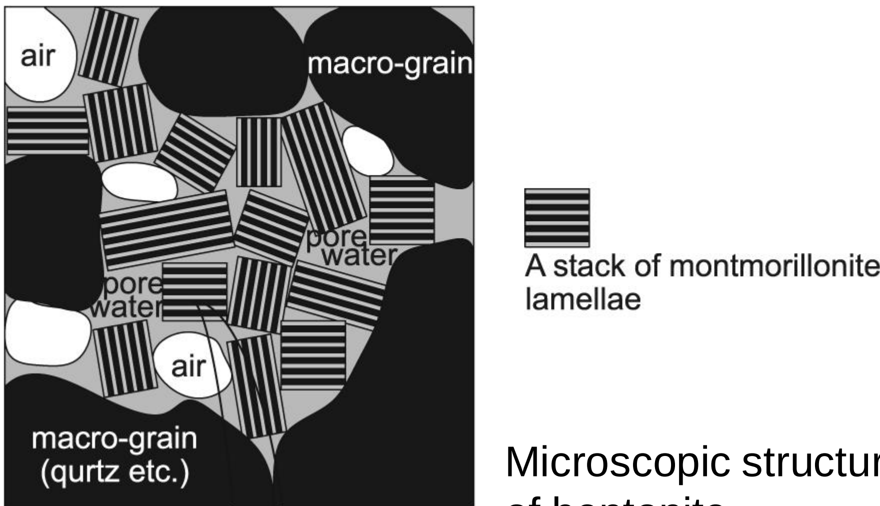
Prediction of Swelling Pressures of Different Types of Bentonite in Dilute Solutions

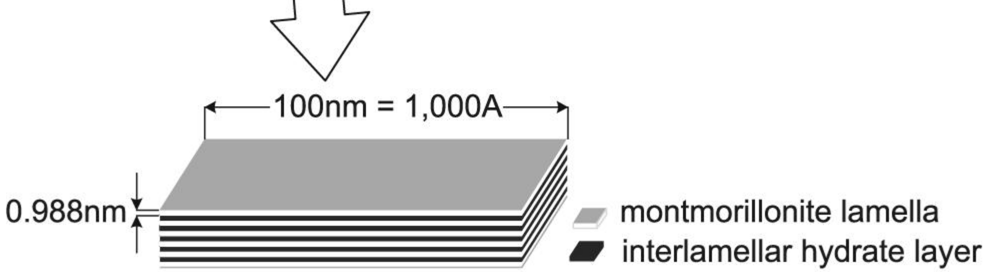
Model development and simulations

Longcheng Liu

Bentonite Buffer



Microscopic structure of bentonite



(b) A stack of montmorillonite lamellae

Candidate buffers

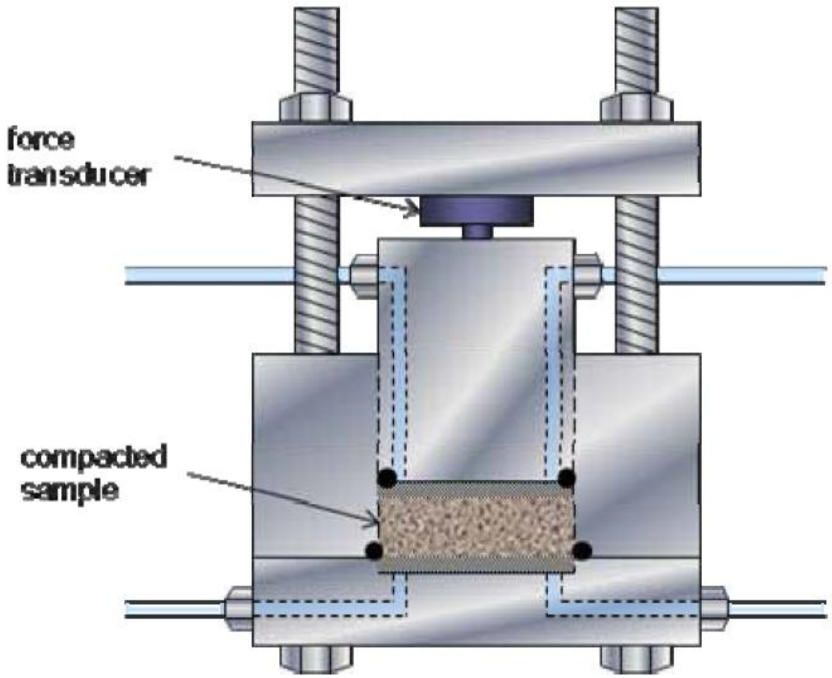
- **MX-80 (Na-bentonite)**
- **Deponit CA-N (Ca-bentonite)**

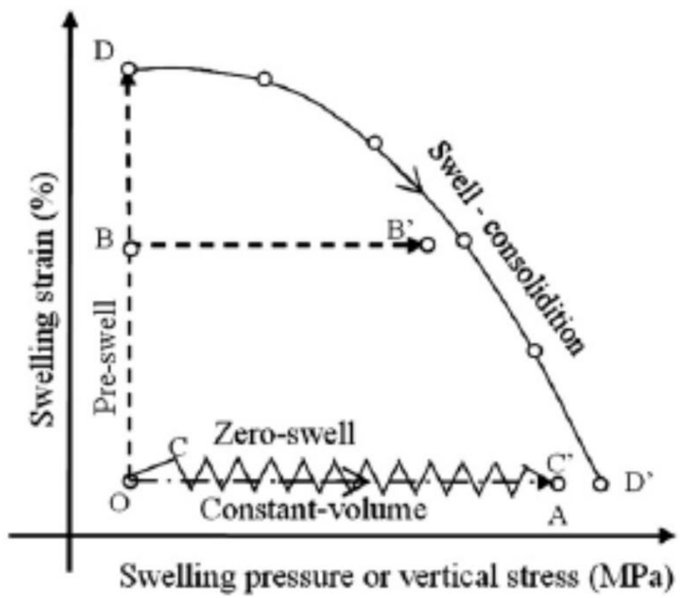
> 80 % smectite

Bentonite clay

Swelling Pressures

➢Measurements





Swelling Pressures

➢ Available models

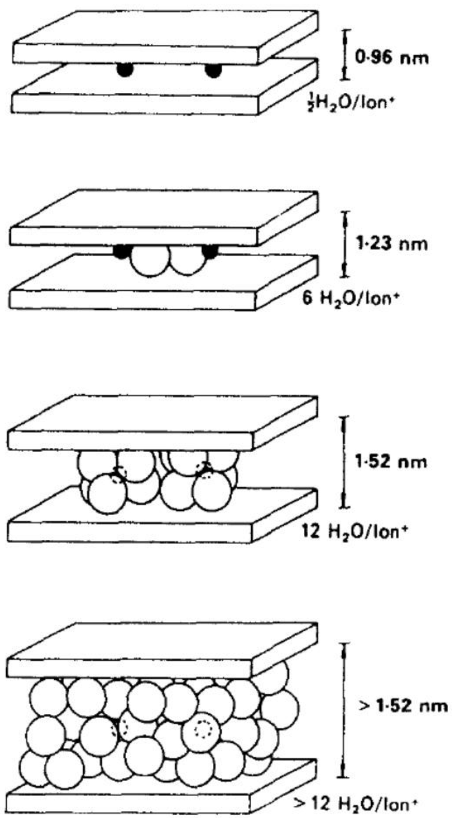
- Empirical models (simple regression expressions)
- Pheonmenological models (like BBM, BExM, etc.)
- Thermodynamic models (based on the fact of $p = s$)
- Diffuse double-layer models (like DLVO, DLVOE, etc.)
- Statistical mechanical models (like DFT, IET, etc.)
- ......

