

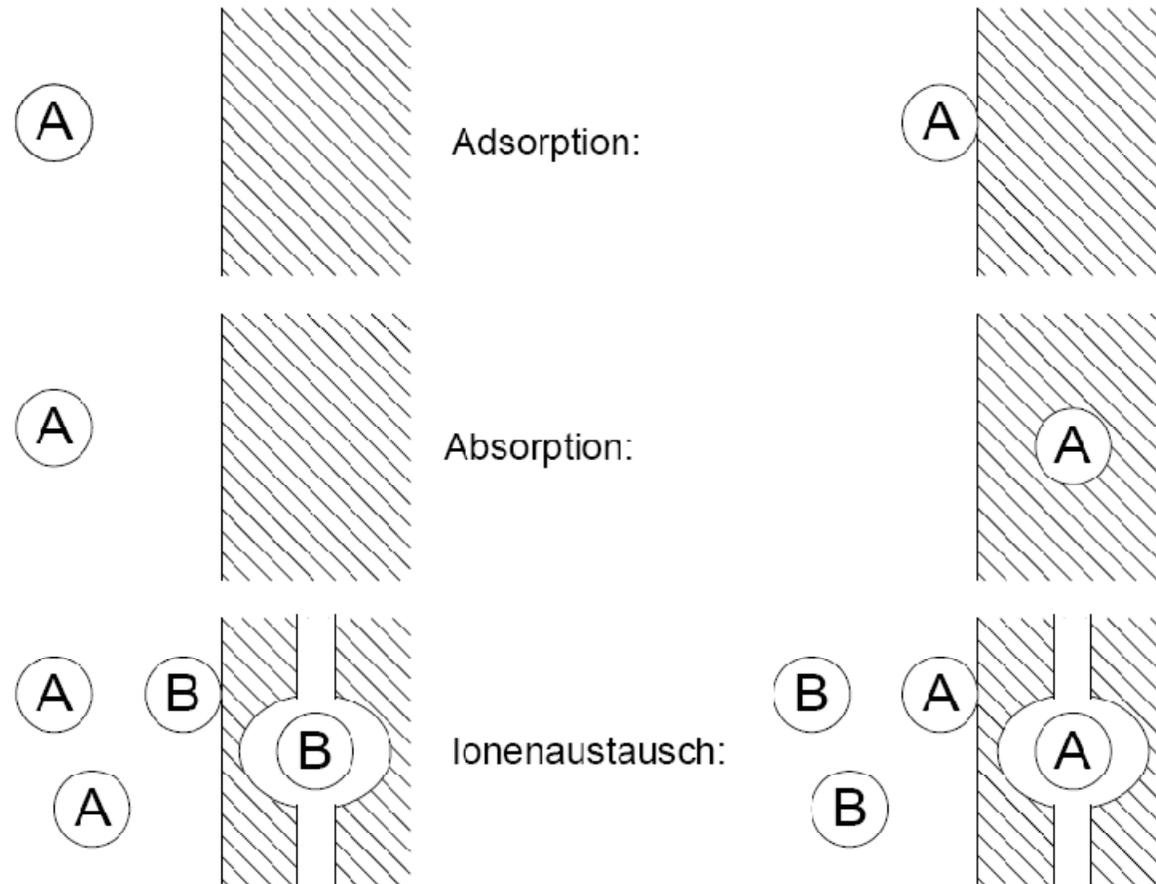
Figure 2.9. Concentrations of different solutions in terrestrial waters in the USA displayed in a frequency plot (Davies and De Wiest, 1966). Reprinted by permission of John Wiley & Sons, Inc.

Appelo C.A.J. & Postma D. (1996) Geochemistry, groundwater and pollution. Balkema, 536 p.

