduate School of Sciences, Hokkaido University

Partitioning of volatile elements on an accreting planet among vapor, silicate melt and molten iron is a key process that controls initial inventories of these elements among the planetary surface and interior. So far, most studies have evaluated it separately for each element by applying gas solubility data and/or element distribution coefficients among liquid phases. Actually, however, volatile elements do form various chemical compounds, which affects fugacities of chemical species that control their amounts in liquid phases. Here we have developed an empirical thermodynamic model solving equilibrium chemical speciation of major volatiles H, C, N and S and their partitioning among vapor, silicate melt and molten iron applying a Gibbs free energy minimization method. Chemical potentials of volatile solutes in liquid phases are modeled from experimental data of gas solubilities into silicate melt and molten iron. Given the bulk elemental composition of Earth's building block by the two component model (Wanke and Dreibus, 1988) and conditions with high temperature (1500 K- 3000 K) and pressure (up to 1000 bar) on a terrestrial magma ocean, our model predicts 1) H_2-rich vapor containing H_2O, CO, CH_4 and SH as secondary species and 2) preferential partitioning of C, N and S into molten metal and significant H_2O partitioning into silicate melt at elevated pressures. These results imply selective removal of C and N from a thick proto atmosphere to the core, which is consistent with the observed strong depletion of C and N from the present Earth's surface and depleted mantle compared to the chondritic proportion of volatile elements. N_2 is the dominant nitrogen species in vapor whereas NH_3/N_2 ratio reaches to order of 10^{-3} to 10^{-1}, which may be large enough to produce significant greenhouse effect and have impacts on prebiotic synthesis of amino acid after the cooling of proto-atmosphere.

Keywords: volatile elements, accretion, partitioning, magma ocean, proto atmosphere