An Experimentally Derived Kinetic Model for Smectite-to-Illite Conversion and Its Use as a Geothermometer

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Abstract: The smectite-to-illite conversion during shale diagenesis has recently been used to constrain the estimate of a basin's thermal history. We have systematically investigated the kinetics for the conversion of a Na-saturated montmorillonite (SWy-1) to a mixed-layer smectite/illite as a function of KCl concentration (from 0.1 to 3 moles/liter) over a temperature range of 250 ° to 325 ° C at 500 bars in cold-seal pressure vessels using gold capsules. The results show that the conversion rate can be described by a simple empirical rate equation: $-dS/dt = A \cdot \exp(-Ea/RT) \cdot [K^+] \cdot S^2$ where S = fraction of smectite layers in the I/S, t = time in seconds, A = frequency factor = 8.08×10^{-4} sec^{-1}, exp = exponential function, Ea = activation Energy = 28 kcal/mole, R = gas constant, 1.987 cal/deg-mole, T = temperature (degree Kelvin), $[K^+]$ = K^+ concentration in molarity (M) in the fluid.

The results also show that Ca^{2+} in solutions barely affects the illitization rate, whereas Mg^{2+} significantly retards the rate. The retardation, however, is not as severe as previously reported. Na^+ ion can significantly retard the rate only if the concentration is high.

We found that by assuming a range 0.0026 − 0.0052 moles/liter (100 − 200 ppm) of K^+, concentrations similar to the value typically reported in oil field brines, the present kinetic model can reasonably predict the extent of the smectite-to-illite conversion for a number of basins from various depths and age. This narrow range of potassium concentrations, therefore, is used to model the smectite-to-illite conversion in shale when the actual chemical information of pore fluid is not available.

The kinetic equation has been tested using field data from a large variety of geologic settings worldwide (i.e., the Gulf of Mexico, Vienna Basin, Salton Trough Geothermal Area, East Taiwan Basin, Huasna Basin, etc). The results show that the equation reasonably predicts the extent of the reaction within our knowledge of the variables involved, such as burial history, thermal gradients, and potassium concentration.

Key Words: Geothermometry • Illite • Kinetics • Smectite • Smectite/illite

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