Swelling Mechanisms

➢Important processes

- Crystalline swelling (interlayer swelling)
- Osmotic swelling (interparticle swelling)
- Breakup of montmorillonite particles (stacks)
- Demixing of exchangeable cations
- Co-volume swelling
- Brownian swelling

Crystalline Swelling



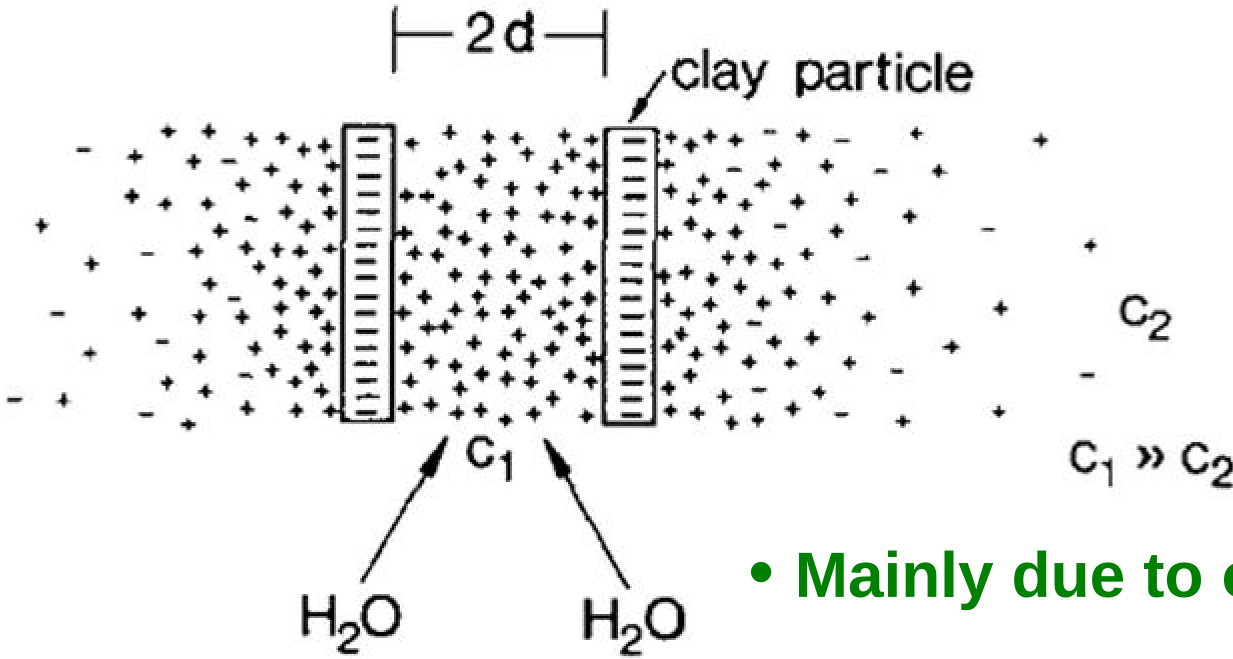
- Mainly due to hydration of cations and surface charge sites
- Take up water layer-wisely layer after layer up to 3 or 4 layers

Basal spacings (in nm)

Exchangeable cation	p_v/p_0 0	0.5	0.7	1
Na^+	0.95	1.24	1.51	M
K^+	1	1.24	d	1.5
Mg^{2+}	0.95	1.43	d	1.92
Ca^{2+}	0.95	1.5	1.5	1.89

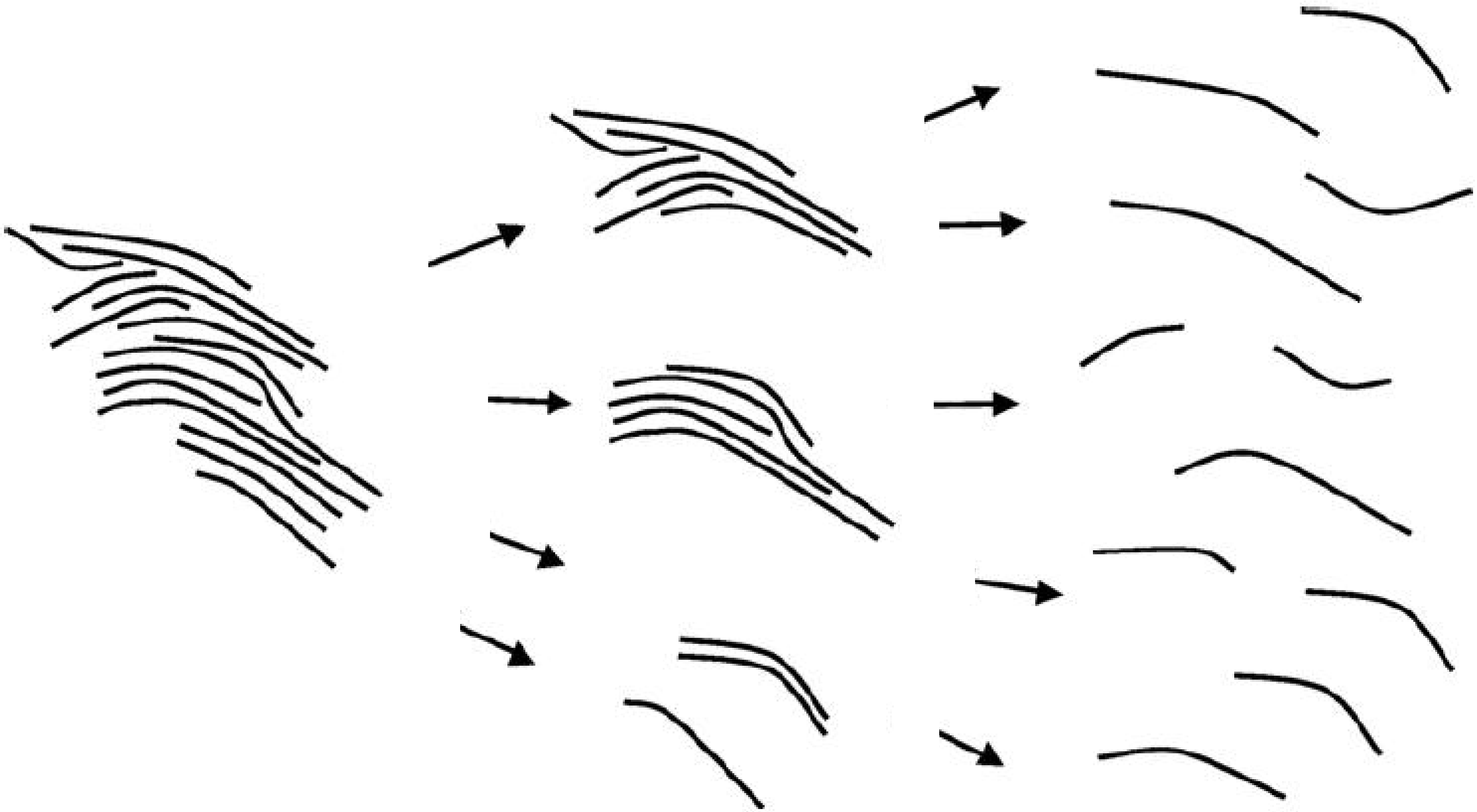
d: diffuse reflections; M: macroscopic swelling.

