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Ca and Sr sorption on Ca-illite experimental study and modelling

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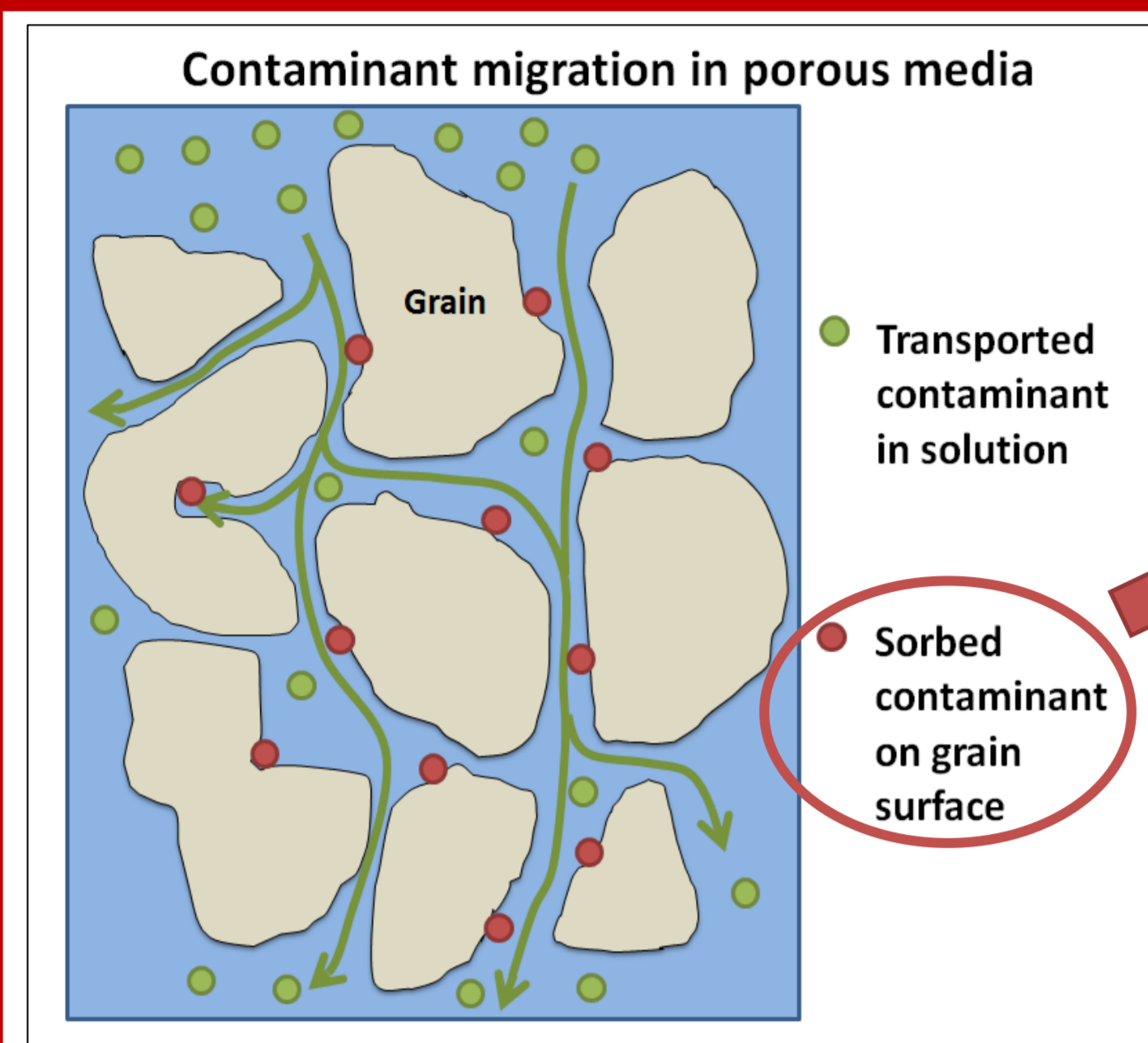
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Context & objectives

