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Model Study of Formation of the Cap Rocks for Geothermal System Using ChemTOUGH2

Sato, T.[+], Sato, M.[+]. Ueda, A.[++], Kato, K.[++]. Kissling, W.M.[+++], and White, S.P.[+++]

[+]Geothermal Energy Research & Development Co., Ltd.,1-22-4,Shinkawa,Chuo-ku, Tokyo, Japan.

tatuya@gerd.co.jp, msato@gerd.co.jp

[++]Mitsubishi Materials Corporation. Central Research Institute, 1-297,Kitabukuro-cho, Saitama-shi, Saitama, Japan.

a-ueda@mmc.co.jp, koikato@mmc.co.jp

.[+++]Industrial Research Limited, Gracefield Research Center, Gracefiled Road, Lowe Hutt, New Zealand.

W.Kissling@irl.cri.nz, S.White@irl.cri.nz

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ABSTRACT

We have developed numerical model of the geothermal system. The aim of this study is to simulate the formation of low permeability cap rocks. The reactive chemical transport simulator ChemTOUGH2 was used to model the kinetic reactions describing precipitation and dissolution of minerals.

First, we developed a numerical model of the natural state of the geothermal system without considering the chemistry of the geothermal fluid. This model was then extended by including reservoir rock, alteration minerals and assuming a chemistry for the source water based on 12 component species.

Using ChemTOUGH2 the evolution of fluid chemistry and rock alteration was traced for several thousand years. The model predicted, in keeping with observation, deposition of clay minerals at the top of the upflow area forming a low permeability cap.

1.INTRODUCTION.

The purpose of the modeling is to study the formation and distribution of altered minerals in the shallow regions of the Sumikawa geothermal field, Japan. In this work, we evaluated the effect of these minerals on the reservoir permeability.

The chemical modeling described in this report has been carried out using the reactive chemical transport code ChemTOUGH2, White (1995). Due to the very intensive nature of this calculation, the domain for the models is limited to a region 3 km × 3 km horizontally by 1.5 km deep that incorporates the hot upflow zone of the geothermal field. This model comprises a subset of the DSGR (Deep-Seated Geothermal Reservoir) model that was constructed before, and contains approximately 20% of the number of computational elements.

2. SUMIKAWA GEOTHERMAL FIELD

The Sumikawa geothermal field is located in the Hachimantai volcanic region of the north district of Japan Main Island. The commercial operation of power generation started in March 1995 with an installed capacity of 50 MWe. The steam-production section was constructed in the southern part of the area as subsurface temperature increases south word. The reinjection section was in the northern part separated from the production section.

For the Sumikawa geothermal system, Bamba and Kubota (1997) proposed geothermal conceptual model from the point of view the thermal history including the knowledge of the fracture – pattern analysis as follows.

1) Heat source: It is thought that a present heat source is in the lower parts of the Hachimantai-Yakeyama volcanic chain. At the period of highest temperature, heat source was located to the north than a present one, or two or more heat sources that were divided in to branches existed.

2) Fracture: It was concluded that the fractures have been formed by the magma-fracturing from the viewpoint that the distribution of fractures are corresponding to the high temperature area and its direction at the period of the highest temperature.

3) Thermal history: The thermal history at this area has been started from the formation of the caprock by the deposition of lacustrine sediments (1.0 – 1.5 Ma). Afterwards, the temperature of the geothermal system increased gradually by the andesitic magma and formed monmorillonite which was a typical swelling clay mineral. As the highest temperature and geothermal secondary minerals were formed at the same time. Toward the present stage, the part of geothermal system was cooled down 70□ or more by down –flow of cold water.

3. MODEL DESCRIPTION

3.1.Model domain

The model domain used for the present work is a subset of the DSGR Sumikawa model. On the DSGR project in Japan, Sumikawa was selected for one of study area, NEDO (2001). In this study, numerical model was developed to estimate the DSGR capacity for Sumikawa.

On ChemTOUGH modeling, we needed to reduce the number of model elements because of the very intensive nature of the calculations. It was found by experiment that about 1000 model elements is the current practical limit. This is determined by the number of chemical species and reactions included in the model, and the speed of the available computers.