Osmotic Swelling

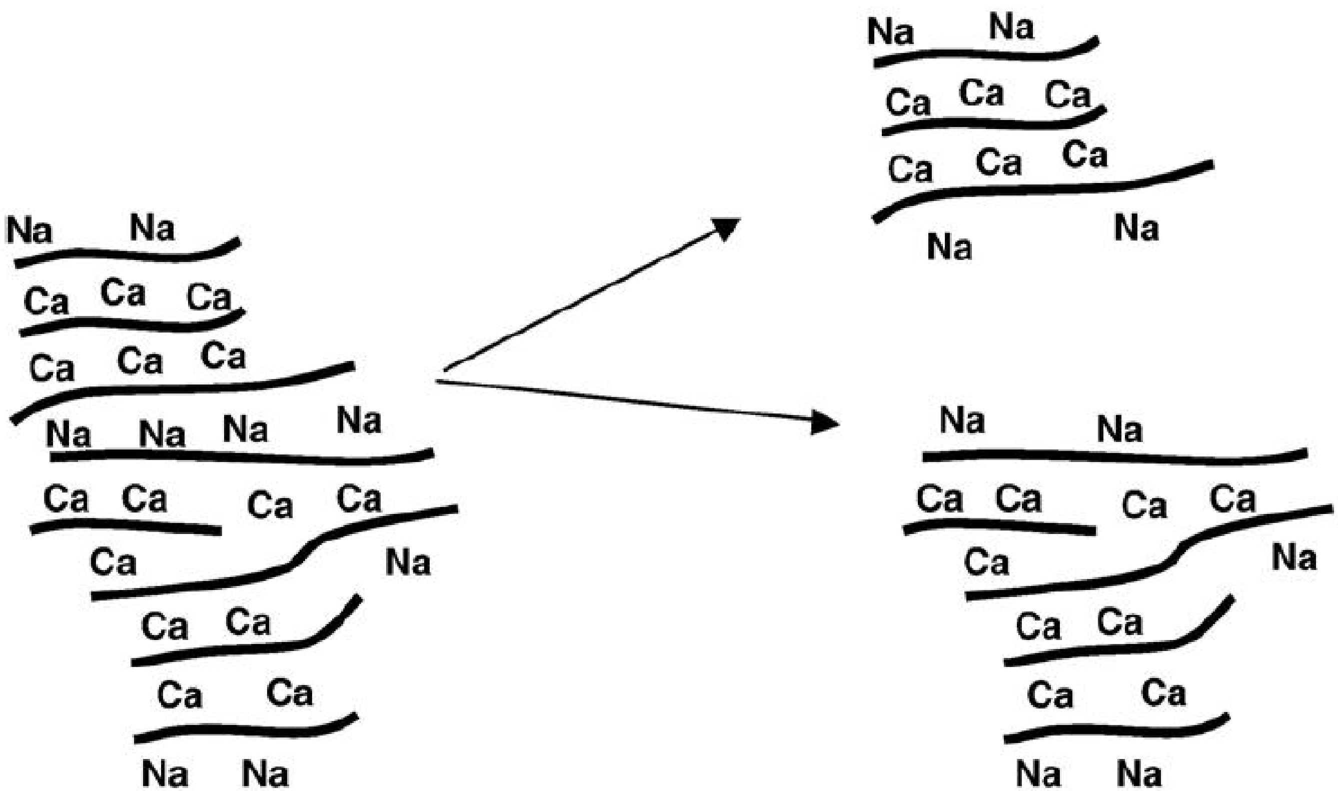


- **Mainly due to overlapping of diffuse double-layers**
- **Depending on the pore water chemistry (v, c, σ, etc.)**