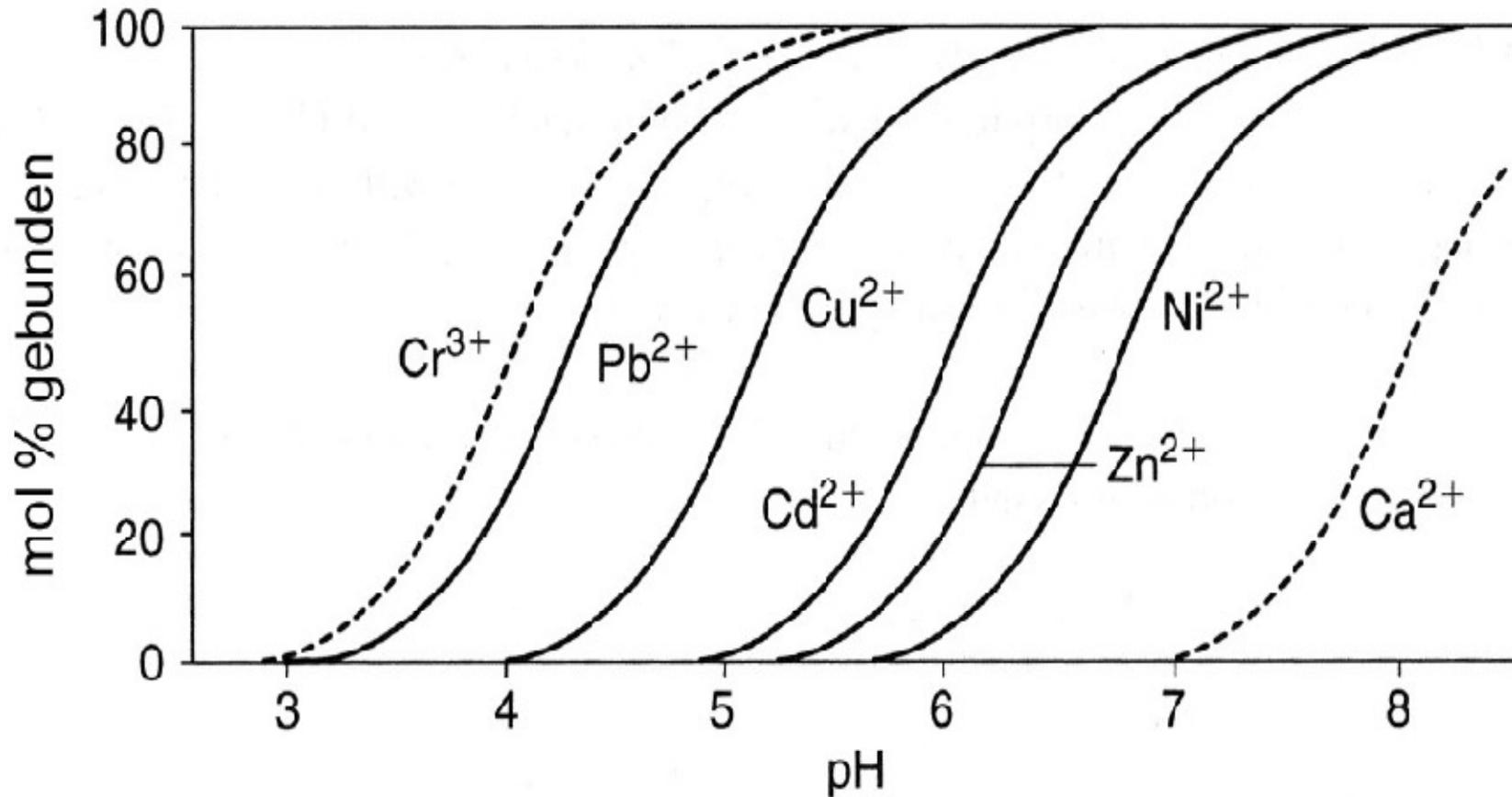
Sorption – Bindung von Stoffen an die Aquifermatrix

