SolEq

Software and tutorials to study

Solution Equilibria:

-- Principles and Applications --

Poster presented at the
IUPAC Congress/General Assembly
July 2001

Summary

Created through

a joint venture by:

•IUPAC Comm. V.5

•Academic Software

Demonstrates applications in:

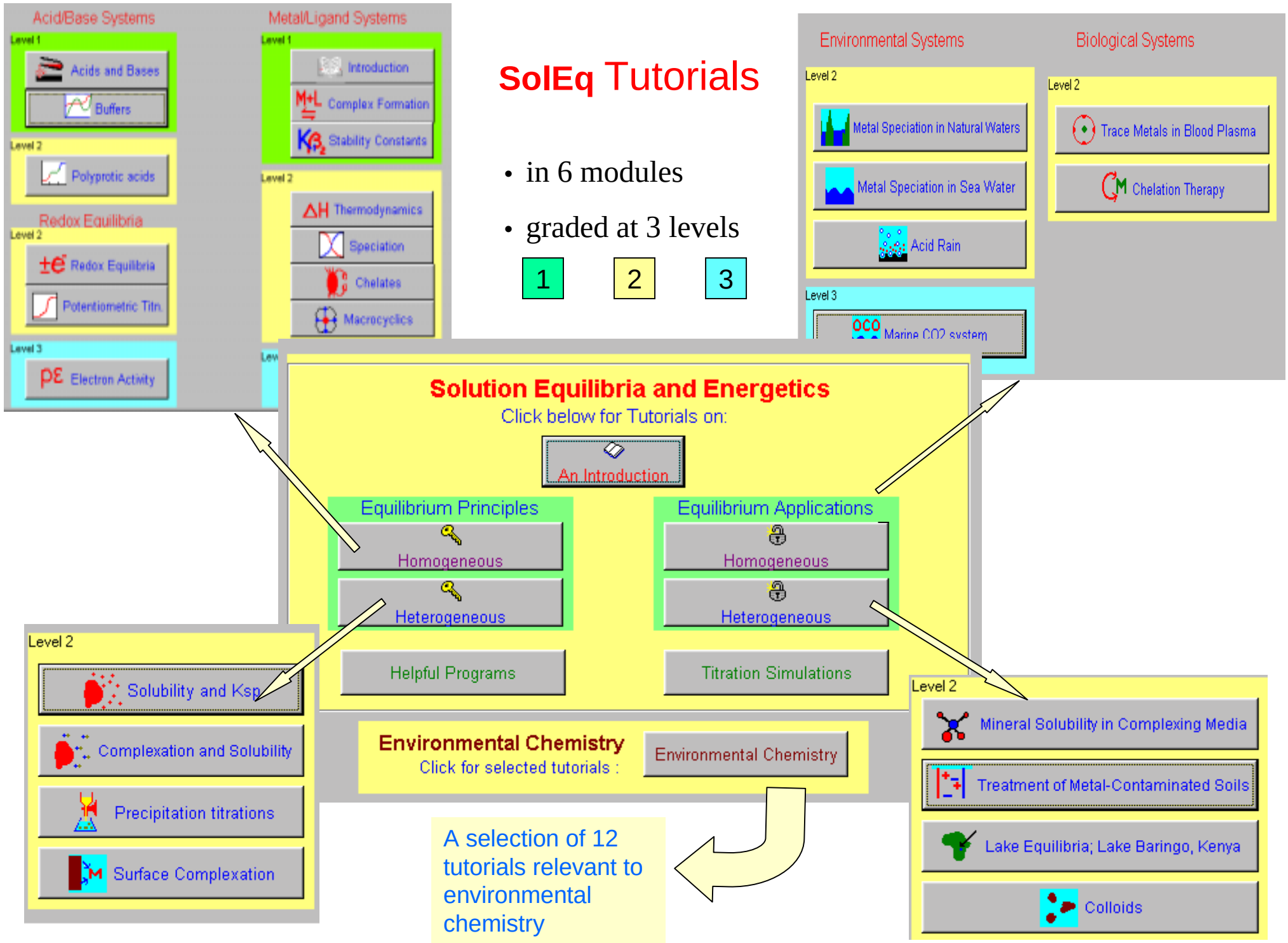
- Environmental chemistry
- Medicinal chemistry
- Industrial chemistry
- Analysis

Teaches principles of:

- Solution equilibria
- Redox reactions
- Complex formation
- Titrations
- Precipitation