Breakup of Mont. Particles

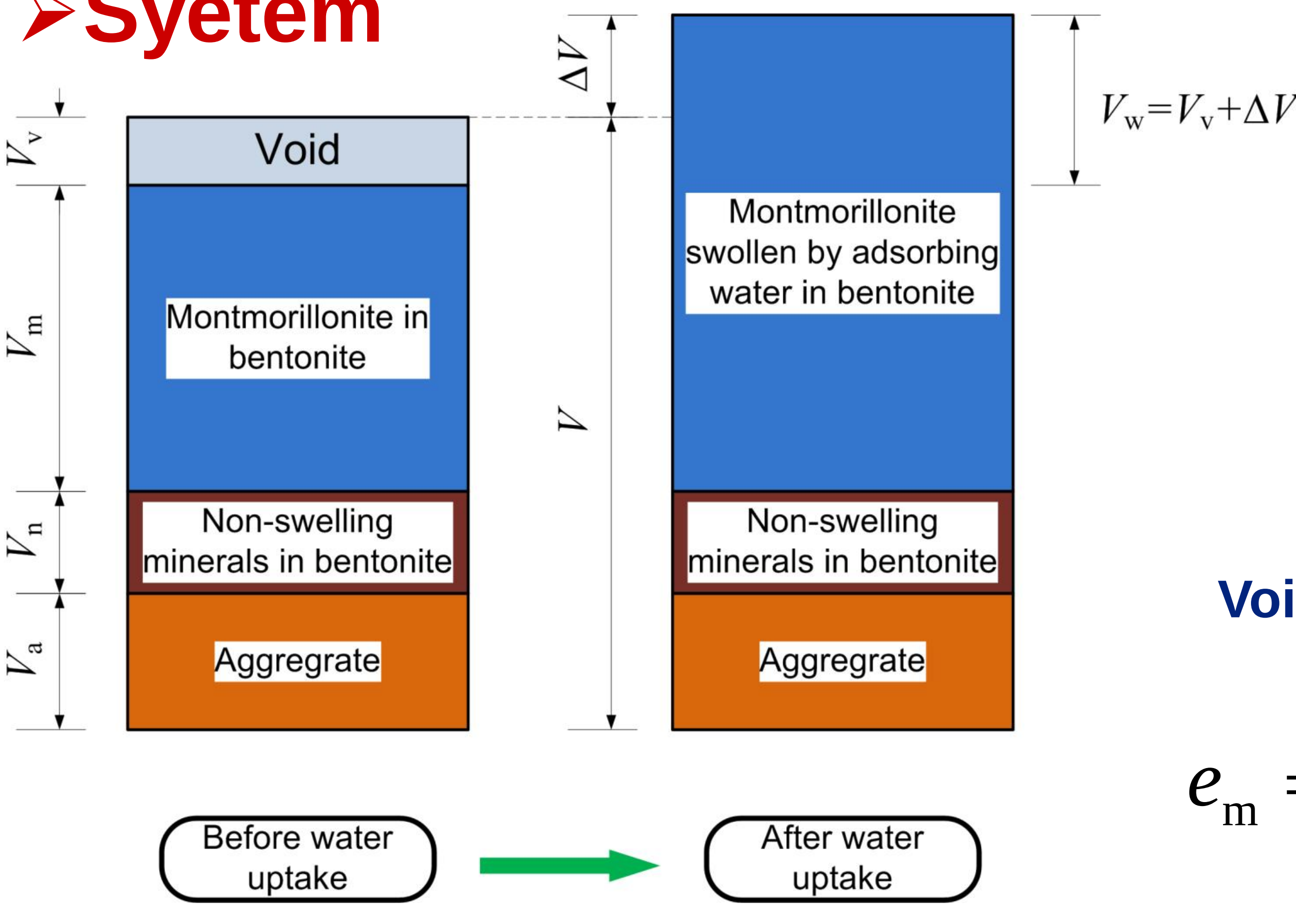


Cation Demixing



Model Development

➢Syetem

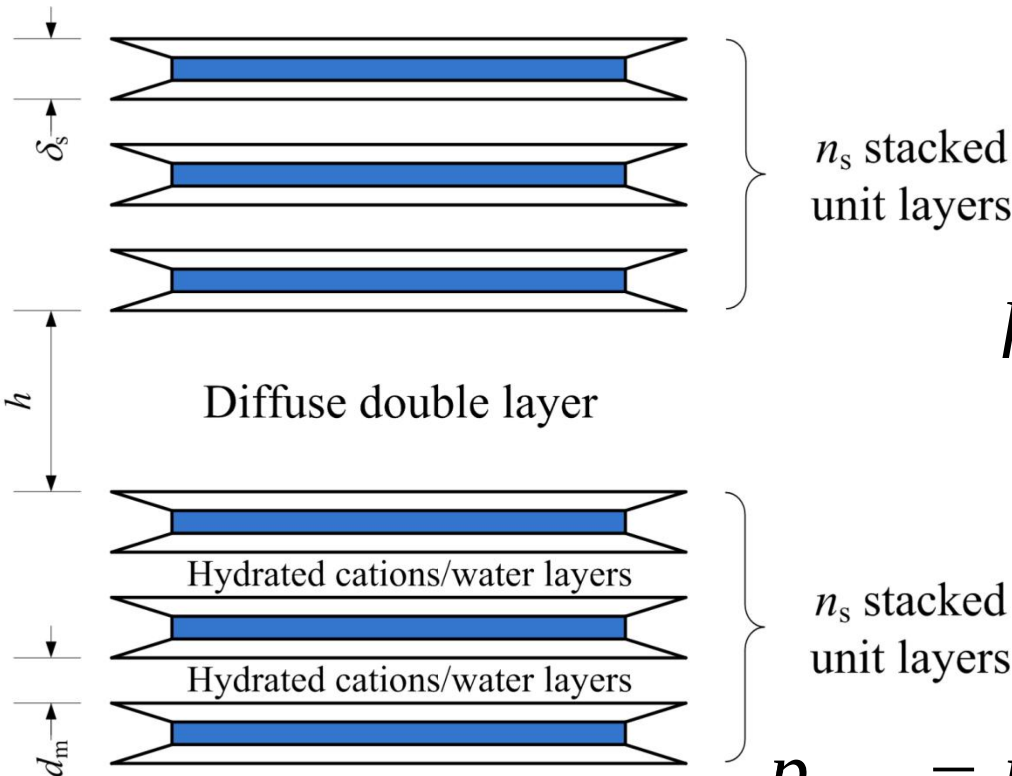


Void raio of mont.

$$e_{\mathrm{m}} = e\frac{\rho_{\mathrm{m}}}{\rho_{\mathrm{s}}}\frac{1}{\alpha C_{\mathrm{m}}}$$

Model Development

➢Fully developed osmotic swelling



Separation distance

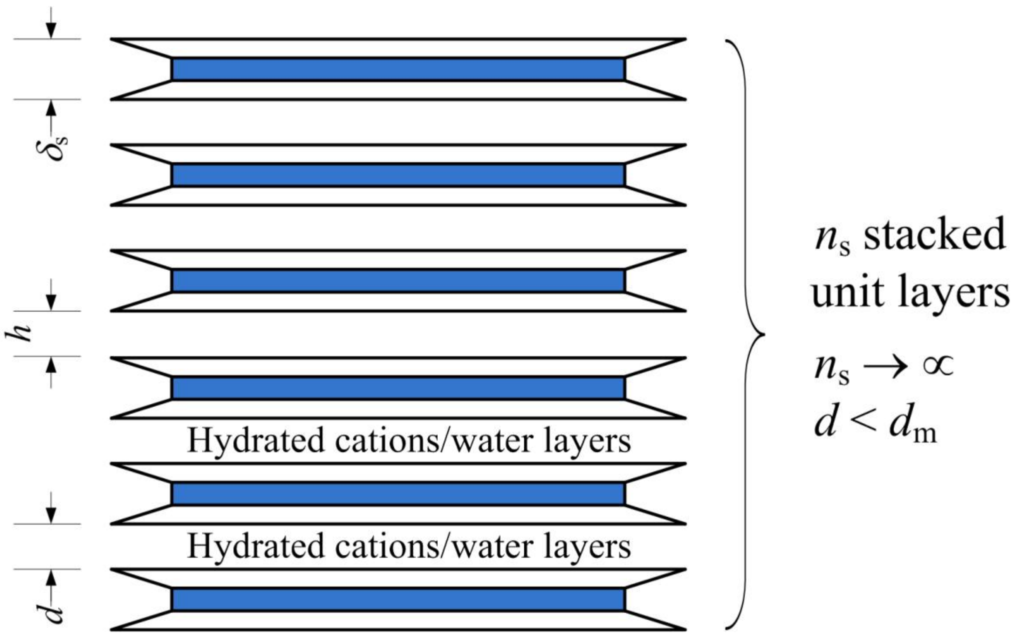
$$h = n_s \delta_s e_m - (n_s - 1) d_m$$

