

Molecular Dynamics Study of Adsorption States of Cesium Ion in Cement Matrix

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Cs⁺ ion is one of radioactive species generated by nuclear electric power. It is one of the most problematic ions because of its long half-life and high mobility. Cement material is considered as a candidate for the solid fixation of Cs⁺ ions, and the engineered barrier for the geological disposal of such radioactive species. The structures of the cement is complicated, and considered as nano-crystalline aggregation phase with two distinct principal local structures, tobermorite and jennite, by the difference of silica-chain length. The goal of this research is to detect which structural or compositional feature is essential to ionic adsorption into cement matrix. By using molecular dynamics simulations, we have studied the aqueous solution-mineral (cement) interfacial systems for two different cement local structures (tobermorite and jennite) and two different solutions (NaCl and CsCl). It was found that Na⁺ ion could form both inner-sphere complex and outer-sphere complex, without full hydration shell and with full hydration shell at the time of adsorption, respectively. In contrast, Cs⁺ ion could only form inner-sphere complex for both mineral cases. Furthermore, it was found that tobermorite presents better binding property than that of jennite. The fact that differences in cement structure and ion species may cause these differences in adsorption state and binding property will enhance our understanding on cement materials in the case of the solid fixation and the geological disposal.

Keywords: Geological Disposal, Cs Fixation, Ionic Adsorption, Molecular Dynamics

Chemical weathering index suitable for Japanese granitic rocks

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The chemical weathering of rocks proceeds mainly by water-rock interactions (Nesbitt, 1979; White and Brantley, 1995). During such weathering, several alkaline and alkali-earth elements are easily leached from rocks, whereas residual elements are redistributed into secondary minerals (Reiche, 1943; Vogel, 1975; Nesbitt et al, 1980; Nesbitt and Young, 1982; Harnois, 1988). This geochemical process has been used as the foundation for indices assessing the extent of chemical weathering of rocks, based on the whole rock chemistry. Many chemical weathering indices have been suggested in the latter part of the 20th century, with 30 or more proposed in the literature (Duzgoren-Aydin et al., 2002).

Granitic rocks are important subjects for the study of rock weathering because they are a major component of the continental surface. Numerous indices have been proposed to estimate their degree of chemical weathering (Ruxton, 1968; Vogel, 1975; Harnois, 1988). They are wide concerns in such fields of geology, environmental science, and civil engineering (Hencher and McNicholl, 1995; Irfan 1996; Nesbitt and Markovics, 1997; Panahi et al., 2000). However, many previous studies are aimed at a narrow space such as a vertical section of outcrop or a drilling core (Nesbitt and Markovics, 1997; Guan, et al., 2001; Kirschbaum, et al., 2005). A problem can arise when such indices are applied to granitic rocks sampled over wider areas at batholithic scale, because such rocks may exhibit considerable chemical variation arising from their individual petrogeneses. The underlying magmatic variation obscures patterns in chemical evolution that result from subsequent weathering (Kamei et al., 2012).

The chemical composition of weathered granitoids produced by chemical evolution during rock weathering overlaps with their original magmatic chemical variation. A useful weathering index should be applicable to a wide range of rocks, and should yield different values for each fresh parent rock and the weathered material (Fedo et al., 1995; Price and Velbel, 2003). Kamei et al. (2012) proposed a practical method for evaluation of the degree of weathering of varied granitoids over wide areas. This improved method eliminates the chemical overlap of petrogenetic effect from the chemical weathering, and can raise many classical weathering indices to practical methods.

In this study, various weathering indices are used to determine the best chemical weathering index for Japanese granitic rocks based on the improved method of Kamei et al. (2012). The result suggests that the indices constructed by mobile CaO and Na₂O with immobile Al₂O₃ fulfill highly function. These elements are essential for plagioclase in the granitic rocks. Many researchers are discussing that the important indicative mineral for Japanese granitoid weathering is plagioclase and biotite (Miura, 1973; Kitagawa, 1999; Fukushi et al., 2000; Utada, 2003; Yokoyama and Matsukura, 2006; Kamei et al., 2012). Generally, modal composition of plagioclase in Japanese granitoids is higher than that of biotite. Therefore, it is not inconsistent with that the weathering indices based on CaO, Na₂O, and Al₂O₃ have highly effect for the Japanese granitic rocks. The best chemical weathering index for Japanese granitic rocks would be an index that constructed by CaO, Na₂O, and Al₂O₃.

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Keywords: granitic rocks, chemical weathering, weathering index

Formation and the feature of Flow-path fractures in a sedimentary rock - A Case study at Horonobe URL -

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In the view point of safety assessing the geological disposal system for high-level radioactive waste, it is essential to understand mass transportation in a hostrock. Therefore characteristics of mass-transport structures such as flow-path fractures must be understand. In this study, we report formation and the feature of flow-path fractures based on geological observation and fracture mapping in a sedimentary rock at the Horonobe Underground Research Laboratory (URL). The flow-path fractures occupy 22.4% of total fractures at the depth from GL-250.5m to GL-350.5m of the Ventilation shaft of the Horonobe URL. In addition, results of thin section observation, element mapping, and isotope analysis of carbonate fillings are shown. These results suggest that the formation process of flow-path fractures includes at least 2 stages; the E-W strike fracture forming stage caused by subsidence and East-West compressive stress and the tension fracture forming stage caused by fracture removal beneath regional uplifting and distressing.

