Effects of temperature, pressure and NaCl concentration on electrical conductivity of geothermal fluid using molecular dynamics

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Understanding the behavior of geothermal fluid is important to achieve the sustainable resource development. Generally, the geothermal fluid behavior is evaluated by geophysical explorations such as Magnetotellurics (MT method). MT method is one of the electromagnetic explorations estimating the subsurface structure from the resistivity distribution under the ground. This method is generally used for understanding the distribution of geothermal fluid because its resistivity is low. It is well known that the electric properties of NaCl fluid depend on temperature, pressure, and ionic concentration of NaCl solution. For the quantitative interpretation of water distribution from resistivity profile illustrated by MT method, it is necessary to investigate the effects of temperature, pressure, and ionic concentration of NaCl solution on the electrical conductivity of the fluid. under geothermal reservoir conditions (hereafter GR situation) However, the existing experimental and simulated data for electrical conductivity of fluid are not insufficient to evaluate these effects on the electrical conductivity of geothermal fluid under GR situation. The goal of this study is to investigate electrical conductivity of NaCl fluid under GR situation to interpret water distribution of geothermal fluid quantitatively. In this study, we investigated electrical conductivity under temperature, pressure and NaCl concentration of 400-600 K, 5-30 MPa and 0.3-2.0 mol/L, respectively. Since it is difficult to measure the electrical conductivity of NaCl fluid under GR situation, we employed molecular dynamics (MD) simulation to estimate electrical conductivity of NaCl fluid. Our calculation used LAMMPS(ver.2017) for MD simulation and the Green-Kubo relations for estimation of electrical conductivity from calculated results by MD simulation. We confirmed the validities of our simulation results by comparing with existing experimental results. As a result, a strong dependence of electrical conductivity on temperature was confirmed. Electrical conductivity increases with temperature and it shows the peak around 550 K of temperature. After this peak, electrical conductivity decreases with the increment of temperature. In the case of 1.0 mol/L of NaCl concentration and 30 MPa of pressure condition, comparing 400K of temperature with 550K of the peak temperature, electrical conductivity increases about 9.2 S/m. At 600 K of temperature, which is after the peak temperature, electrical conductivity decreases 0.8 S/m. These trends are consistent with previous experimental results. Meanwhile, the pressure dependence of electrical conductivity was not confirmed in GR situation in our calculated results (1.4%). Our simulation results indicate that NaCl concentration has the largest effect on the electrical conductivity of the three parameters as temperature, pressure and NaCl concentration under GR situation. In the case of 500 K of temperature and 30 MPa of pressure condition, electrical conductivity increases about 31 S/m with the increment of 0.3-2.0 mol/L of NaCl concentration. The database of electrical conductivity of NaCl fluid under GR situation in this study is expected to contribute to the more precise interpretation of the electromagnetic exploration.

Keywords: electrical conductivity, molecular dynamics, geothermal fluid, magnetotellulic