The model covers an area 3 km × 3 km, which is roughly centered on the location of the highest temperature geothermal upflow. In relation to the DSGR Sumikawa model, the boundaries of the model lie in the range $-6000 < \times < -3000$ and $-4500 < y < -1500$. The model extends to $z = -1500$ m vertically. This limit is chosen to avoid the extremely hot conditions (> 350 °C), which occur at greater depths, because no experimental information is available for chemical reaction rates or equilibrium constants at these temperatures.

Elements (from the DSGR model) within the limits given above remain as active elements in the present model and have evolving thermodynamic (P,T,S) and chemical conditions. Those elements lying outside the above limits (but connecting to elements within the domain) act as boundary elements for the present model, and must have appropriately assigned thermodynamic and chemical states. How these conditions are calculated and assigned is explained in the section "Initial conditions" below.

3.2.Chemical species, reactions and mineralogy

The models presented in this report include the following 13 primary chemicals species:

> H2O, H+, Ca++, Mg++, Na+, Cl-, SiO2(aq), HCO3-, SO4--, K+, Al+++, Fe++, HS-.

These species are considered to be the minimum essential to represent the changes in mineral content expected at Sumikawa. In addition to the primary species, there are 38 secondary chemical species:

> Al(OH)2+, Al(SO4)2-, Al13O4(OH), Al2(OH)2, Al3(OH)4 , AlO2- , AlOH++, AlSO4+, CO2(aq), CO3-- , CaCO3(aq), CaCl+, CaCl2(aq), CaHCO3+, CaOH+, CaSO4(aq), H2SO4(aq), HAlO2(aq), HCl(aq), HSO4-, HSiO3-, KCl(aq), KHSO4(aq), KOH(aq), KSO4-, Mg4(OH)4, MgCO3(aq), MgCl+, MgHCO3+, MgSO4(aq), NaAlO2(aq), NaCO3-, NaCl(aq), NaHCO3(aq), NaHSiO3(aq), NaOH(aq), NaSO4-, OH-

The 17 minerals included in the model are:

> Calcite, Albite-l, Anorthite, K-Feldspar, Kaolinite, Laumontite, Muscovite, Quartz, SiO2(am), Wairakite, Anhydrite, Epidote, Gypsum, Pyrophlite, Calcium Montmorillonite, Sodium Montmorillonite, Enstatite.

3.3.Thermodynamic data

The SOLTHERM database, Reed (1982), provides equilibrium constants as a function of temperature for all the reactions considered in this work up to a temperature of 350^{o}C. It appears none of the widely available chemical databases provides data above this temperature explicitly. The program SUPCRT92, Johnson *et al (*1992), and associated databases provide a theoretical prediction of equilibrium constants for almost all the reactions of interest at temperatures up to 415^{o} C. There is excellent agreement between theoretical predictions of SUPCRT92 and the SOLTHERM database in regions where they overlap.

It is not possible to calculate the activity coefficients for charged species near the critical point of water. The approach we have taken is to use the values for equilibrium constants and activity coefficients for 350^{o}C for all temperatures greater than 350^{o}C.

3.4.Thermodynamic initial state

The thermodynamic initial state for the models was obtained by running the model that was based on the DSGR model, using the super-critical version of TOUGH2, Kissling and White (1999). Because the current modeling is concerned only with the relatively shallow part of the Sumikawa reservoir (above z = −1500), layers below this in the DSGR model were discarded for the calculation of the thermodynamic initial state.

The thermodynamic states calculated in this way were adopted as the initial state for temperatures, pressures and saturations in the Sumikawa chemical models. For the chemical models, bottom layer (to −1500 msl) was adopted as the bottom boundary, and lateral elements outside the 3 km × 3 km model domain were set to be boundary elements. The conditions in these boundary elements remain fixed throughout all of the simulations. The next section describes how the chemistry in these boundary elements was determined.

3.5. Chemical initial state

For each model, the initial chemistry was calculated in two stages - one to define the chemistry of the cool lateral boundaries of the reservoir, and one for the high temperature lower boundary of the model. This approach was necessary because of the very different fluid chemistry in the ‘hot’ and ‘cold’ parts of the reservoir. This section describes these calculations in more detail.