- Reversibel
- Irreversibel

Austausch
- spezifische
Adsorption



Bindungsstärke und pH-Abhängigkeit



Empirische Beschreibung der Sorption

Sorptionsisothermen

Lineare Regressions-Iso

$$C^* = K_d \cdot C$$

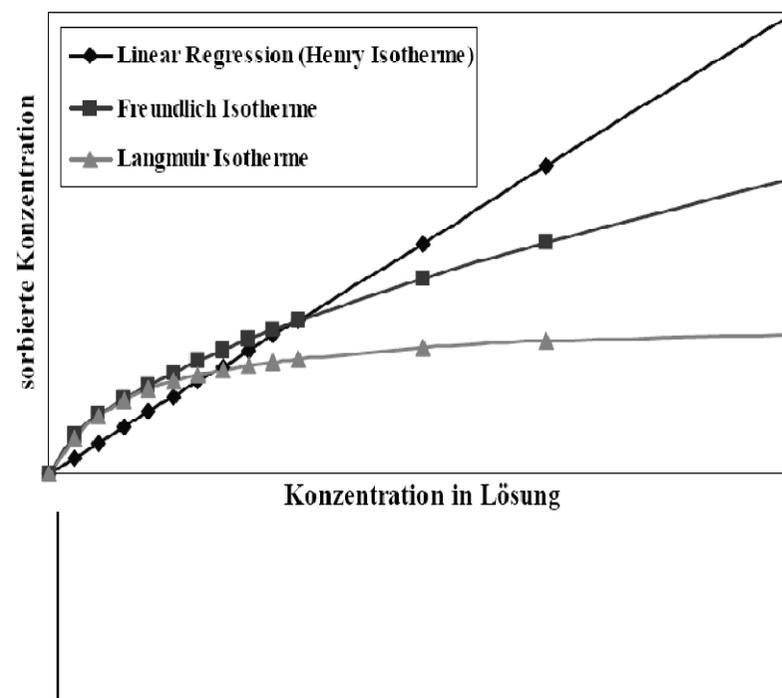
Freundlich Isotherme

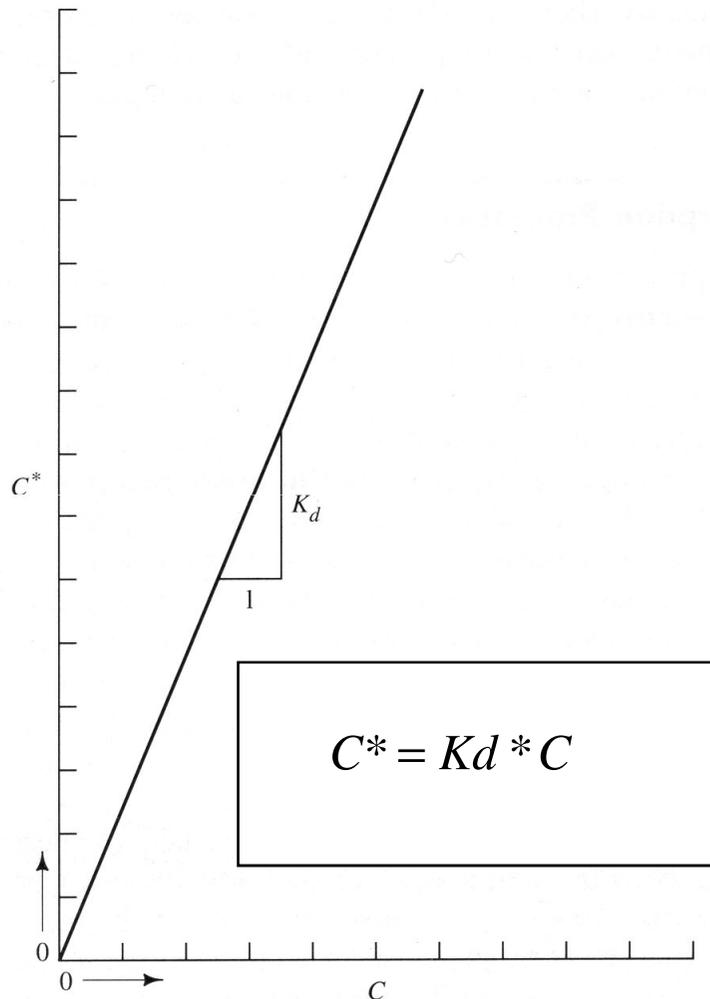
$$C^* = K_d \cdot C^n$$

Langmuir Isotherme

$$C^* = \frac{a \cdot b \cdot C}{1 + a \cdot C}$$

C=Konz. Lösung
C*=Konz. Feststoff
K_d=Gleichgewichts-
konstante
a,b Konstanten





Linear sorption isotherm with C^* versus C plotting as a straight line.

Verteilungskoeffizient = Steigung der linearen Sorptionsisotherme (Henry)

- C^* : Masse der am Mineral sorbierten Substanz (mg/kg)
 C : Konzentration der Substanz im Wasser (mg/L)
 K_d : Verteilungskoeffizient (L/kg)

