# Estimating Illitization Kinetics

**Ed Matteo and Yifeng Wang**
**Sandia National Labs**

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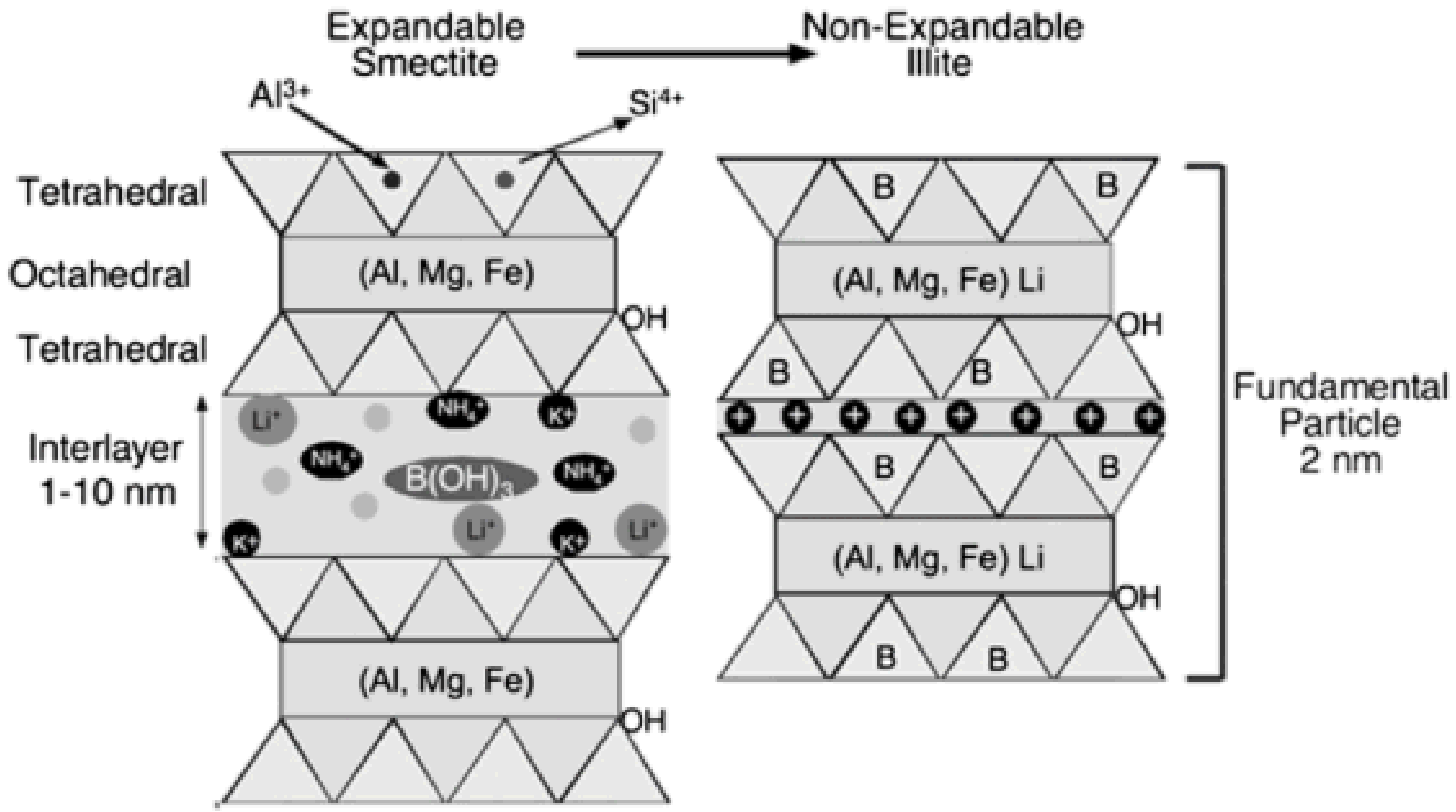
# Overview

