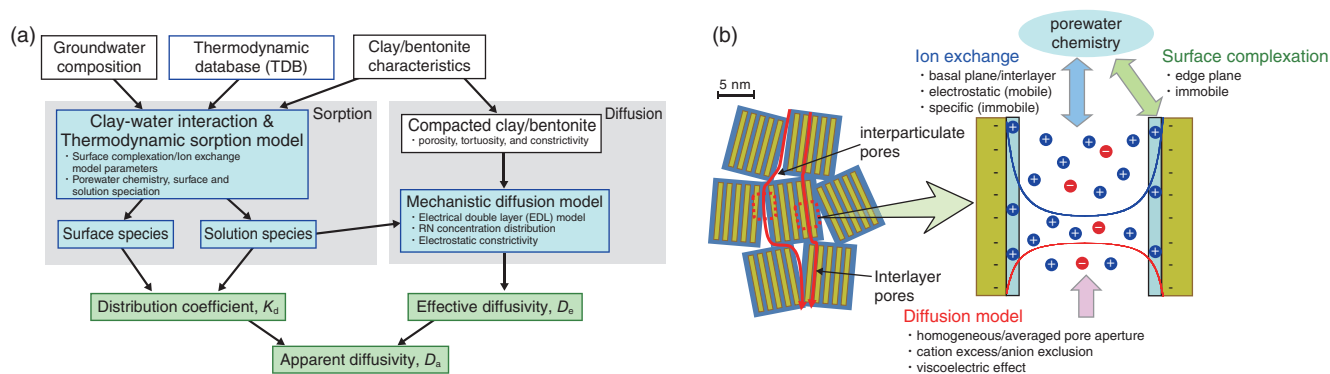# 8-12 Prediction of Radionuclide Migration in a Buffer Material
— Development of an ISD Model in Compacted Bentonites —

Fig.8-27 Framework and conceptual sketches of the ISD model in compacted bentonite
The ISD model is based on (a) a consistent combination of the clay-water interaction, sorption, and diffusion models; (b) coupling of the thermodynamic sorption model (ion exchange and surface complexation) and the EDL diffusion model in homogeneous pores.
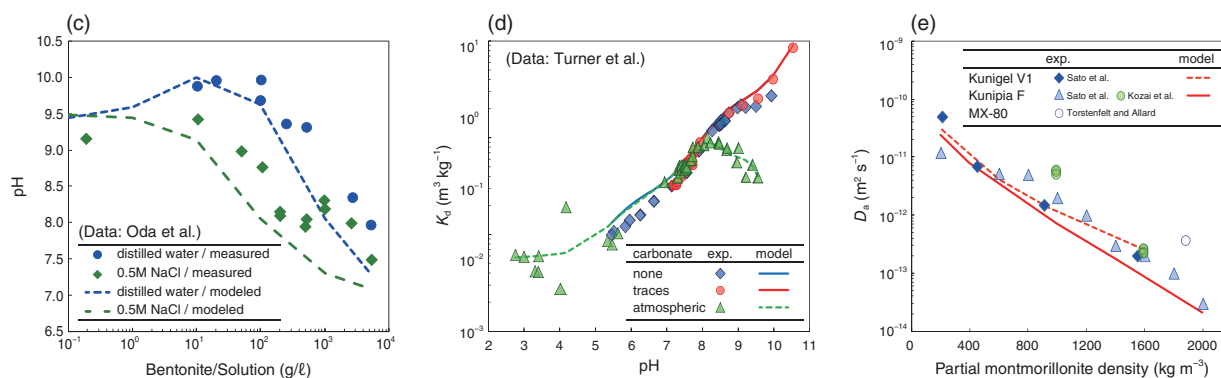
Fig.8-28 Applicability of the ISD model for predicting porewater chemistry, sorption, and diffusion
The ISD model was successfully tested for (c) pH in porewater, (d) K_d of Np(V) under a wide range of conditions, and (e) D_a of Np(V) as a function of partial montmorillonite density.

Sorption and diffusion of radionuclides in compacted bentonite are key processes in the safe geological disposal of radioactive waste. Quantitative understanding of the sorption and diffusion behavior of radionuclides, typically expressed as distribution coefficients (K_d) and effective diffusivities (D_e), are essential for safety assessment (SA). Geochemical variability and uncertainty, as well as their effects upon sorption and diffusion, usually have to be considered for SA. It is not feasible, however, to experimentally determine K_d and D_e values for all possible geochemical conditions. For this purpose, an integrated sorption and diffusion (ISD) model in compacted bentonite with nanoscale complex pore structures has been developed to achieve a consistent combination of the clay–water interaction, sorption, and diffusion models (Fig.8-27).

The basic premise considered in the ISD model was to consistently use the same model design and parameters to describe sorption/diffusion as well as porewater chemistry. A 1-site non-electrostatic surface complexation model in combination with a 1-site ion exchange model was used as the sorption model. The basic model, derived from surface titration data for purified montmorillonite, was parameterized on the basis of published sorption datasets for various radionuclides in dispersed systems, which cover a range of key geochemical conditions. The pH and sorption trends for Np(V) can be quantitatively described by the model considering a full suite of surface species including hydrolytic and carbonate species (Figs.8-28(c) and (d)).

The diffusion model based on the electrical double layer (EDL) describing relative ionic concentrations and viscoelectric effects at the negatively charged clay surface is connected to a simplified homogeneous pore model. The diffusion model component was integrated with the clay–water interaction and sorption models. The ISD model was successfully tested for Np(V) with a complex chemistry (Fig.8-28(e)) using published diffusion data (D_a, D_e) as a function of the partial montmorillonite density. It can therefore be concluded that the ISD model developed here is able to adequately explain the sorption and diffusion behavior of various radionuclides with a complex chemistry in compacted bentonites.

References
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