In the first stage, the chemistry of the reservoir was calculated using a simplified fluid chemistry including H+, OH- and trace amounts of the other primary species. The results from this calculation define the chemical equilibrium throughout the reservoir at time ‘zero’, and also to set the chemical conditions in the lateral boundary elements of the model.

Initial runs of ChemTOUGH revealed a tendency for the fluid in the cool part of the model (outside the upflow zone) to become moderately acidic, with a pH of about 5.5. The reason for this was traced to there being insufficient OH- in the reservoir fluid to maintain near-neutral conditions, and an excess of Al3+, which tended to remove OH- from solution. Once this was established, the quantities of H+, OH- and Al3+ were adjusted and the model was run for a sufficient period to establish chemical equilibrium with near-neutral pH throughout the reservoir. This state was used to specify the initial chemistry in a model without the input of any geothermal chemistry.

The second stage of the calculation is used to define the chemical equilibrium in the high-temperature boundary elements at the base of the model. To do this, a fluid chemistry nearer to that measured (or inferred) for the upflow region of Sumikawa was defined, and bought to equilibrium for each lower boundary element. The aim of this was to achieve a slightly acidic pH solution containing sufficient primary species to permit the formation of the observed clays and minerals such as montmorillonite, kaolinite, laumonite, and wairakite.

The initial chemical state of the model was constructed by using a combination of the results for the first and second stages described above. This defined the initial chemical state within the model domain, and in the lateral (low temperature) and lower (high temperature) boundaries of the model.

Although the chemical compositions of the fluid in these elements do vary, Table 1 shows the compositions of a ‘typical’ upflow element, which has a temperature of 366 °C.

Table 1:Chemical compositions of a typical upflow element.

Species	Concentration (gm/l)
H+	0.1565D-06 (pH = 6.8)
Ca++	0.3734D-06
Mg++	0.6383D-17
Na+	0.8543D-01
Cl-	0.1537D-01
SiO2(aq)	0.5507D+00
HCO3-	0.1103D-04
SO4--	0.4011D-04
K+	0.1712D-01
Al+++	0.1385D-30
Fe++	0.1000D-07
HS-	0.1000D-07

3.6. Initial Mineralogy

There are four ‘primary’ minerals present at the start of the model simulations. The predominant minerals are K-feldspar and quartz, with small amounts of calcite and enstatite. These correspond to ‘andesitic’ rocks, and are present in the initial assemblage in the proportions listed in the table below. These minerals provide the raw materials for the formation of other secondary minerals, including the montmorillonite group. The magnesium silicate enstatite is included to provide a source of magnesium for the formation of montmorillonite. The initial mineral assemblage contains no albite or anorthite, as the equilibrium calculated using these minerals was found to produce an initial pH which was too high. Removal of these minerals allowed an approximately neutral initial pH (Table 2).

Table 2:Initial minerals present in the ChemTOUGH simulation.

Mineral	Relative
Calcite	1
Albite	1000
Anorthite	1000
K-Feldspar	1000
Quartz	1000
Enstatite	10

3.7. Simulation period

Due to the intensive nature of the calculations involving reacting, transporting chemical species, it is not possible to specify a maximum simulation time. Instead, simulations are run for the longest practical periods, typically a few days at a time. For models of the size presented in this report, this typically allows simulations of periods of a few thousand years. This is sufficient to demonstrate some significant chemical and mineral evolution within the geothermal reservoir.

4. RESULTS

Chemical models have been run to 50000 years. Calculated temperature was fit to observed temperature distribution. There are existent concentration for calcite, anorthite, Ca-montmorillonite, albite, K-feldspar, laumontite, muscovite, quarts, wairakite and enstatite. There are low or non-existent concentrations for kaolinite, amorphous silica, anhydrite, epidote, gypsum, pyrophilite and Na-montmorilloite.