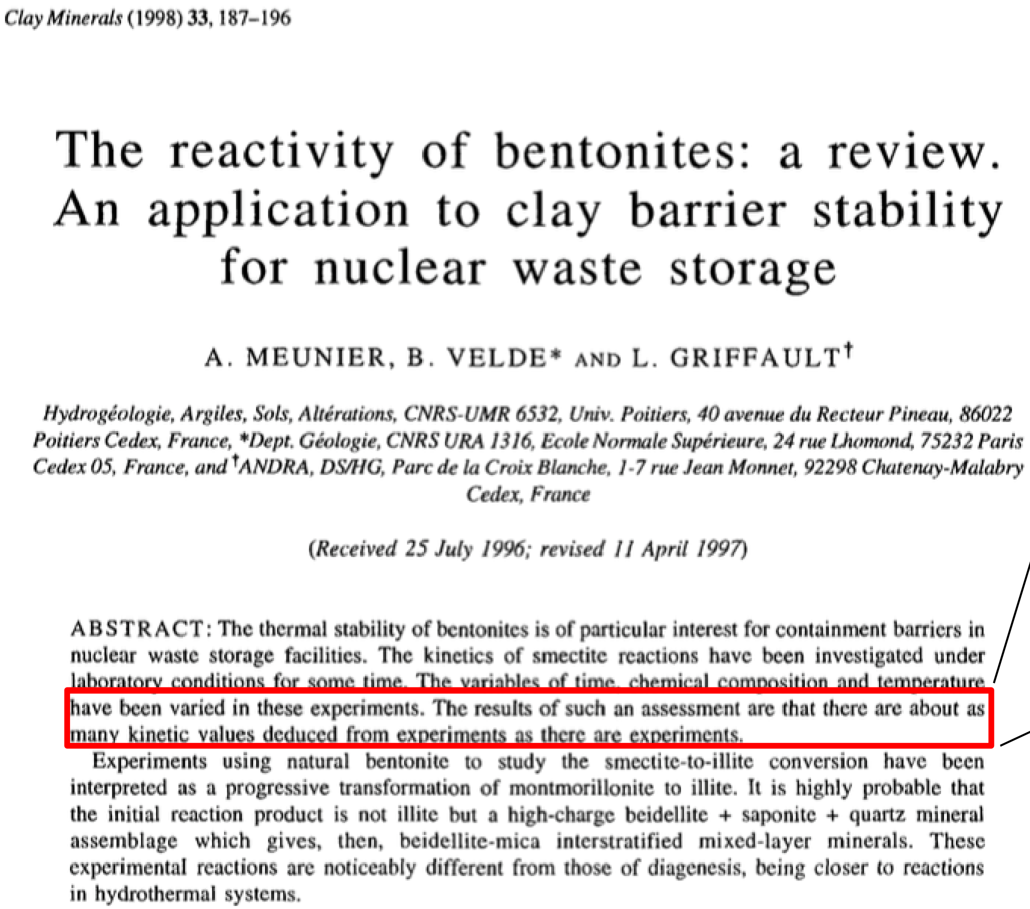
- **Brief Background**
- **Deriving an Empirical Illitization Expression**
- **Sensitivity analysis for [$K^+$], $E_a$ , and Temperature**

# Smectite to Illite Tranistion (low surface charge to high surface charge)



*https://www.researchgate.net/publication/301490033_Stable_isotope_constraints_on_the_origin_of_kaolin_deposits_from_Variscan_granitoids_of_Galicia_NW_Spain/figures?lo=1*

# Seems like a simple process, yet there are some discrepancies w.r.t. kinetics



*Clay Minerals* (1998) **33**, 187–196

## The reactivity of bentonites: a review. An application to clay barrier stability for nuclear waste storage

A. MEUNIER, B. VELDE* AND L. GRIFFAULT[†]

*Hydrogéologie, Argiles, Sols, Altérations, CNRS-UMR 6532, Univ. Poitiers, 40 avenue du Recteur Pineau, 86022 Poitiers Cedex, France, *Dept. Géologie, CNRS URA 1316, Ecole Normale Supérieure, 24 rue Lhomond, 75232 Paris Cedex 05, France, and †ANDRA, DS/HG, Parc de la Croix Blanche, 1-7 rue Jean Monnet, 92298 Chatenay-Malabry Cedex, France*