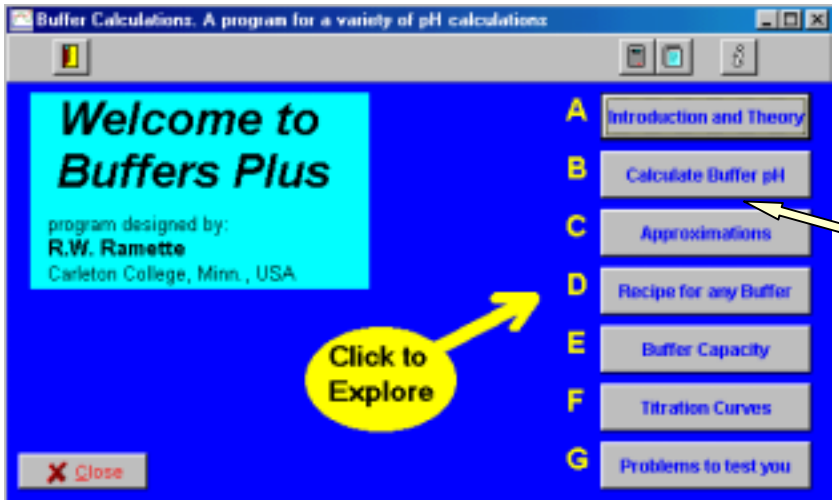
Features:

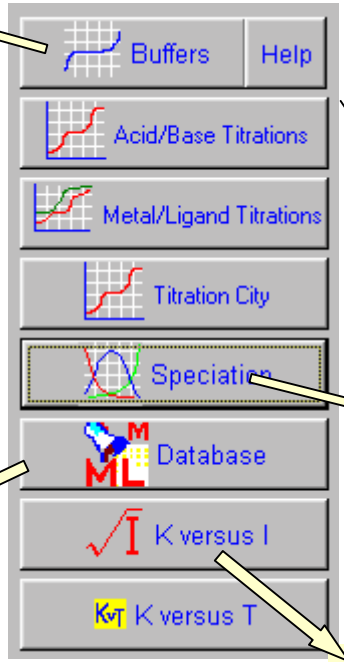
- Speciation software
- Buffer simulations
- Titration simulations
- Equilibrium database


Acid/Base Systems
Level 1
Acids and Bases
Buffers
Level 2
Polyprotic acids
Redox Equilibria
Level 2
Redox Equilibria
Potentiometric Titn.
Level 3
pε Electron Activity
Metal/Ligand Systems
Level 1
Introduction
M+L Complex Formation
Stability Constants
Level 2
ΔH Thermodynamics
Speciation
Chelates
Macrocyclics
SolEq Tutorials
• in 6 modules
• graded at 3 levels
1
2
3
Environmental Systems
Level 2
Metal Speciation in Natural Waters
Metal Speciation in Sea Water
Acid Rain
Level 3
Marine CO2 system
Biological Systems
Level 2
Trace Metals in Blood Plasma
Chelation Therapy
Solution Equilibria and Energetics
Click below for Tutorials on:
An Introduction
Equilibrium Principles
Homogeneous
Heterogeneous
Equilibrium Applications
Homogeneous
Heterogeneous
Helpful Programs
Titration Simulations
Level 2
Solubility and Ksp
Complexation and Solubility
Precipitation titrations
Surface Complexation
Environmental Chemistry
Click for selected tutorials :
Environmental Chemistry
A selection of 12 tutorials relevant to environmental chemistry
Level 2
Mineral Solubility in Complexing Media
Treatment of Metal-Contaminated Soils
Lake Equilibria; Lake Baringo, Kenya
Colloids

Helpful programs

Software to drive the tutorials and exercises - accessible interactively from all tutorials