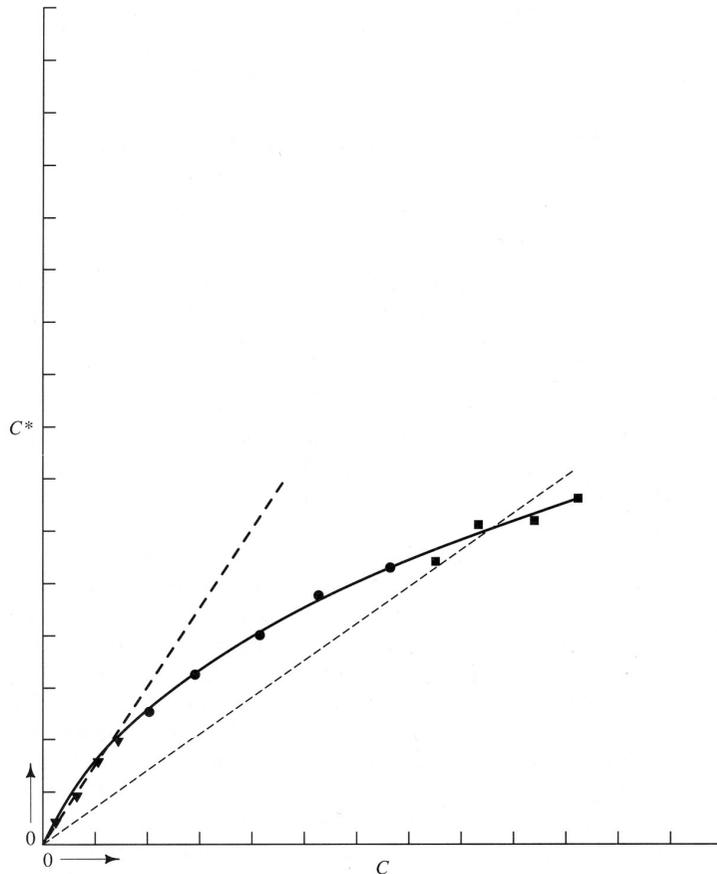
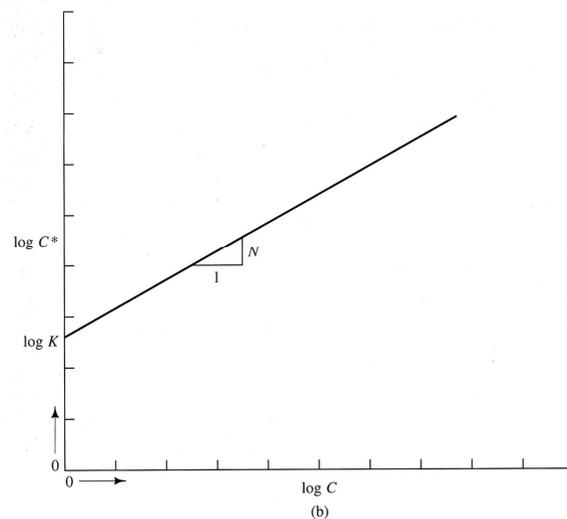
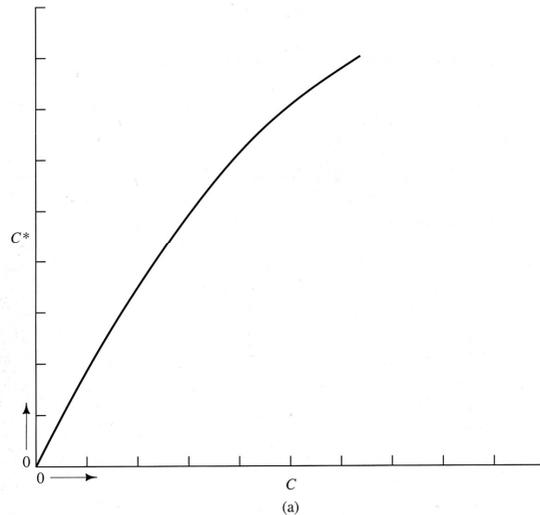


FIGURE 3.3 Nonlinear sorption isotherms can be misinterpreted as linear sorption isotherms if a small data set is extrapolated out of its range. The subset of the data represented by triangles can be interpreted as a linear sorption isotherm, as can the data subset consisting of squares. However, if the complete data set, which includes the triangles, circles, and squares, is used, it can be seen that the isotherm is nonlinear.