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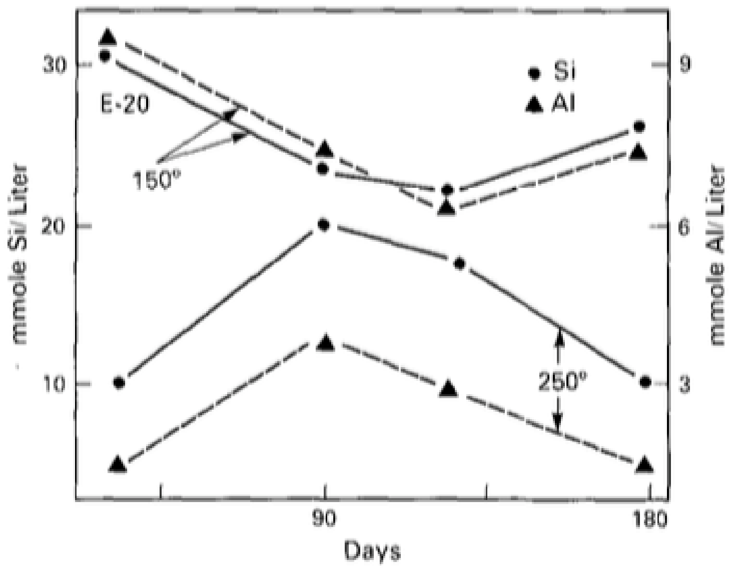
ABSTRACT: The thermal stability of bentonites is of particular interest for containment barriers in nuclear waste storage facilities. The kinetics of smectite reactions have been investigated under laboratory conditions for some time. The variables of time, chemical composition and temperature have been varied in these experiments. The results of such an assessment are that there are about as many kinetic values deduced from experiments as there are experiments.

Experiments using natural bentonite to study the smectite-to-illite conversion have been interpreted as a progressive transformation of montmorillonite to illite. It is highly probable that the initial reaction product is not illite but a high-charge beidellite + saponite + quartz mineral assemblage which gives, then, beidellite-mica interstratified mixed-layer minerals. These experimental reactions are noticeably different from those of diagenesis, being closer to reactions in hydrothermal systems.

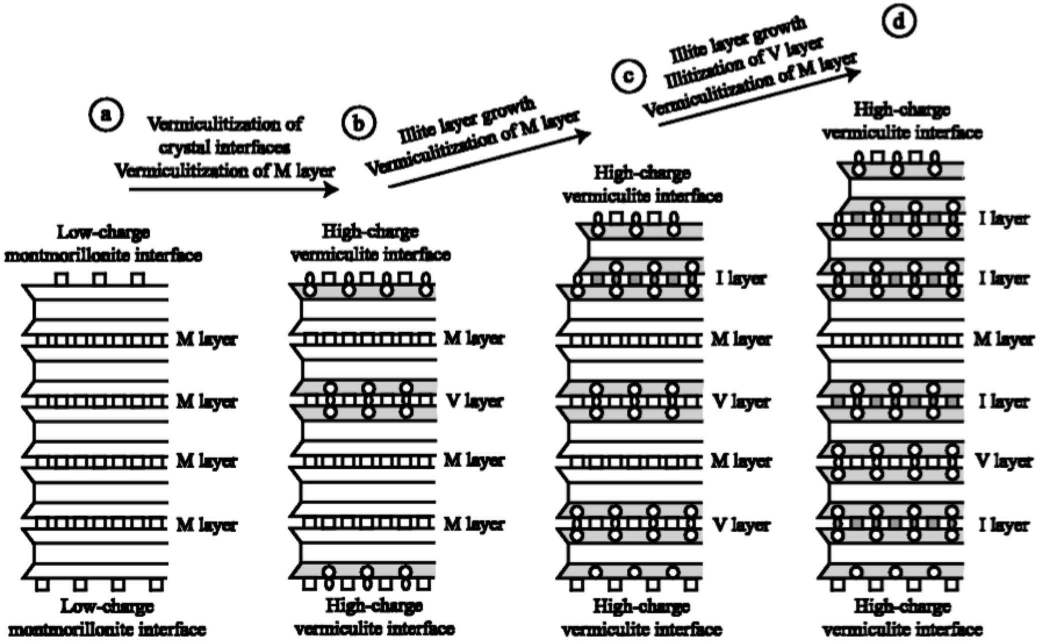
*The results of such an assessment are that there are about as many kinetic values deduced from experiments as there are experiments. [!!!]*