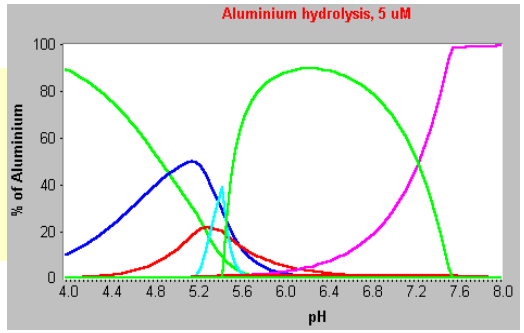




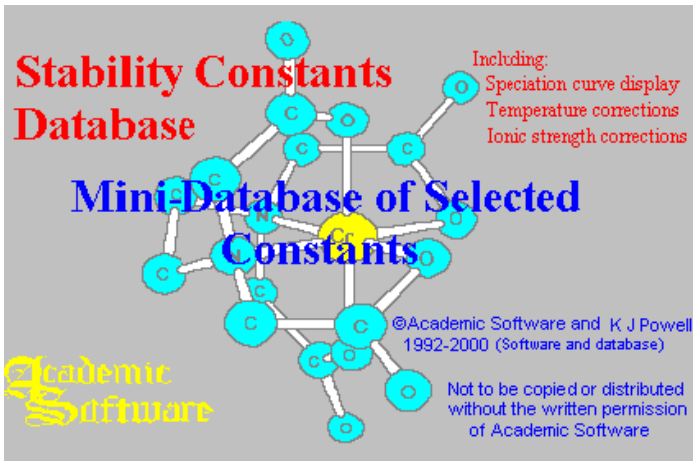
Simulate, in real-time:

- acid-base
- metal-ligand
- redox titrations

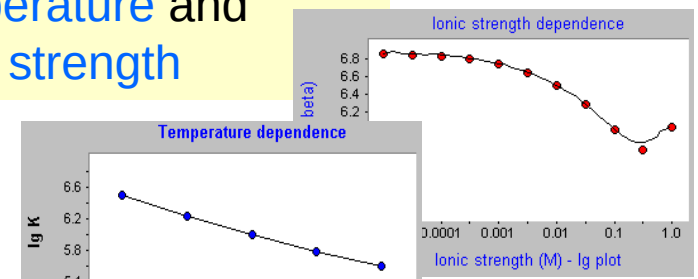
A powerful speciation package



A database of 18000 metal-ligand complex stability constants



To correct stability constants for temperature and ionic strength



Softbook Format

A typical page - from the tutorial '*Colloids*'

Toolbar links to database, speciation software

Hypertext link

- to explanation
- to diagram

Colloids

Colloid coagulation 1 | Colloid coagulation 2 | Colloid coagulation 3 | Colloid coagulation 4 | Cation hydrolysis | Bridging 1

Cation Hydrolysis

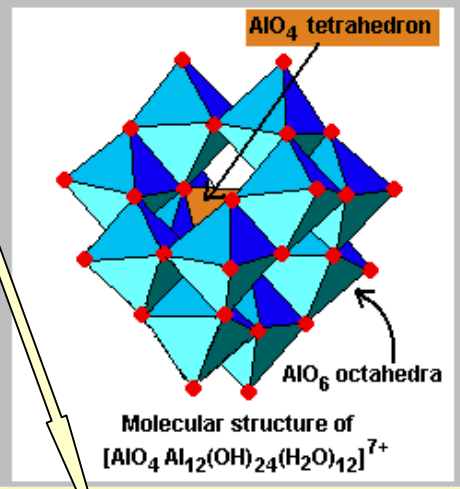
Significant hydrolysis occurs for metal ions of high charge. Trivalent ions have stepwise pK_a ($-\lg {}^*K_n$) values in the range 3-7. $Al(H_2O)_6^{3+}$ has **$-\lg {}^*K_n$ values** of 4.9, 5.5 and 6.7 (n = 1-3). Thus in weakly acidic dilute solution it exists as a mixture of weak conjugate acids and bases (see **speciation**).

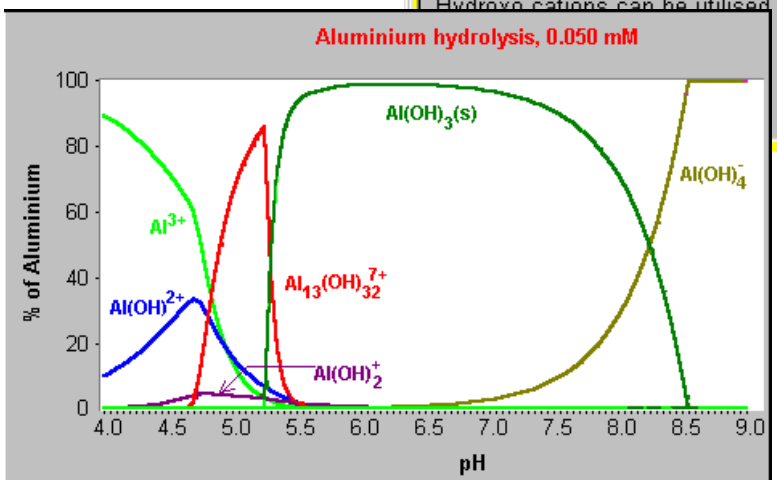
Polymeric ions form in more concentrated solution by sharing of -OH groups, *e.g.* :

$13Al(H_2O)_6^{3+} = Al_{13}O_4(OH)_{24}^{7+} + 32H_3O^+ + 18H_2O$.