Nichtlineare Sorptionsisotherme

- C^* : Masse der am Mineral sorbierten Substanz (mg/kg)
- C : Konzentration der Substanz im Wasser (mg/L)

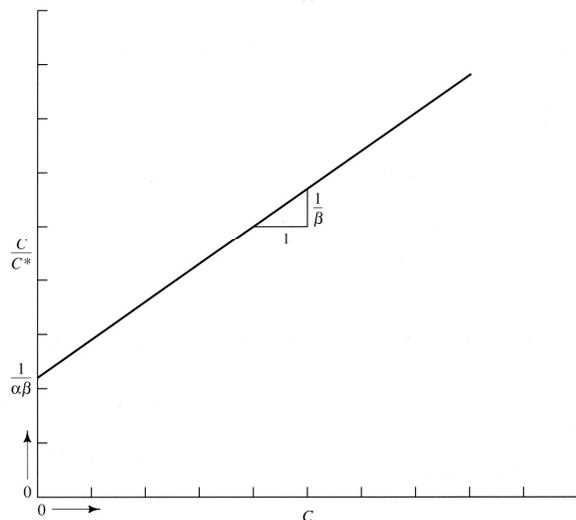
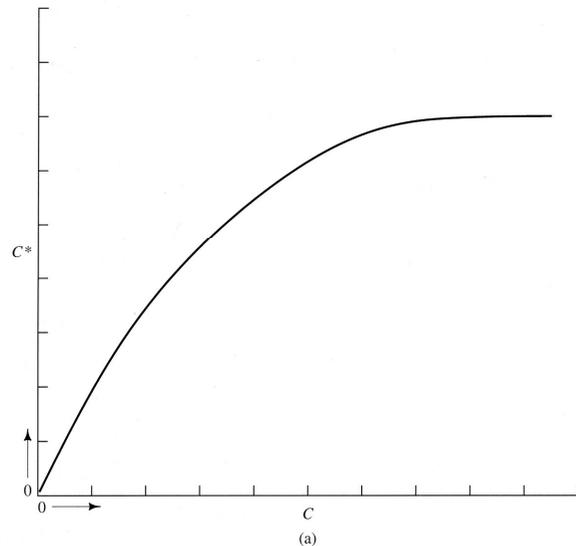
Freundlich Sorptionsisotherme



- C^* : Masse der am Mineral sorbierten Substanz (mg/kg)
 C : Konzentration der Substanz im Wasser (mg/L)
 K_d : Verteilungskoeffizient (L/kg)

$$C^* = K_d * C^n$$

Langmuir Sorptionsisotherme



- C^* : Masse der am Mineral sorbierten Substanz (mg/kg)
- C : Konzentration der Substanz im Wasser (mg/L)
- a, b : Konstanten

$$C^* = \frac{a * b * C}{1 + a * C}$$

Langmuir-Isotherme

Bei der Langmuir-Isotherme erreicht der Sorptionsprozess einen Grenzwert:

$$C_s = \frac{a \cdot b \cdot C_w}{1 + a \cdot C_w}$$

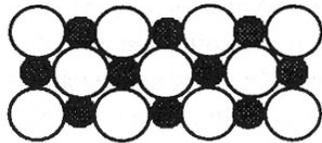
- a : Sorptions-Konstante als Funktion der Bindungsenergie (L/mg) b
: maximal sorbierbare Masse der Substanz
C_s : Masse der am Mineral sorbierten Substanz (mg/kg)
C_w : Konzentration der Substanz im Wasser (mg/L)

$$R_f = 1 + \frac{Bd}{q} \cdot \left[\frac{a \cdot b}{(1 + a \cdot C_w)^2} \right]$$

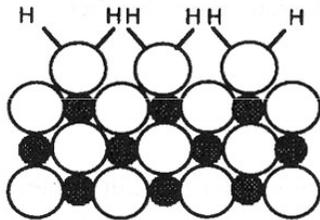
- R_f : Retardationsfaktor
B_d : Feststoffdichte
q : Wassergehalt

Oberflächenkomplexierung

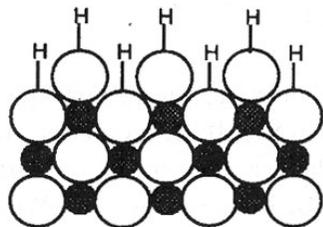
Original-Oberfläche - Metalle
mit unvollständiger Koordination