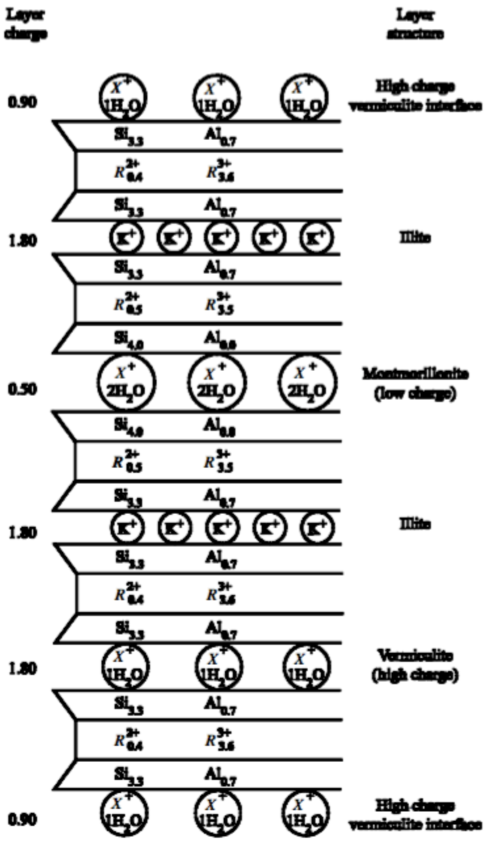
# Howard and Roy, 1985

- **Highlights**
  - High T(>200 ºC) and Low T (150 ºC) mechanisms? Al re-precipiataion at High T
  - Low T diffusion controlled process? Doesn’t fit mechanisms
  - Activation energies much lower than other studies (sol’n composition)
  - Water: clay ratio
  - Surface area?



# Meunier et al. 2000 – Vermiculite as an intermediary between I-S





- $-\frac{dS}{dt} = [K^+] \cdot S_0^2 \cdot A \cdot exp\left(-\frac{E_a}{RT}\right)$

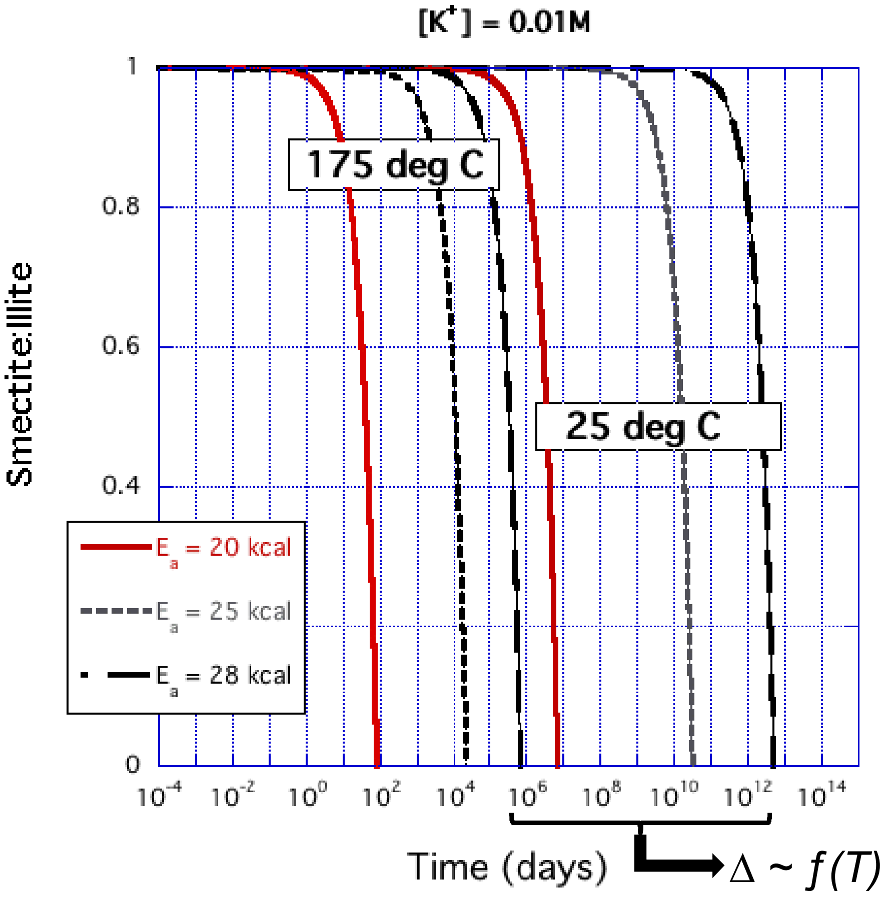
- *S* =1
- $-\frac{dS}{dt} = [K^+] \cdot A \cdot exp\left(-\frac{E_a}{RT}\right)$

