Department of Chemistry
Chair of Instrumental Analytical Chemistry

UNIVERSITÄT DUISBURG ESSEN

Water Chemistry: Intro

Your Lecturer: Prof. Dr. Torsten C. Schmidt

- Diploma, Chemistry, 1994
  PhD, Analytical Chemistry, 1997
  (+ law studies 1994-1997)

- Postdoc Environmental Chemistry
  1998-2002

- Group Leader Environmental
  Chemistry and Analysis
  2002-2006

- Chair of Instrumental Analysis
  since 01.02.2006

- Scientific Director for Water
  Chemistry, IWW since 01.12.2006

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EBERHARD KARLS UNIVERSITÄT TÜBINGEN

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IWW

http://www.uni-duisburg-essen.de/iac

Your Assistant: Dirk Steinmann

PhD Student - University Duisburg-Essen - Germany

UNIVERSITÄT DUISBURG ESSEN

Since 2007	**PhD** **Instrumental Analytical Chemistry** **University of Duisburg-Essen**
PhD Thesis	*"Coupling of HT-HPLC/IRMS"* University of Duisburg-Essen
2005 – 2007	**MSc in Water Science** **University of Duisburg-Essen**
Master Thesis (2007)	*" Construction of an Interface for HPLC/FID"* University of Duisburg-Essen
2002 – 2005	**BSc in Water Science** **University of Duisburg-Essen**
Bachelor Thesis (2005)	*" Biofilm monitoring in soils using BIOX"* *CESI & University of Bicocca, Milan (Italy)*

Contact: dirk.steinmann@uni-due.de

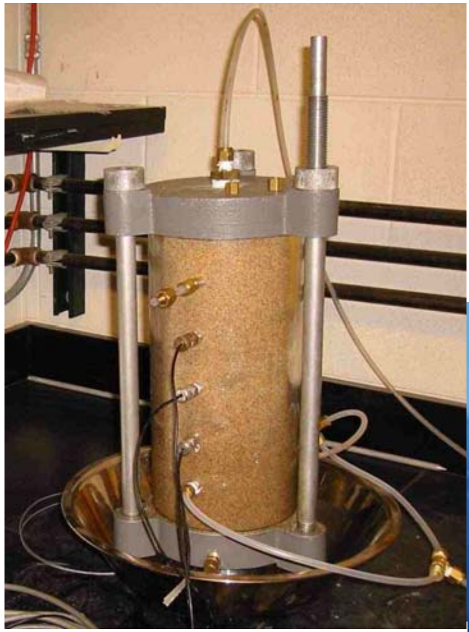
Your Assistants: Alexandra Jarocki

PhD Student - University Duisburg-Essen - Germany

Since 2007	**PhD** **Instrumental Analytical Chemistry** **University of Duisburg-Essen**
PhD Thesis	*“Die Fenton Reaktion (Fe^{2+} + H_2O_2): Unter welchen Bedingungen entstehen OH Radikale und/oder Fe(IV)”* *University of Duisburg-Essen*
2005 – 2007	**MSc in Water Science** **University of Duisburg-Essen**
Master Thesis (2007)	*“ OH-Radical Production in the Peroxone Process – Competition Studies”* *University of Duisburg-Essen*
2002 – 2005	**BSc in Water Science** **University of Duisburg-Essen**
Bachelor Thesis (2005)	*“Erarbeitung eines Analyseverfahrens zur Bestimmung von Nitrosaminen in Wässern unterschiedlicher Matrices”* *IWW Mülheim*