Swelling pressure

$$p_{OMS} = p_{DDL}(h, c, v) - p_{vdW}(h)$$

Model Development

- **Just initiated crystalline swelling**



Separation distance

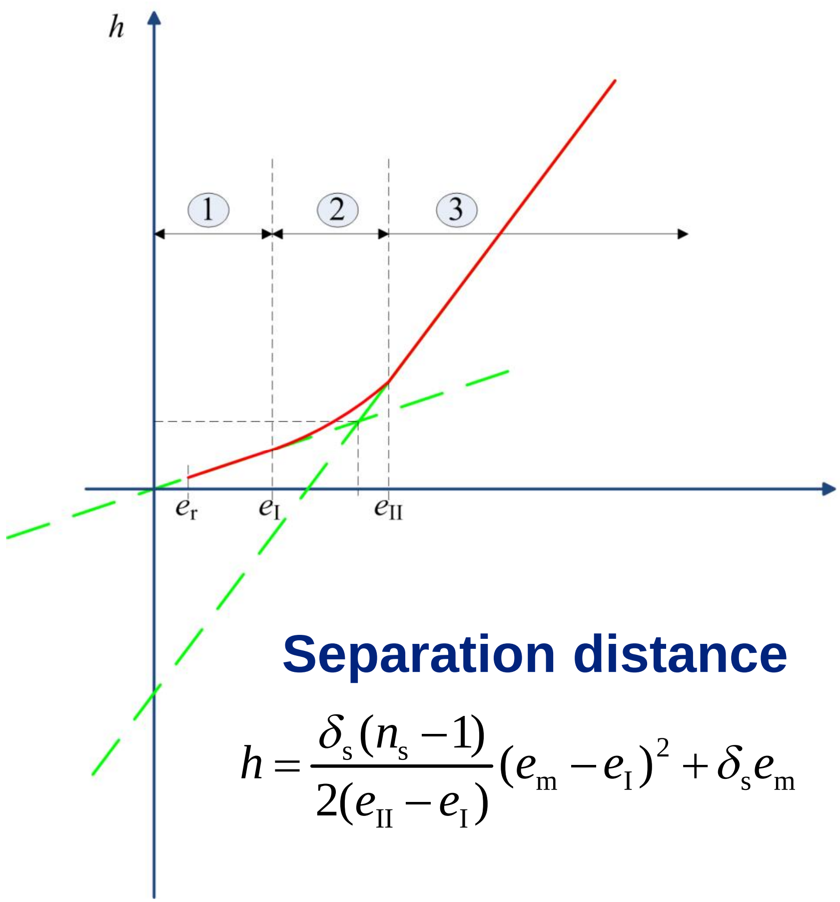
$$h = \delta_s e_m$$

Swelling pressure

$$p_{CSS} = s = k \exp(-h/l)$$

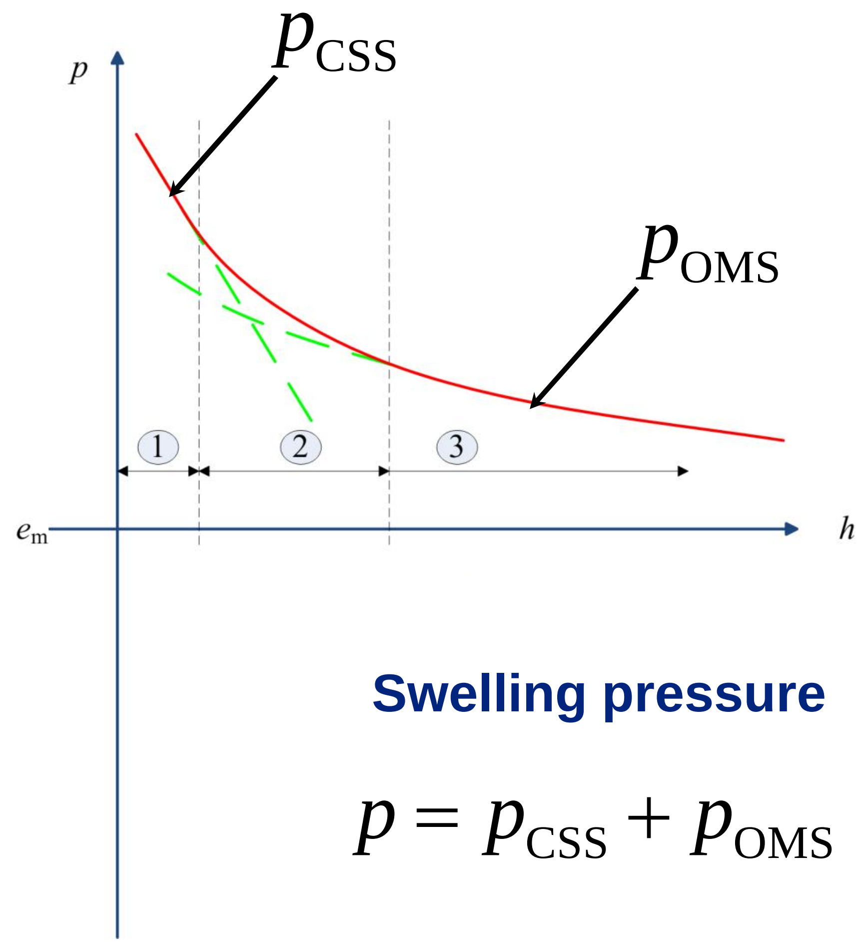
Model Development

➢Transition region



Separation distance

$$h = \frac{\delta_s (n_s - 1)}{2(e_{II} - e_I)} (e_m - e_I)^2 + \delta_s e_m$$