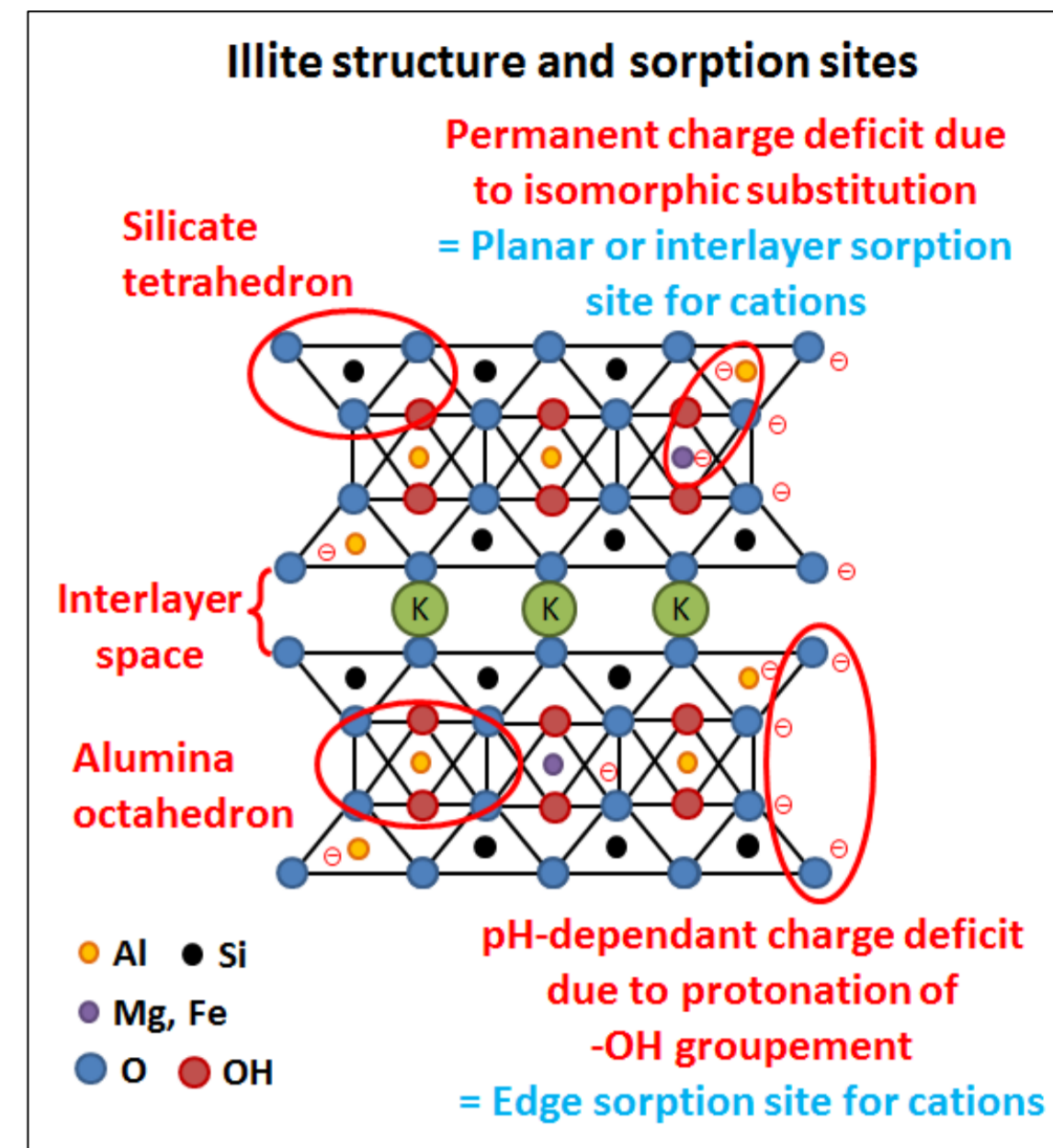


To ensure the environmental monitoring of nuclear sites, **sorption models** enabling the prediction of **contaminant migration** in soils and aquifers need to be developed.