The $Al_{13}O_4(OH)_{24}^{7+}$ polymer is well characterised. Its structure indicates a central AlO_4 tetrahedron, surrounded by AlO_6 octahedra that link by sharing of edges and vertices.

Hydroxo cations can be utilised to achieve coagulation





$^*K_1$	$Al(H_2O)_6^{3+} + H_2O = Al(OH)(H_2O)_5^{2+} + H_3O^+$	$-\lg {}^*K_1 = 4.9$
$^*K_2$	$Al(OH)(H_2O)_5^{3+} + H_2O = Al(OH)_2(H_2O)_4^+ + H_3O^+$	$-\lg {}^*K_2 = 5.5$
$^*K_3$	$Al(OH)_2(H_2O)_4^+ + H_2O = Al(OH)_3 + H_3O^+$	$-\lg {}^*K_3 = 6.7$

SolEq: built-in exercises

Selectivity

Title | Introduction | Overview | Class A/B 1 | Class A/B 2 | Soft-Soft 1 | Soft-Soft 2 | Hard-Hard | Energetics 1 | Energe

Class A – Class B classification 2

Donor preference for cations varies dramatically with cation position in the periodic table.

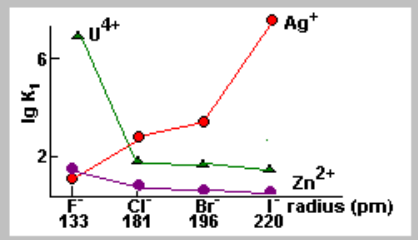
Class A: **Tendency to complex with hard metal ions**

N >> P > As > Sb
O >> S > Se > Te
F^- >> Cl^- > Br^- > I^-

Class B: **Tendency to complex with soft metal ions**

N << P > As > Sb
O << S < Se ≈ Te
F^- < Cl^- < Br^- << I^-

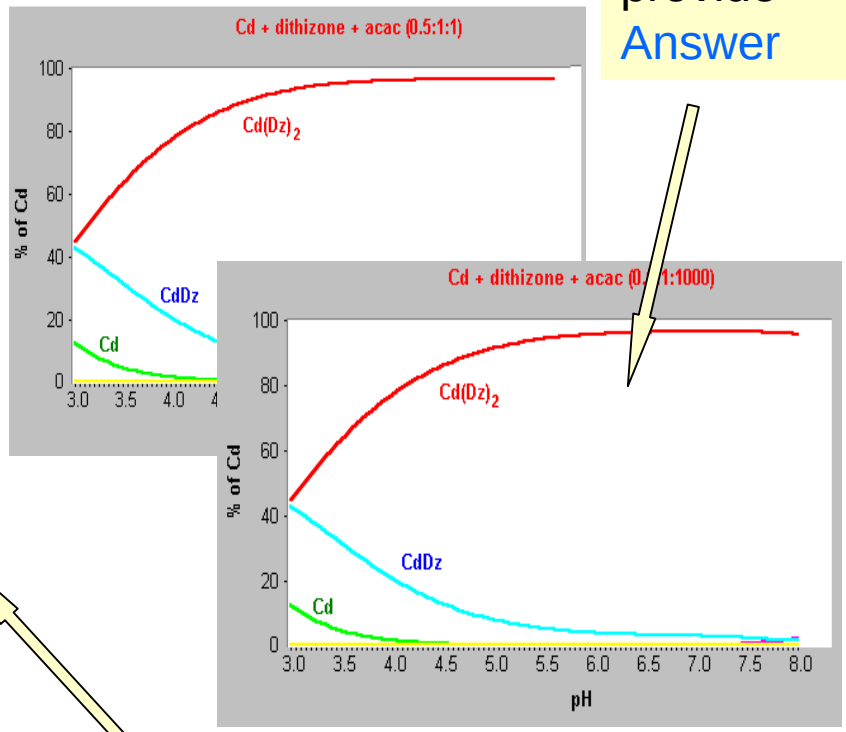
The combination of ligand and cation can be **highly selective**. The figure illustrates distinctive Class A character (U^{4+}) and Class B character (Ag^+) toward the halide ligands. Zn^{2+} represents a Borderline (transition) case.



Exercise

The 'softness' or 'hardness' of a donor atom may **vary** according to its bonding within the ligand.