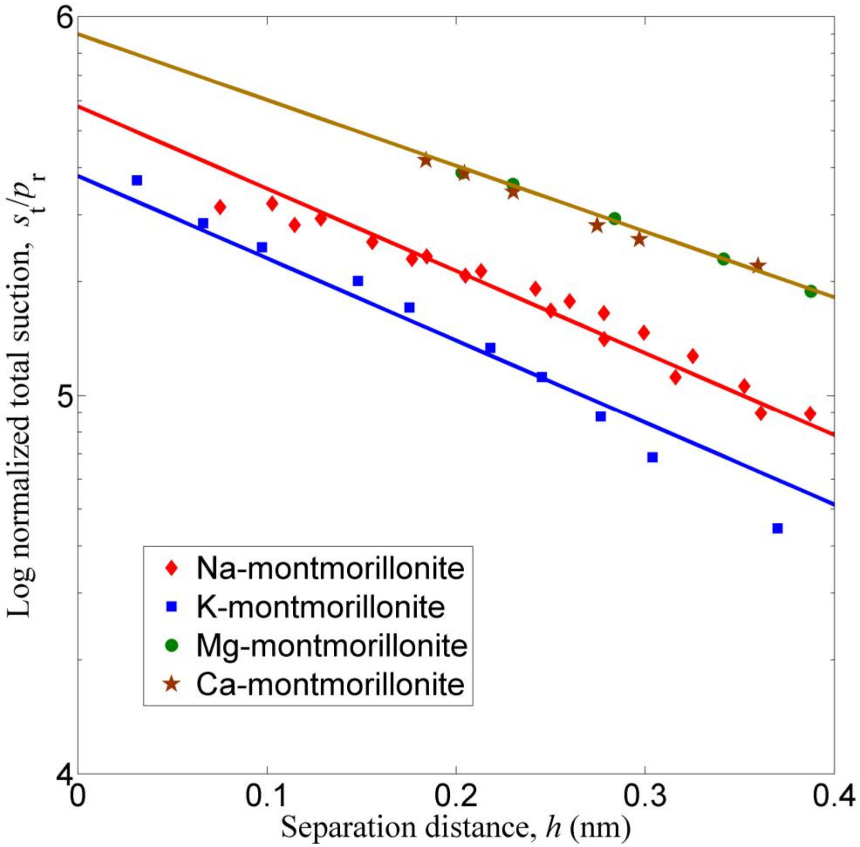


Swelling pressure

$$p = p_{CSS} + p_{OMS}$$

Model Parameters

➢Determination of *k* and *l*

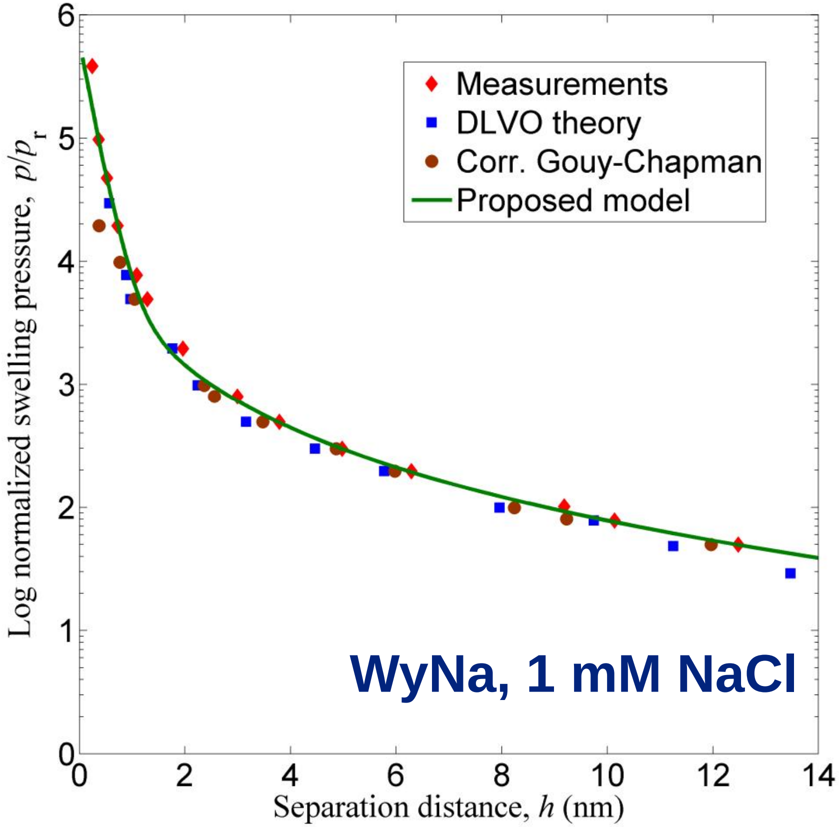


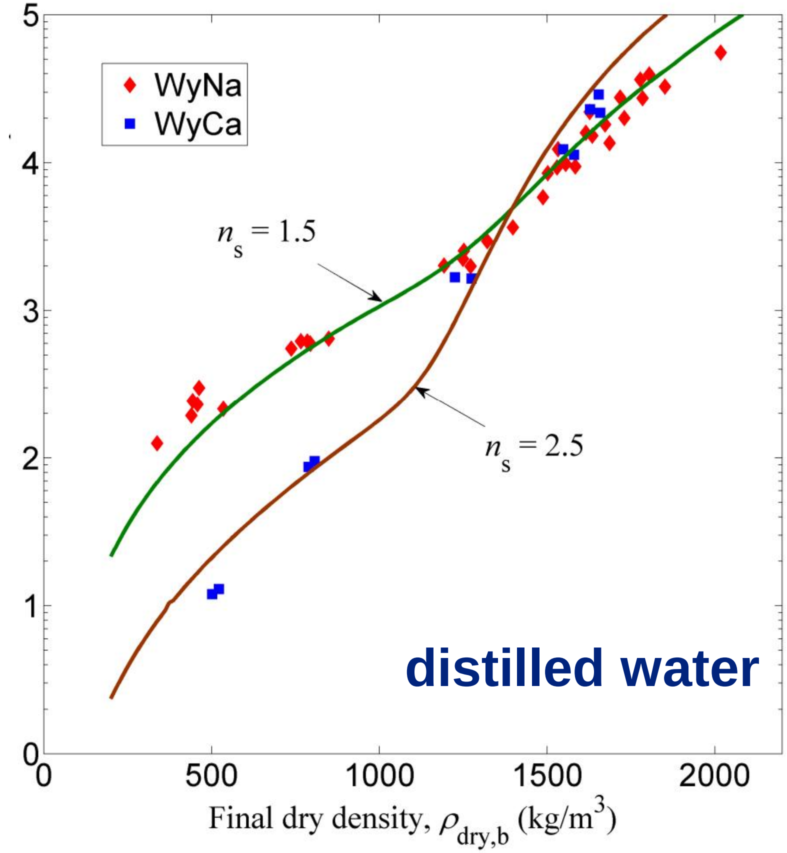
- **The only unknown parameter is n_s**
- **The others can be determined independently**

Types	Pre-exponential factor *k* (Pa)	Decay length *l* (nm)
Na-mont.	5.8×10^8	0.20
K-mont.	3.8×10^8	0.20
Mg-mont.	9.0×10^8	0.25
Ca-mont.	9.0×10^8	0.25

