Molecular simulation of density fluctuation of H_2O and H_2O-NaCl solutions under supercritical conditions

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Supercritical fluids, which the density of the liquid phase and the vapor phase are equal, have characteristic properties on chemical reactivity, solubility, and ionic product. The fluids are under the condition higher temperature and higher pressure than the critical point. Geofluids, which is mainly composed in H_2O-NaCl are sometimes identified as supercritical state in deep areas such as earth’s crust, deep-sea hydrothermal vents and deep-drilling for geothermal well. The physicochemical properties of supercritical geofluids are important to understand these areas.
Molecules of supercritical fluid are heterogeneously distributed, and forming density fluctuation. The characteristic properties of supercritical fluids are said to be mainly due to the density fluctuation. Direct observation on the density fluctuation is obtained by small-angle X-ray scattering (SAXS) (Nishikawa *et al*., 1996) and visible light spectroscopy (Tsuchiya and Hirano, 2007; Sekiguchi *et al*., 2013). On the other hand, molecular dynamics simulations of supercritical fluids have been performed focused on the molecular cluster size (Istok *et al*., 2008). Here, we performed molecular dynamics simulations of H_2O system and H_2O-NaCl system at high temperature conditions around the critical point.
H_2O molecules and H_2O-NaCl molecules were prepared in a cubic box. In order to evaluate the density fluctuation, “bin analysis method” was used. This method divides the cubic box into small cubes with equal volumes, and the number of molecules in each boxes was counted at each time steps. The distribution of the number of molecules in each small boxes has a normal distribution and some amount of standard deviation. Large standard deviation means that the density fluctuation is large. As the result of the simulations, the density fluctuation of H_2O and H_2O-NaCl was maxima around the critical point.
In our poster, we will show the behavior of NaCl concentration dependence, and discuss about the effect of Na^+ and Cl^- ion.

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