Recently, a **multi-site ion exchanger model** based on the **Multi-site Ion Exchanger Theory**^[1] has **successfully** been applied to evaluate the **sorption** of a **contaminant** in a **natural soil** under **static** and **dynamic conditions**^[2,3].

Need of a **database** containing **sorption properties** of **pure minerals** present in the studied environment

Lack of Ca and Sr sorption data onto illite

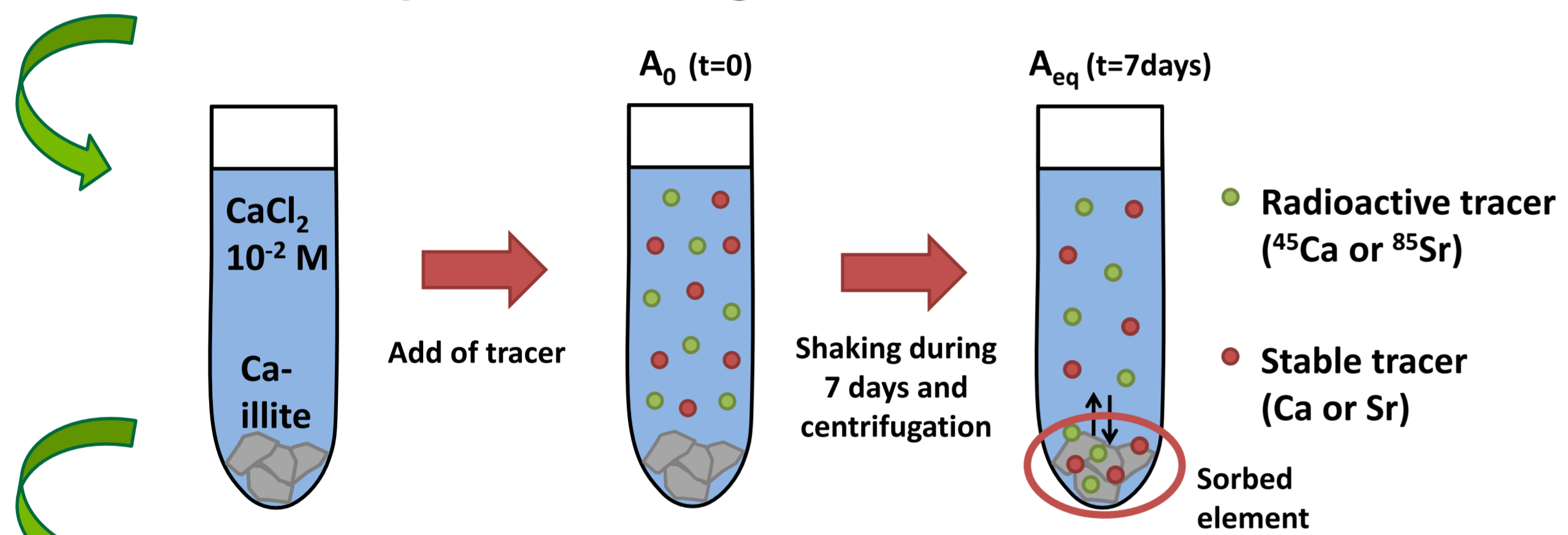


Methodology & results

Acquisition of sorption data on pure minerals

Determination of selectivity coefficients

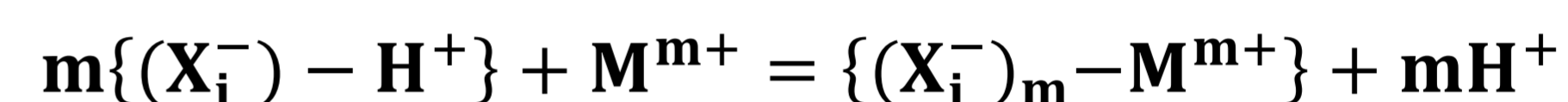
Batch experiments using radioactive tracers