- $-\int dS = [K^+] \cdot A \int exp\left(-\frac{E_a}{RT}\right) dt$
- $S = -[K^+] \cdot A \cdot exp\left(-\frac{E_a}{RT}\right) t + C$

- @ *t*=0, *S*=1 -> C=1

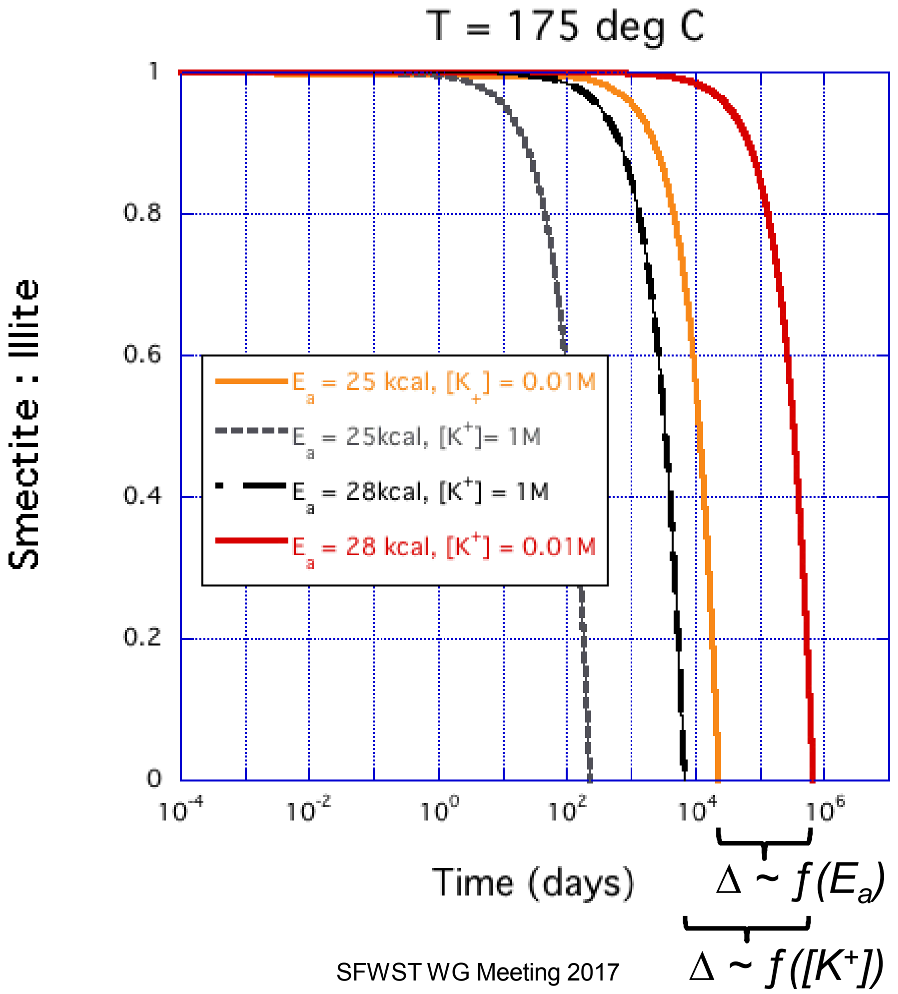
- $S = 1 - [K^+] \cdot A \cdot exp\left(-\frac{E_a}{RT}\right) t$

# Sensitivity of [$K^+$], $E_a$, and T



$\Delta \sim f(T)$

# Sensitivity of [$K^+$], $E_a$, and T



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