Model Predictions

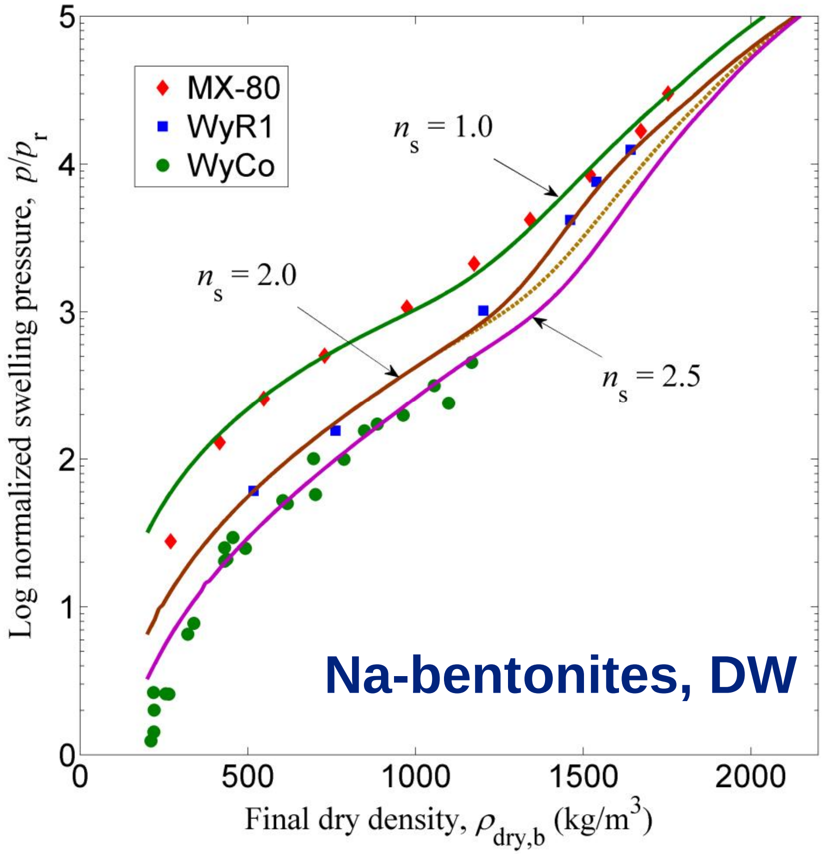
➢Benchmark tests

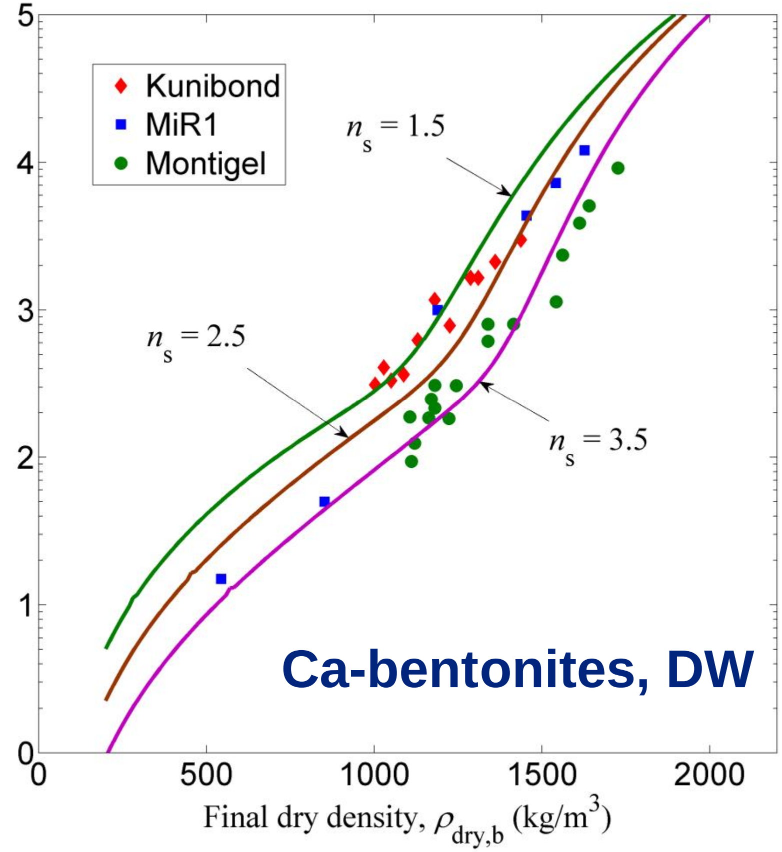




Model Predictions

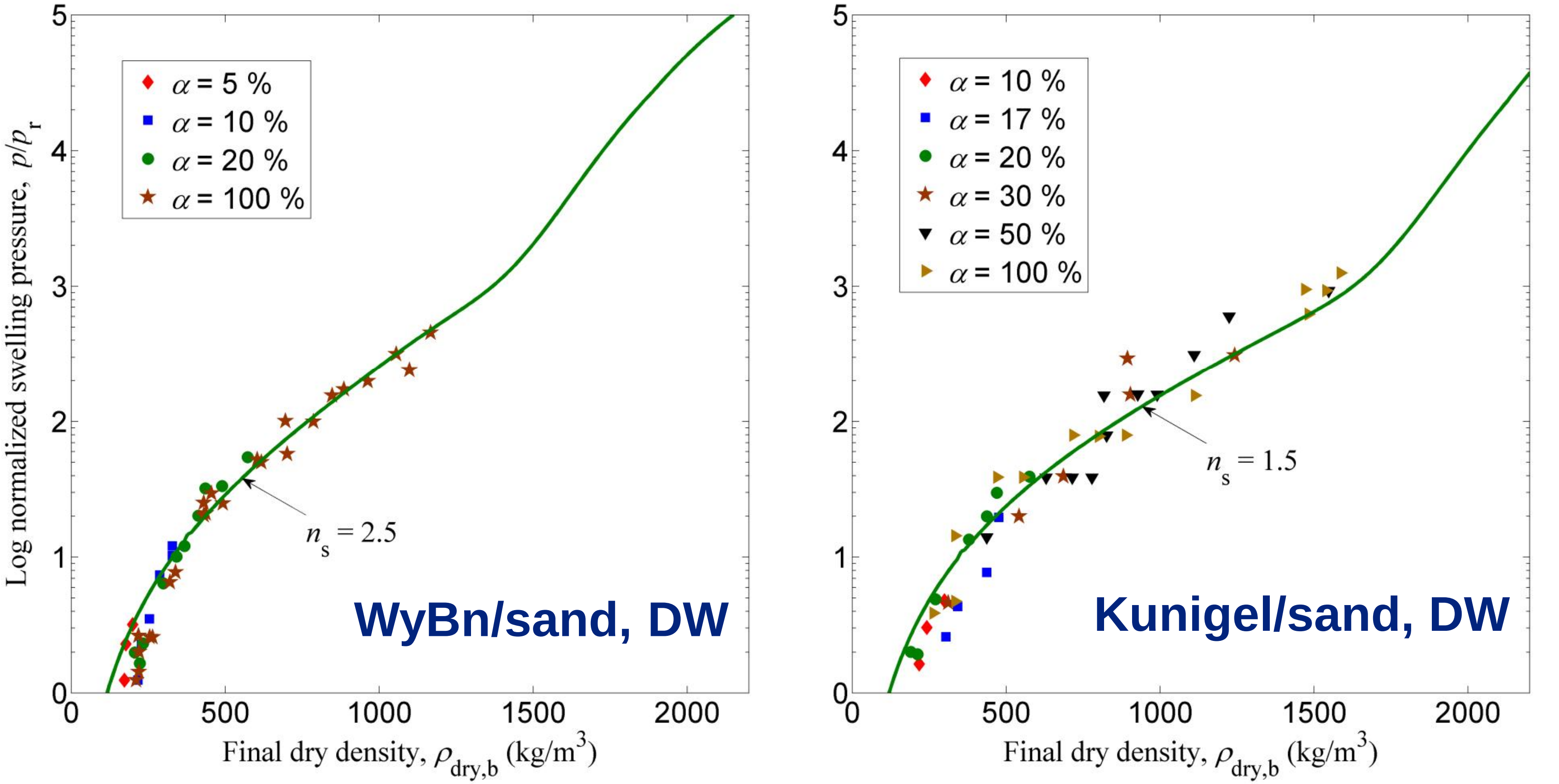
➢Natural bentonites





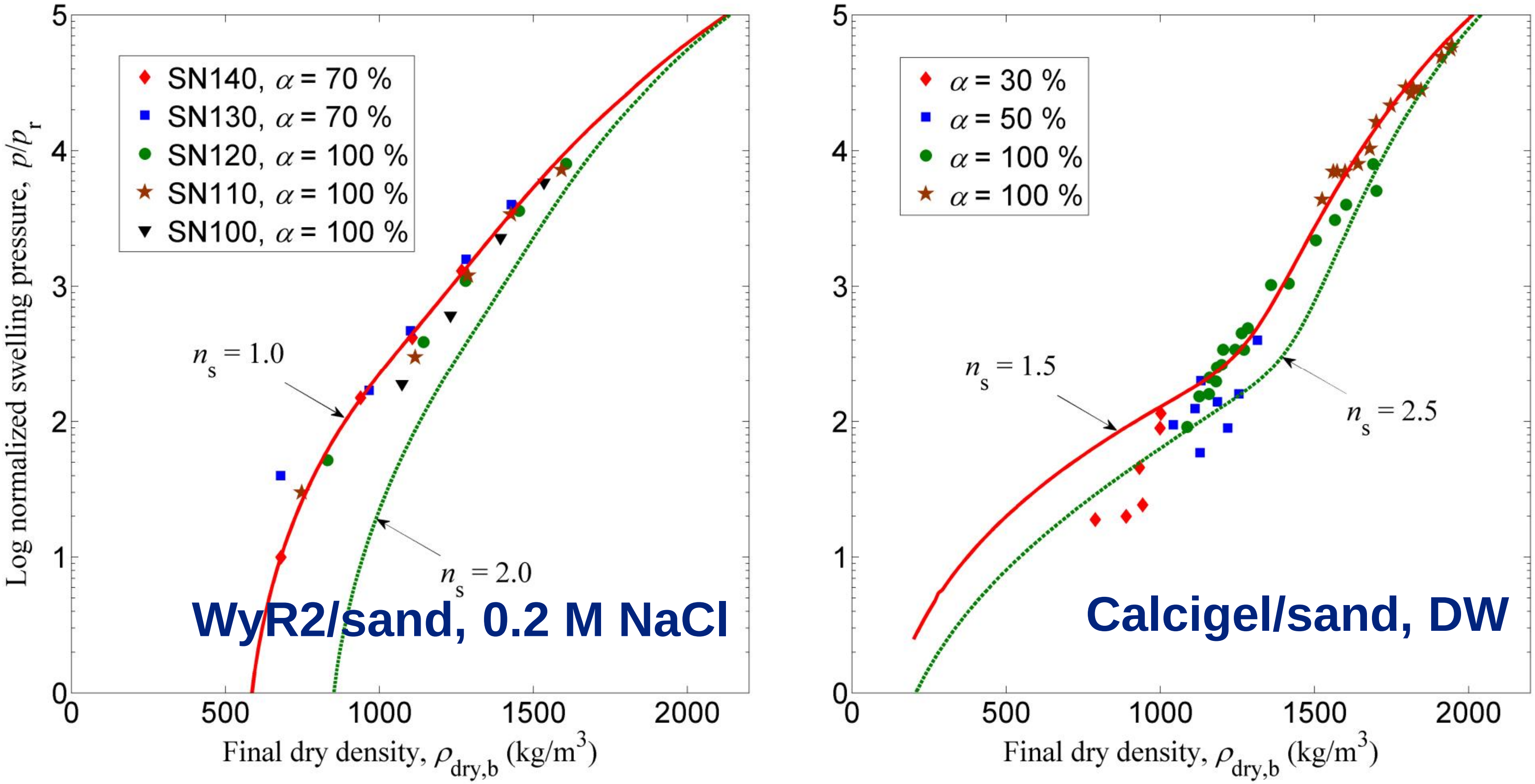
Model Predictions

- **Bentonite/sand mixtures**



Model Predictions

➢ **Bentonite/sand mixtures**