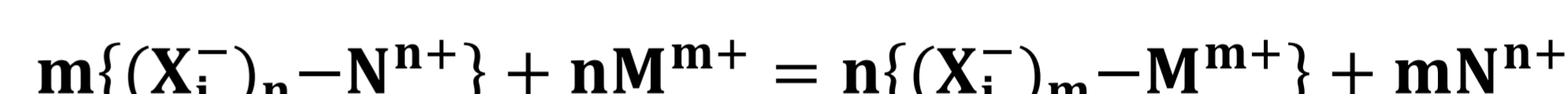
$$K_d = \frac{[M]_{\text{sorbed}}}{[M]_{\text{eq}}} = \left(\frac{A_0}{A_{\text{eq}}} - 1 \right) \cdot \frac{V_{\text{solution}}}{m_{\text{solid}}}$$

Multi-site Ion Exchanger Theory^[1]

Ion exchange equation on a X_i site between major cation M^{m+} and H⁺:



Ion exchange equation on a X_i site between major cation M^{m+} and trace element Nⁿ⁺:



Selectivity coefficients :

Components of the database

$$K_{mH^+/M^{m+}}^{*i} = \frac{[(X_i^-)_m - M^{m+}](H^+)^m}{[(X_i^-) - H^+]^m (M^{m+})}$$

$$K_{mN^{n+}/nM^{m+}}^{*i} = \frac{[(X_i^-)_m - M^{m+}]^n (N^{n+})^m}{[(X_i^-)_n - N^{n+}]^m (M^{m+})^n}$$

