Noble gases in geothermal waters as tracers for deep fluid circulation

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Introduction

Dissolved noble gases make excellent environmental tracers to study physical processes in groundwater and other aquatic environments. Especially helium isotopes have been widely used to trace residence time and deep circulation in groundwater systems.

Elevated ^{3}He/^{4}He isotope ratios were found in areas with increased geothermal resource potential in the Basin and Range Province, western United States [1]. The authors suggest that high ^{3}He/^{4}He anomalies, i.e., areas with admixture of mantle-derived helium in groundwater, indicate enhanced crustal permeability coupled with local zones of deep fluid production and/or hidden magmatic activity.

As part of a geothermal exploration project, samples were collected from five warm and hot springs in southern and central Yukon, Canada. All samples were analyzed for noble gas abundances of He, Ne, Ar, Kr, Xe and the isotope ratios ^{3}He/^{4}He, ^{20}Ne/^{22}Ne, and ^{36}Ar/^{40}Ar, as well as stable isotopes (^{2}H, ^{18}O), tritium (^{3}H), and routine inorganic chemistry.

Results and Conclusions

All samples contained a significant component of mantle-derived helium which is characterized by a higher ^{3}He/^{4}He isotope ratio compared to crustal helium. The presence of a mantle-derived helium component typically suggests the existence of a deep fluid pathway, usually a steeply inclined fault or fault zone. This is in agreement with the conceptual models for the warm and hot springs which include a deep circulation system for meteoric water to reach a sub-surface heat source and a suitable, fast conduit back to surface.

However, it remains unknown whether the noble gas signatures from the warm and hot springs represent local anomalies being characteristic for areas with geothermal resource potential. If this is the case, noble gas data, especially helium isotope ratios, could be used as an exploration tool for geothermal resource assessments once background values have been established. More noble gas data from both thermal waters and cold groundwater in the wider areas of known warm and hot springs would be required to answer this question.

[1] Kennedy and van Soest (2007) *Science*. **318**, 1433-1436.

Molecular Dynamics study of Aqueous Solution: solubility calculation with kinetic and thermodynamic approaches

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Aqueous solutions are fundamental to chemistry, biology, geology and technology. Predicting the shape of growing crystals is of essential importance for industrious crystallization process. In geology, crystalization is also one of the most siginifcant phenomenon to be better understood.

The rock-salt crystal structure is the stable solid phase in contact with a saturated solution of NaCl at atomspheric pressure and at room or higher temperature, while the dihydrate is stable solid phase in contact with a saturated solution of NaCl below 0.1°C. The question is that how this different stable solid phase in contact will be reflected from the hydration structure of the solutions(namely, how the hydration structure varies with temperature), how the different hydration structure will influence the salt-solution interfacial structure and eventually affect the crystal growth. Solubility is one of the significant and measurable properties, which is directly related to these three particular aspects: 1)crystal growth; 2) salt-solution interfacial structure and 3) the ionic hydration structure.

Here, we have investigated the salt-solution interface system and the salt solution single-phase system at different temperatures by using molecular dynamics. The solubilities were calculated by using the direct calculation and the free energy calculation, which are kinetic approach and thermodynamic approach, respectively. The direct calculation employs a salt-solution combined system. When the system is equilibrated, the concentration in the solution area is the solubility. In the free energy calculation, we calculate separately the chemical potential of two systems: solid and solution. And the two chemical potential values are compared. When the chemical potential of the solution phase is equal to the chemical potential of the solid phase, the concentration of the solution system is the solubility.

Very interestingly, it was found that the crystal shapes obtained from the direct calculations are significantly different between high and low temperatures: while the clusters were observed at the crystal surface at low temperatures, the layered rock salt structure is formed at high temperatures. We found that the clustering behavior is tightly conncted with the adsorbed water.

The calculated solubilties from two different approaches have a general good agreement, where the values at low temperatures exhibit slightly lager deviation than those at high temperatures. We remarked that the solubility value from the direct calculation might be affected by the kinetic reasons: the newly formed crystal structure and the adsorbed water molecules.