Koordinations-Sphäre vervollständigt durch Wassermoleküle

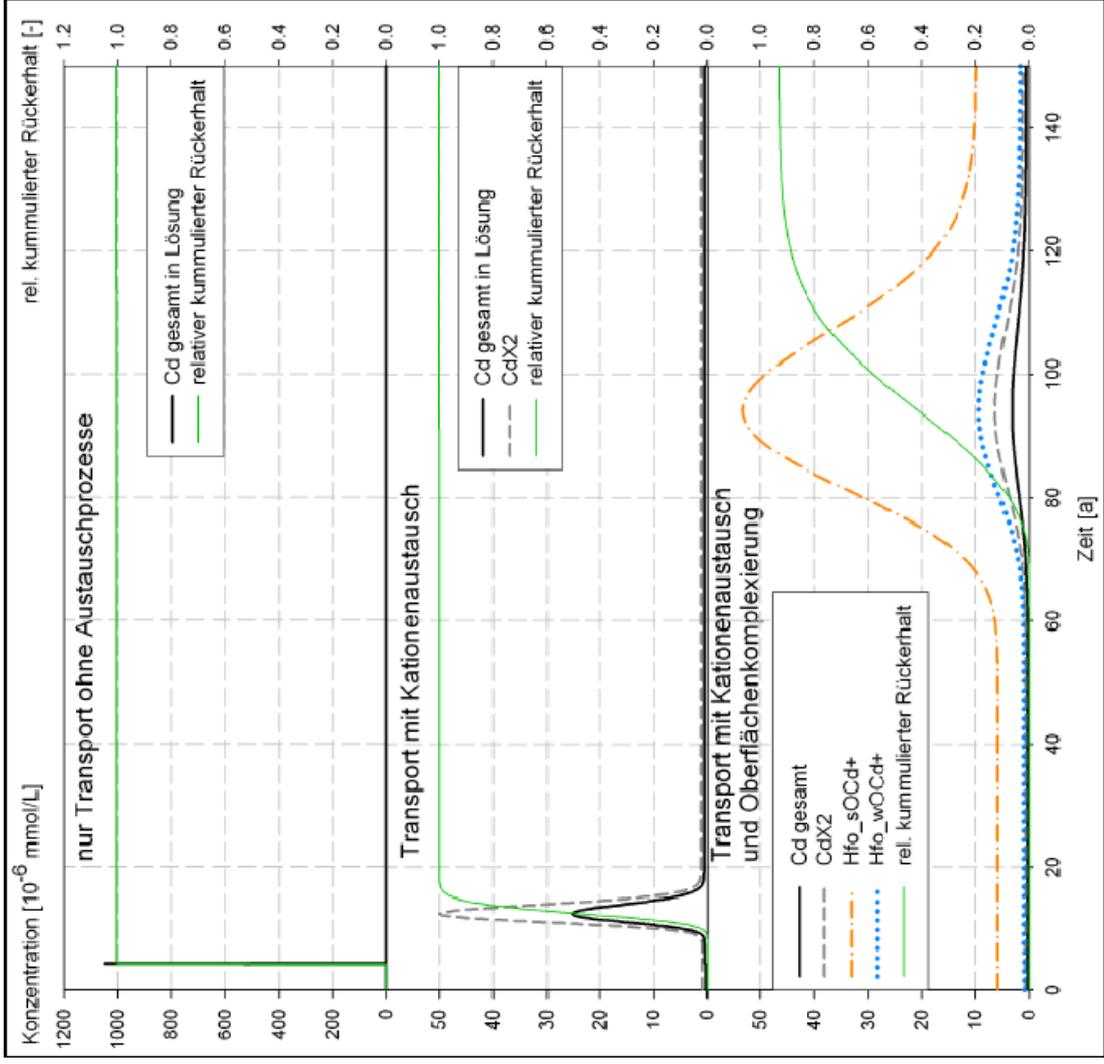


Protonen-Neuordnung zur Bildung
von Oberflächen-Hydroxyl-Gruppen



● Metallion ○ Sauerstoff

Abb. 13 Prozeß der
Oberflächenkomplexierung
(nach Drever 1997)



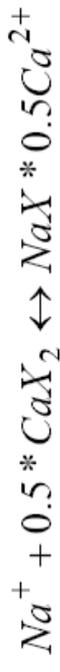


$$K_B^A = \frac{\{A^+ R^-\} * \{B^+\}}{\{A^+\} * \{B^+ R^-\}} = \frac{\{A^+ R^-\} / \{A^+\}}{\{B^+ R^-\} / \{B^+\}}$$

With A⁺, B⁺ = monovalent ions

R = exchanger

K_x = selectivity coefficient



$$K_{Ca}^{Na} = \frac{\{NaX\} * \{Ca^{2+}\}^{0.5}}{\{CaX_2\} * \{Na^+\}}$$

With X= exchanger

K_x = selectivity coefficient