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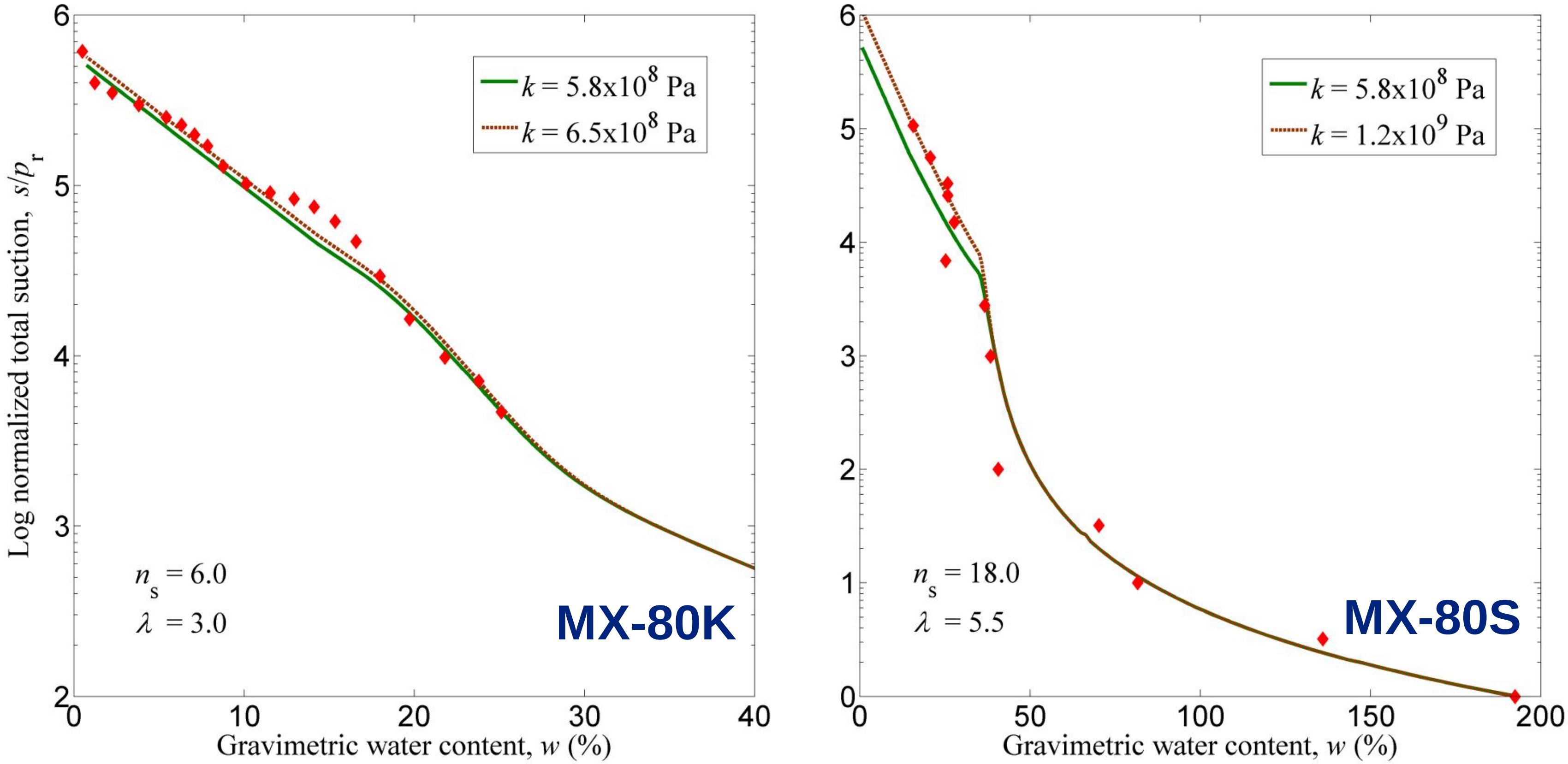
Model Predictions

➢Water retention curves



Conclusions

- A mechanistic model is developed
- The predictions agree well with experiments
- The only unknown parameter is n_s
- It also works well for water retention curves
- The n_s parameter and its dependence on the types of bentonite and the electrolyte, etc. need to be further investigated