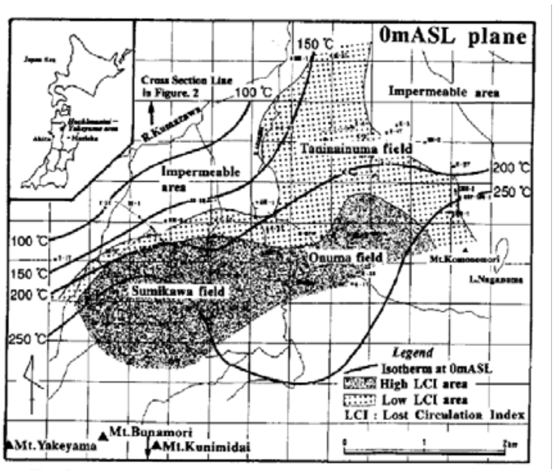

Figure □: The Sumikawa geothermal field (Bamba and Kubota,1997).

Bamba and Kubota (1997) showed distribution of lower most elevation of montmorillonite (Figure 2) and isograd elevation of wairakite (Figure 3). We compared them with calculated distribution.

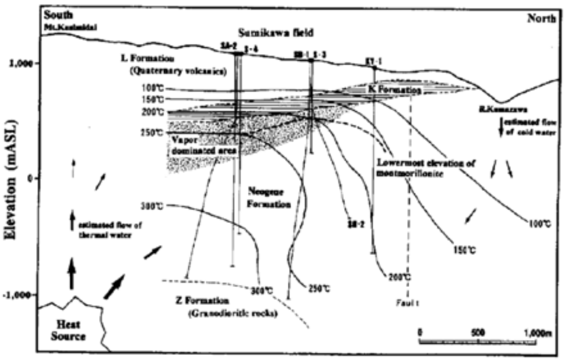

Figure 2:Cross section of the Sumukawa geothermal field, Bamba and Kubota (1997).

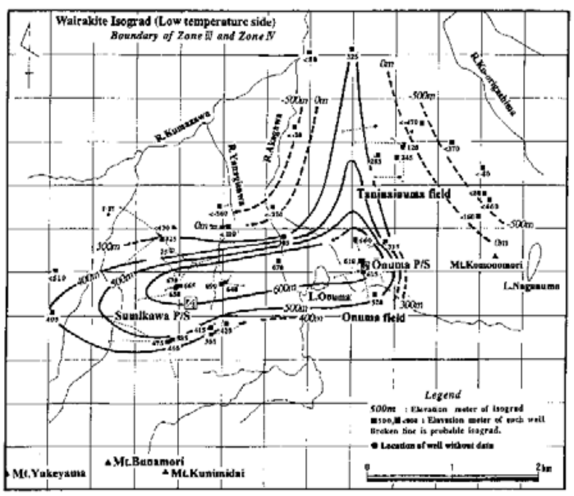

Figure 3: Wairakite isograd elevation (Bamba and Kubota, 1997).

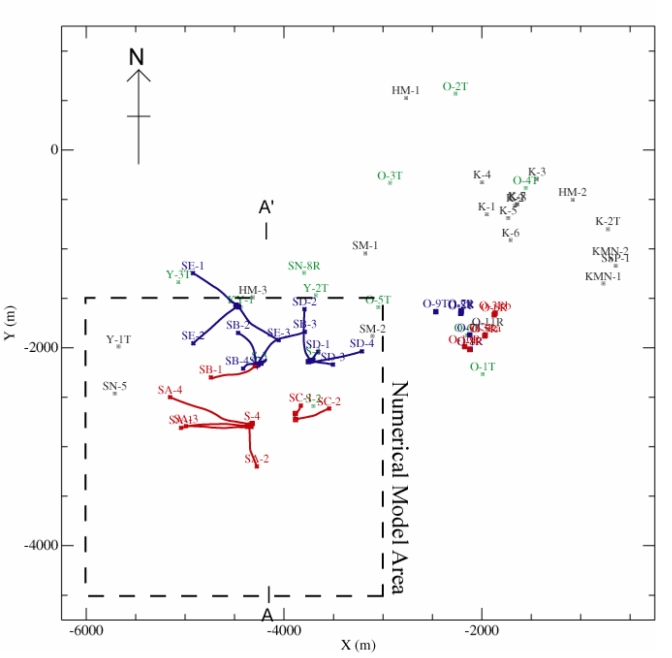

Figure 4:Numerical model area.