Computed curves provide Answer



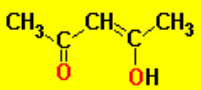
Click here to reveal the Exercise

Exercise:

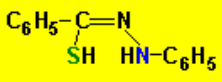
The strong preference of a Hard (or Soft) metal ion for a Hard (or Soft) donor can be illustrated by calculating the distribution of the ion between two dissimilar competing ligands.

Use *Species* to calculate the distribution of Cd^{2+} between the 'hard' O-donor ligand acetylacetone (penta-2,4-dione, acac) and the 'soft' S-donor, dithizone. Input data are in the file *Cd_Dz.spc*. Vary the [acac] by a factor of 1000 to see what effect that has on the calculated distribution.

Deduce from this result whether Cd^{2+} is showing Class A or Class B behaviour.



Acetylacetone



Dithizone

Access SPECIES file and software via toolbar icon

Titration simulations

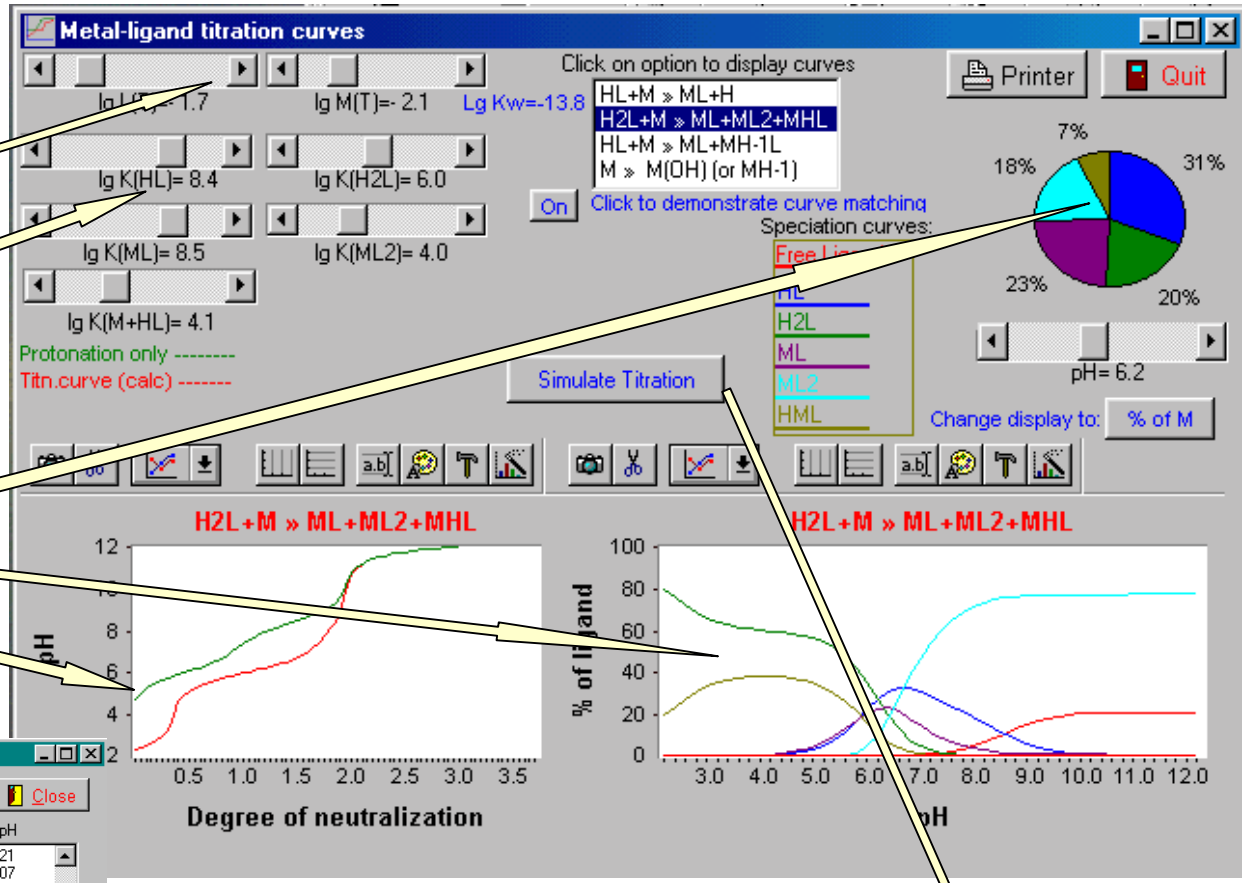
All parameters can be varied.