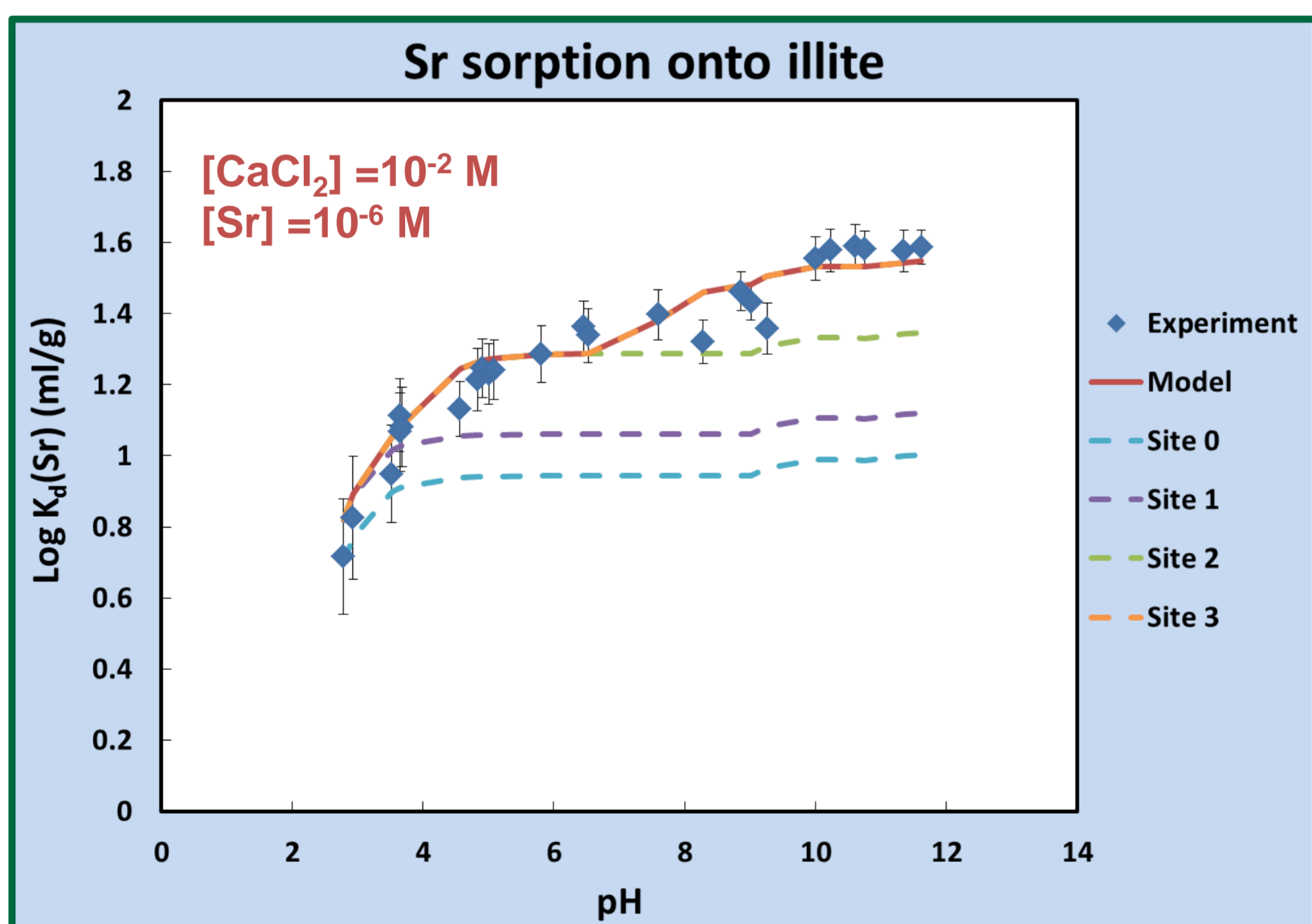
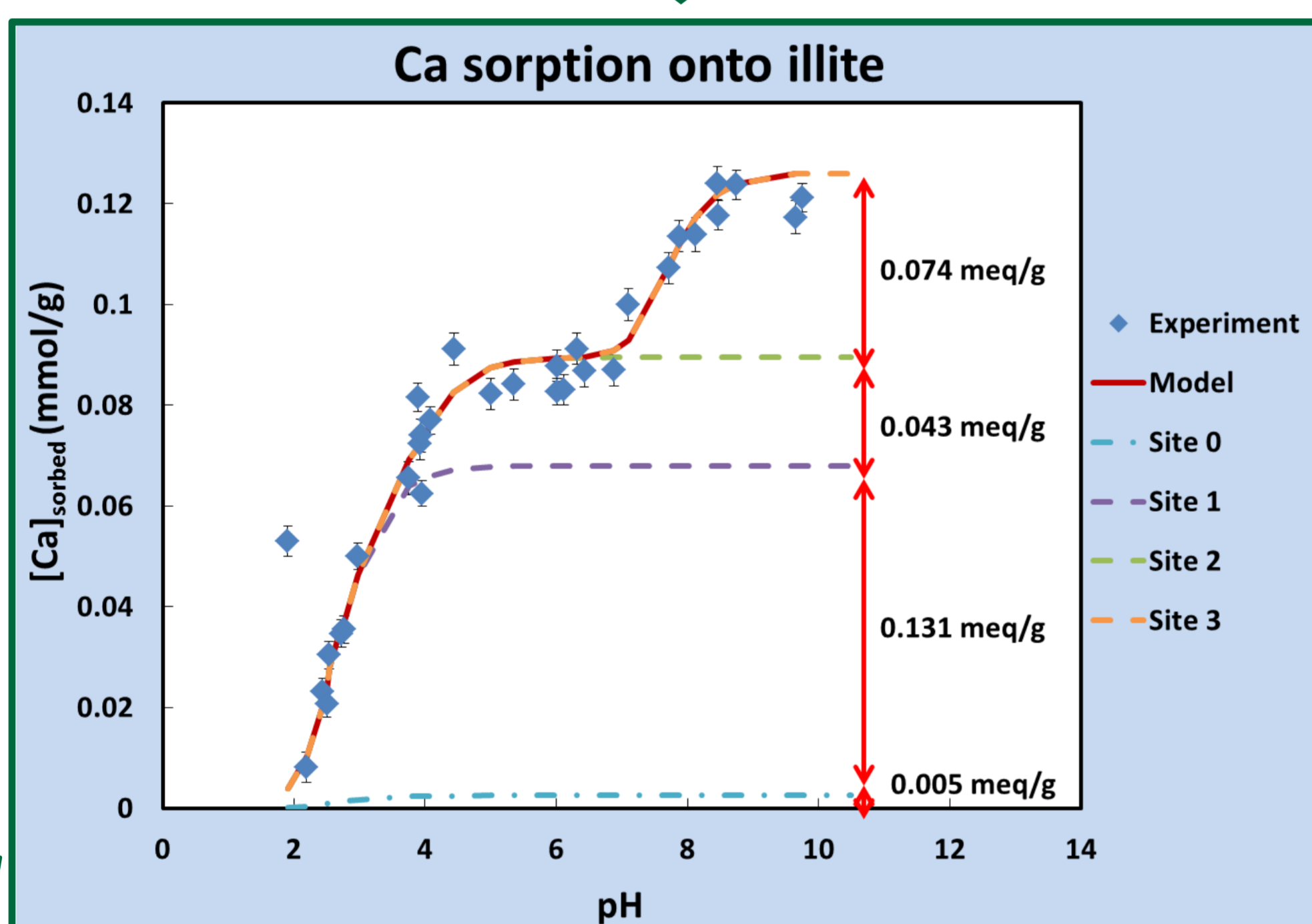
$$K_d = \frac{\sum_i [(X_i^-)_m - M^{m+}]}{[M^{m+}]}$$