Figure 5 shows cross section of montmorillonite distribution with calculated temperature distribution. Filled color contour shows distribution of montmorillonite concentration and dash line shows temperature distribution. There is high concentration of montmorillonite upper up flow zone.

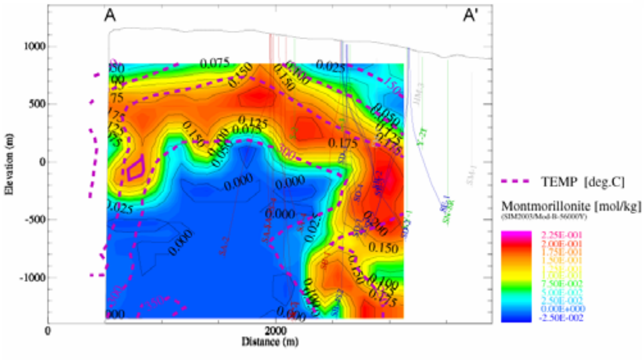

Figure 5:Cross section of calculated montmorillonite concentration and temperature distribution (after 50,000years).

Figure 6 shows cross section of calculated montmorillonite distribution with lower most elevation of observed one, Bamba and Kubota (1997). Filled color contour shows calculated result and thick dash line shows observed one. Center of dome of the calculated montmorillonite was south than observed one. Bamba and Kubota (1997) said, heat source was located to the north than a present one. It was consistency with result of chemical simulation.

Figure 7 shows cross section of wairakite distribution with calculated temperature distribution. Figure 8 and 9 shows cross section and iso-surface of calculated wairakite distribution with observed one, Bamba and Kubota (1997). Center of dome of the calculated wairakite distribution was south than observed one.

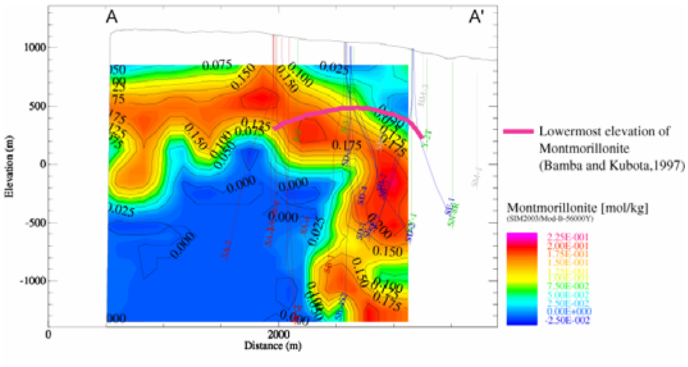

Figure 6: Cross section of calculated montmorillonite concentration (after 50,000years) and observed one.

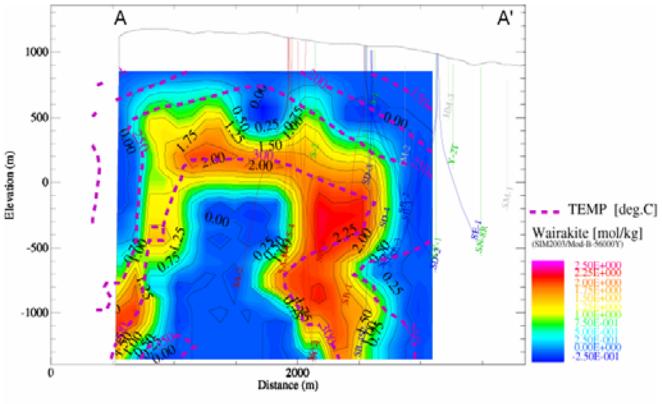

Figure 7:Cross section of calculated wairakite concentration and temperature distribution (after 50,000years).

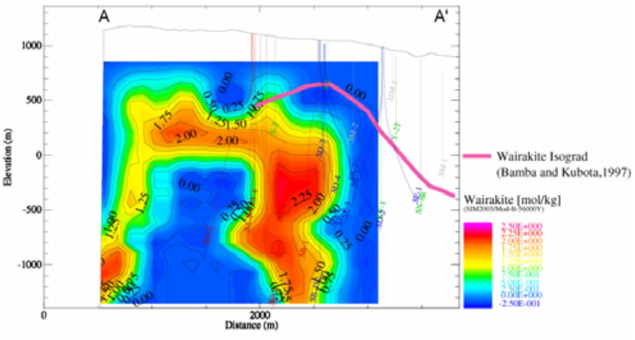

Figure 8: Cross section of calculated wairakite concentration (after 50,000years) and observed one.