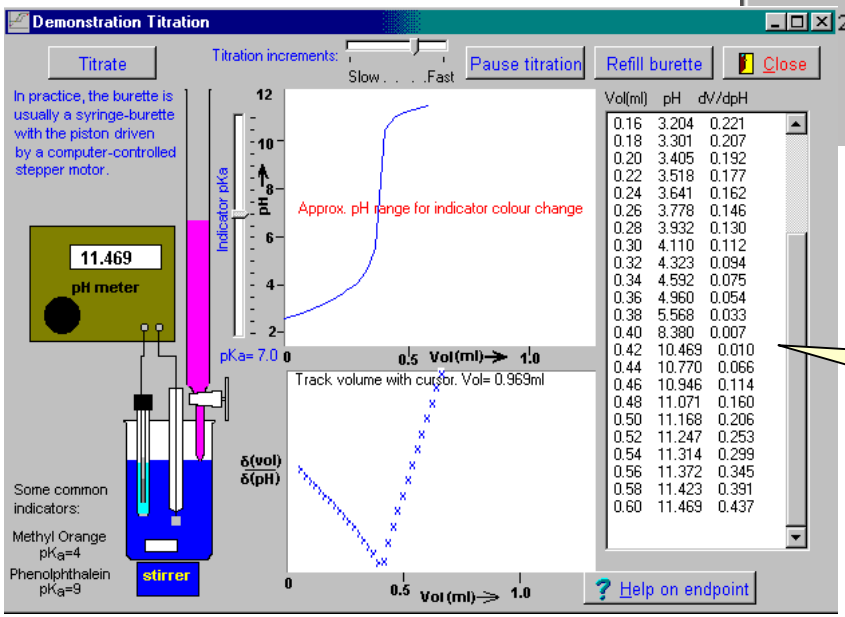
Curves re-drawn in real time.

Vary any concentration

Vary any constant

- Speciation as a pie-chart
- Speciation curves
- Titration curves





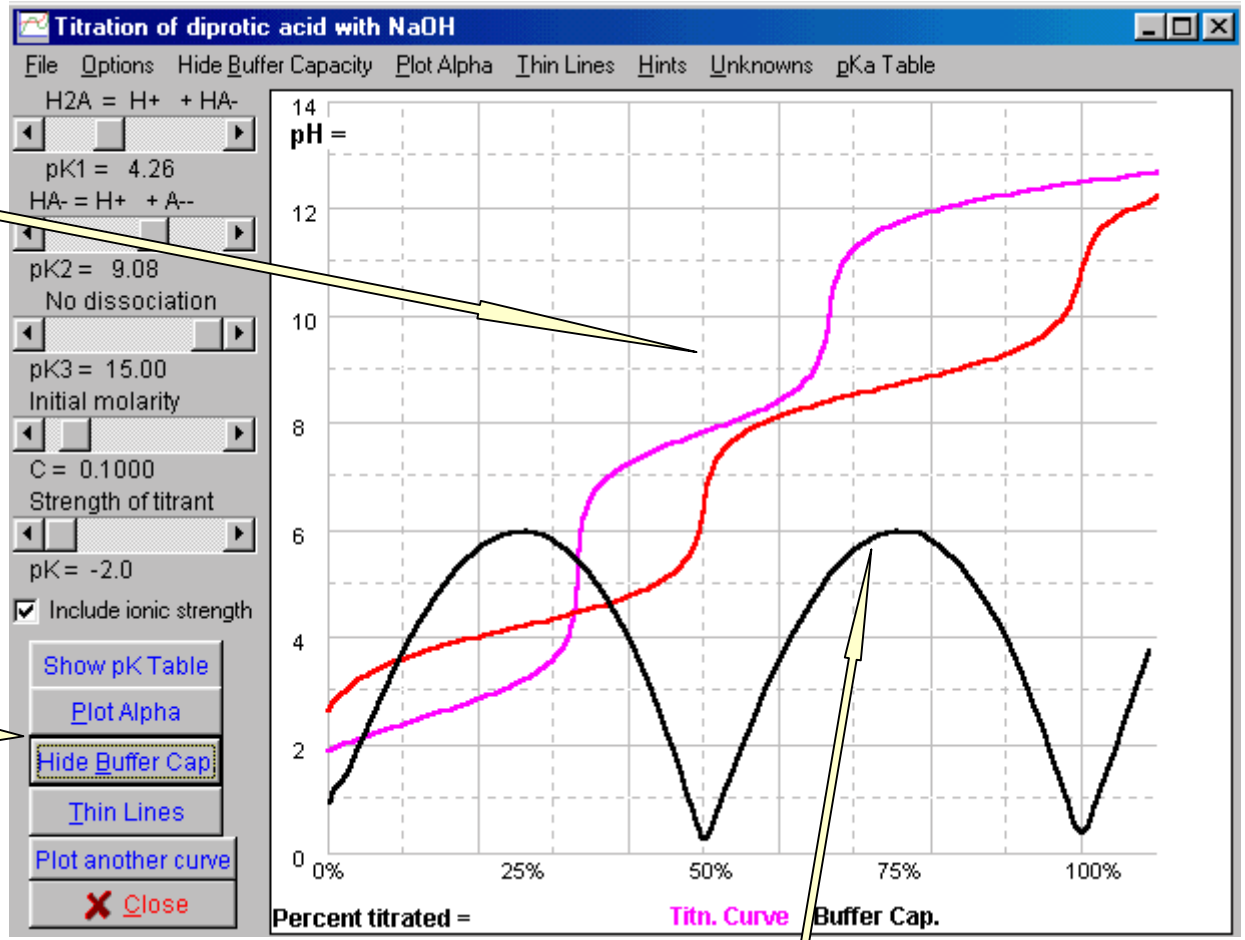
Real-time titration simulation with end-point calculation