This study presents the formation process of flow-path fractures as mass-transport structures in a sedimentary rock. In the future study, we will evaluate changes of flow-path structures from the view point of geological long-term stability.

Keywords: Flow-path, fracture, sedimentary rock, Horonobe

Multiscale Fracture Analysis and Regional Groundwater Flow Estimation of a Granitic Body: a Case Study of Tono Area

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Clarifying the hydraulic properties of geologic media is an important problem that is common to various fields in the geosciences. Especially, in the field of geological disposal of radioactive waste which utilizes the storage characteristics of the geologic structure, the estimation of groundwater flow system of the target area is essential for the safety evaluation. Groundwater flow in the hard rock-mass area is strongly affected by fractures and/or weathering and alternation zone. It is important to estimate the spatial distribution of fractures, weathering and alternation zone in regional scale, after clarifying the relationship between them and permeability of rocks.

Tono area (Gifu prefecture), situated in Central Japan, was selected for a case study of such hydraulic characterization. The study area is overlain the late Cretaceous Toki granite that is the basement rock. We applied GEOFRAC (Koike *et al.*, 2012) which is a geostatistical method that simulates regional fracture distribution by incorporating the directions (strikes and dips) of the sampled fracture data. In addition, a permeability test and property analyses of microcracks using rock-core samples were carried out. From these results, the variation of permeability depending on degrees of weathering and alternation of rock-core samples was clarified. The other important feature was that permeability increased toward the fracture plane and along the dominant directions of the cracks. These directions corresponded with the predominant directions obtained using the 3D simulated fractures with GEOFRAC. The existence of the similar trend of fracture directions at different scales; mm to km scale, which is caused by regional stress field, faulting and so on, was also detected.

The permeability dataset obtained from the hydraulic tests of borehole investigation was observed to correlate positively with the size of the simulated fractures. By integrating the hydraulic conductivity calculated based on that positive correlation with the results of GEOFRAC, a 3D permeability model covering the study area of 12 km (E-W) by 8 km (N-S) with a depth range of 1.5 km was constructed using sequential Gaussian simulation. Finally, MODFLOW, one of the computing modular using 3D finite-difference flow model, was applied to this model to estimate the regional groundwater flow system. The result clarified the anisotropic behavior of flows near faults, which was in agreement with the configuration in the continuous simulated fractures.

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References

Koike, K., Liu, C., Sanga, T. (2012): Incorporation of fracture directions into 3D geostatistical methods for a rock fracture system, *Environmental Earth Sciences*, vol. 66, no. 5, pp. 1403-1414.

Keywords: fracture system, geostatistics, groundwater, hydraulic conductivity, MODFLOW, Toki granite

Relationship between stress and groundwater around TRIES area - consideration taking into account poroelasticity -

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Tono Research Institute of Earthquake Science (TRIES) have developed a borehole stress meter for continuous observation and multi-component borehole instruments. At the present time about 15 borehole stations are in operation. We have investigated crustal movements and behavior of underground water. In one place stress meter and a commercial water pressure meter are installed in the same borehole. Spring water was generated by boring work approximately 300m from these instruments. The water pressure and vertical stress component recorded the same variation in concurrence with this. This indicates that the developed stress meter is reliable.

Both meters recorded the same waveforms originated by 2011 Tohoku earthquake where epicenter distance is about 600km. The amplitude of stress meter is twice larger than water pressure meter and the trace is 0.35second ahead in stress meter. We have more comparisons between two meters like tidal variation and so on. These observation facts are explained by taking into account poroelasticity of surrounded media.

We will present interpretation explaining the observation facts.

Keywords: stressmeter, water-pressure gauge, behavior of groundwater, poroelasticity

Geographic distribution of $^3\text{He}/^4\text{He}$ ratios along seismic source faults in Japan

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It is well known that mantle degassing does not occur homogeneously over the Earth's surface. The elevated $^3\text{He}/^4\text{He}$ ratios found in volcanic regions and tectonically active areas are higher than the atmospheric values. This distribution is interpreted to indicate transfer of mantle volatiles into the crust by processes or mechanisms such as magmatic intrusion, continental underplating and lithospheric rifting. This study was undertaken to elucidate the geographic distribution of $^3\text{He}/^4\text{He}$ ratios around seismic source faults in Japan, using helium isotope data obtained from gas samples. Several case studies suggest that there is a significant trend of high ^3He emanations along the trace of active faults, resulting in leakage of mantle volatiles through crustal pathways (faults) due to more frequent development of higher permeability pathways and/or upwelling of mantle fluids through the ductile lower crust. From the viewpoint of site selection and implementation of a geological disposal facility, helium isotopes may be regarded as a tool for investigating and/or mapping concealed active faults with no surface expression.

Keywords: helium isotope, active fault