Site saturation over pH

Identification of 4 site concentrations

Acquisition of selectivity coefficients K_{H⁺/Ca²⁺}^{*i}

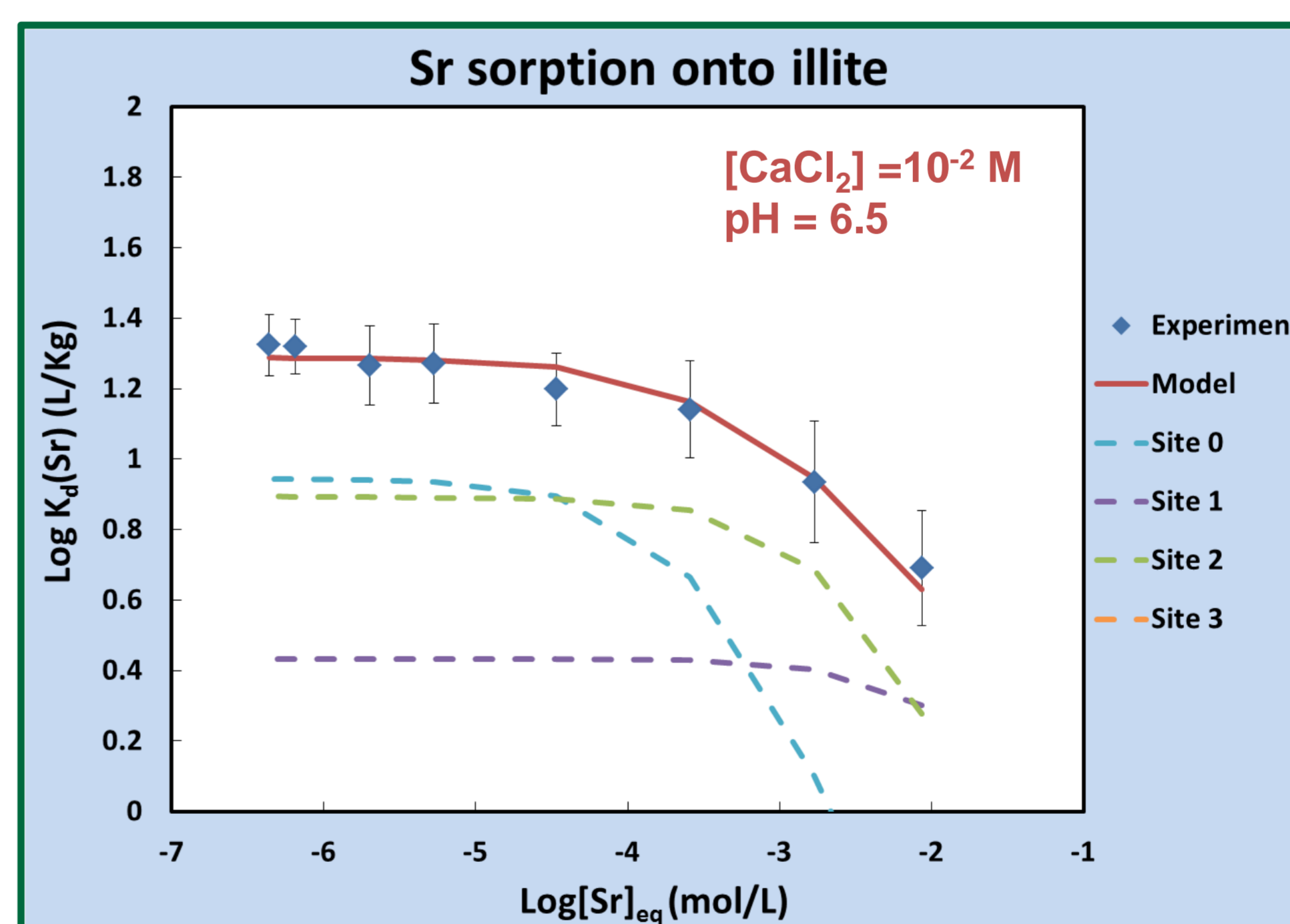
Sorption site	Concentration (mol/kg of dry solid) [4]	Log K _{H⁺/Ca²⁺} ^{*i}	Log K _{H⁺/Sr²⁺} ^{*i}
Site 0	0.005	-0.80 ± 0.19	0.74 ± 0.20
Site 1	0.131 ^[4]	-2.21 ± 0.08	-2.60 ± 0.80
Site 2	0.043 ^[4]	-4.54 ± 0.23	-3.97 ± 0.16
Site 3	0.074 ^[4]	-12.01 ± 0.20	-11.53 ± 0.12



K_d ↑ over pH

Fitting with the 4 sites previously identified

Acquisition of selectivity coefficients K_{H⁺/Sr²⁺}^{*i}



K_d ↓ over Sr concentration

Higher sorption at low Sr concentration

Acquisition of selectivity coefficients K_{H⁺/Sr²⁺}^{*i}

Conclusions & perspectives

Conclusion :

- ✓ Acquisition of **Ca** and **Sr** sorption data in a CaCl₂ background solution on a conditioned **Ca-illite** under static conditions
- ✓ Sorption data **well reproduced** by the **Multi-site Ion Exchanger Theory**^[1] considering **4 types of sites** and their concentrations
- ✓ Determination of **selectivity coefficients** between cations **Ca²⁺**, **Sr²⁺** and **H⁺**

Perspectives :

- **Selectivity coefficients** obtained has been used under static and dynamic conditions to model **Ca** or **Sr** sorption on complex solids composed in part of **illite**
- Same methodology will be used to model **Cs** sorption on complex solids composed in part of **illite** under static and dynamic conditions

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[4] Gorgeon L. Contribution à la modélisation physico-chimique de la rétention de radioéléments à vie longue par des matériaux argileux. Thèse de doctorat, Université Pierre et Marie Curie (Paris VI), Paris, 1994.