Lecture demonstrations

Vary acid-base systems in real-time:

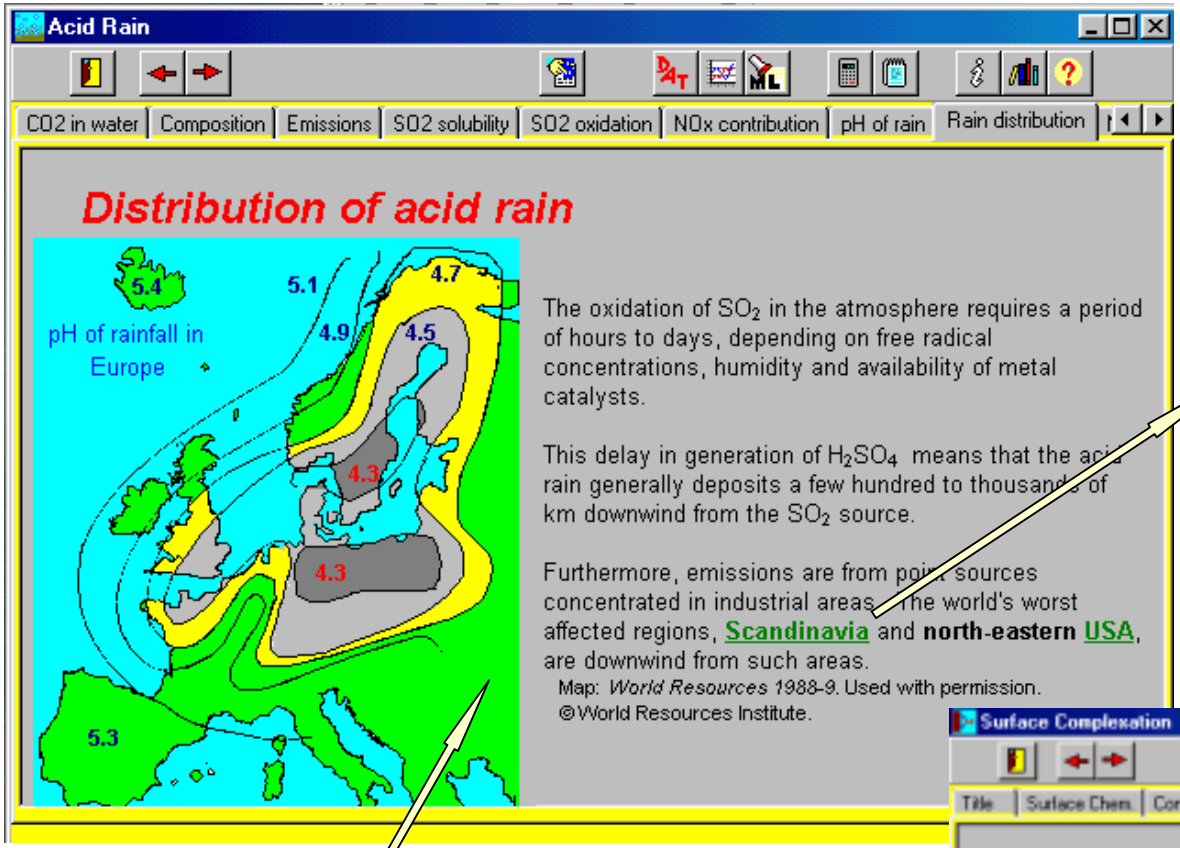
Plot multiple curves, each with different pK values