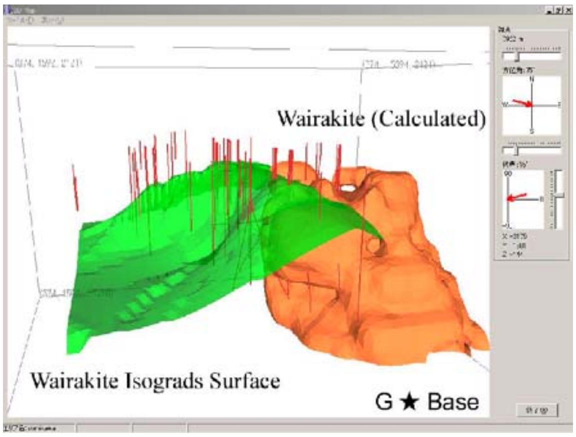

Figure 9:Iso-surface of calculated wairakite distribution

Here, the porosity change due to montmorillonite is plotted. The changes in porosity are calculated by concentration changes for mineral multiplied by its respective molar volume. The changes in porosity are relative to the initial porosity, and are measured in cc mineral/cc rock. A positive change on the plot indicates deposition of a mineral and therefore a decrease in porosity.

Figure 10 shows iso-surfaces of 2% porosity change calculated for the deposition of montmorillonite. There is no dissolution of montmorillonite, so there are no iso-surfaces corresponding to negative changes in porosity.

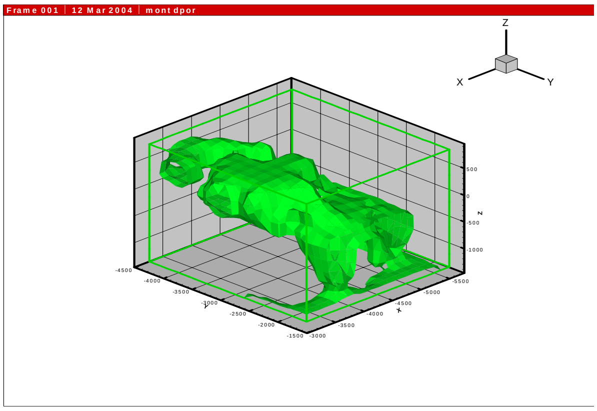

Figure 10: Iso-surface for porosity change of +2% due to deposition of montmorillonite.

5.CONCLUSIONS

In this paper, distribution of calculated montmorillonite and wairakite was compared with observed one.

Of the other minerals were included in the model calcite formed around and above the upflow zone, while anorthite dissolves in the same region as montmorillonite. Albite remains almost constant throughout the reservoir except for the shallow regions. K-feldspar and enstatite are correlated with the anorthite, indicating that it is dissolving to form calcite and Ca-montmorillonite. Laumontite is found to form only outside the highest temperature parts of the reservoir, while muscovite is precipitated weakly in the same regions as calcite and Ca-montmorillonite. Quartz shows unusual behaviour associated with its reverse solubility at high temperature. Finally wairakite forms in the same regions as calcite and montmorillonite, but over a larger range of temperature, resulting in broader regions of this mineral. The models show low or zero concentrations of kaolinite, amorphous silica, anhydrite, epidote, gypsum, pyrophilite and Na-montmorillonite.

Center of dome of the calculated montmorillonite was south than observed one. If concentration of montmorillonite increased, it had effect to reduce porosity. Bamba and Kubota (1997) said, heat source was located to the north than a present one. Also they said, it is possible that fractures were filled by montmorillonite. And these were cap rocks. It was consistency with result of chemical simulation.

This paper has presented chemical model of the Sumikawa geothermal system. Through this study, it was shown that chemical modeling was useful for considering thermal history of geothermal system. We expect to apply this method for another geothermal system.

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