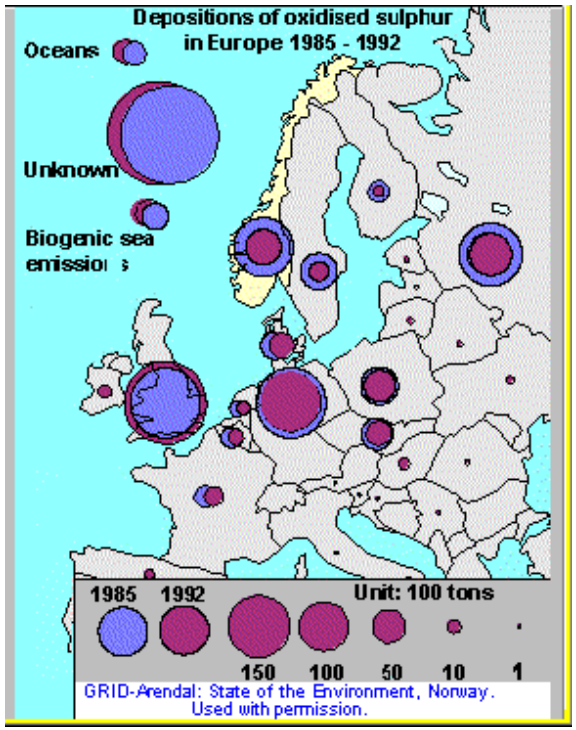
Show buffer capacity and α plots



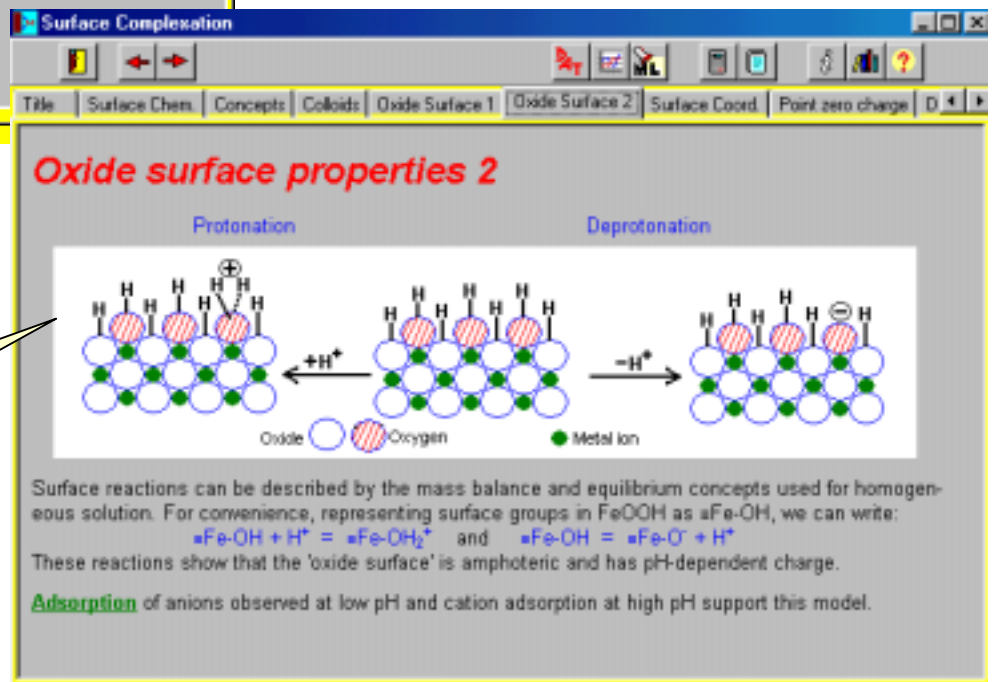
Show how to generate high buffer capacity at a specified pH

Environmental Chemistry





A page from: *Acid Rain*



A page from: *Surface complexation*

SolEq: A unique, interactive learning method

- A first in Chemistry
- A first in Solution Equilibria
- A first in Environmental Chemistry

A joint venture project:

- Project partners: Academic Software and IUPAC
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- Principal programmer: L.D. Pettit Lesp@acadsoft.co.uk
- Marketing: by Academic Software www.acadsoft.co.uk

For demonstration downloads: http://www.acadsoft.co.uk