Contact: alexandra.jarocki@uni-due.de

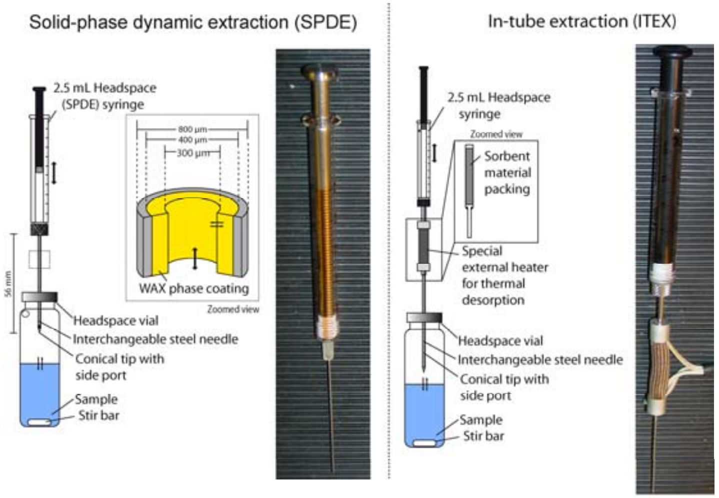
Fields of Research



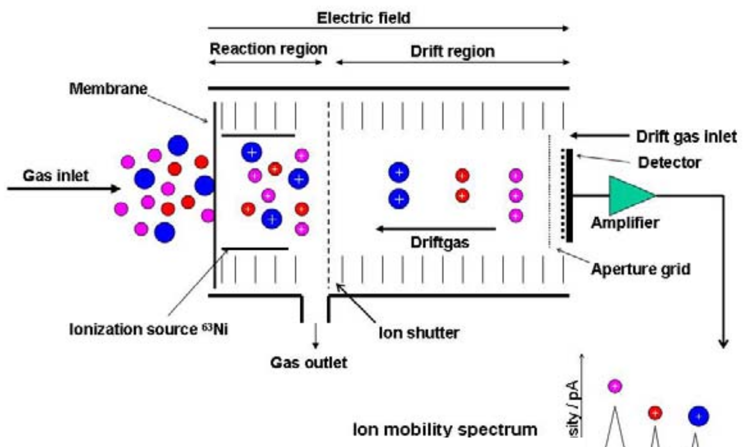
Analytical Methods

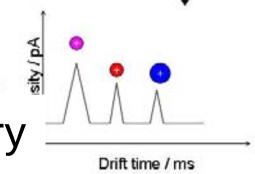
Processes

Fields of Research: Analytical Chemistry

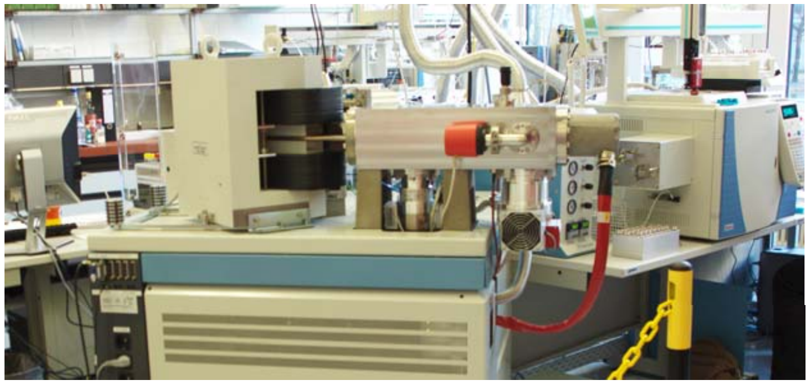


Microextraction Techniques
Dr. Maik Jochmann

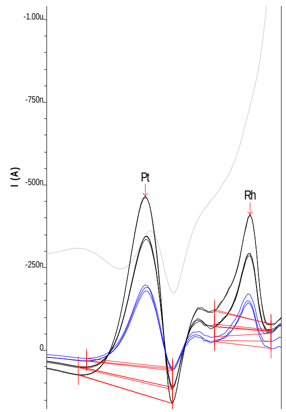


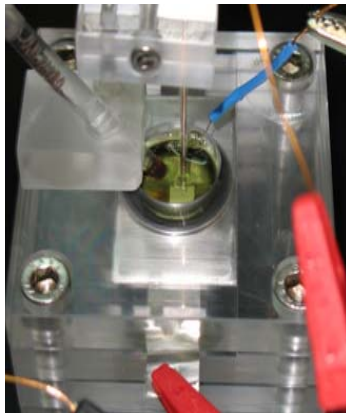


Ion Mobility Spectrometry
PD Dr. Ursula Telgheder



Stable Isotope Analysis
Dr. Maik Jochmann



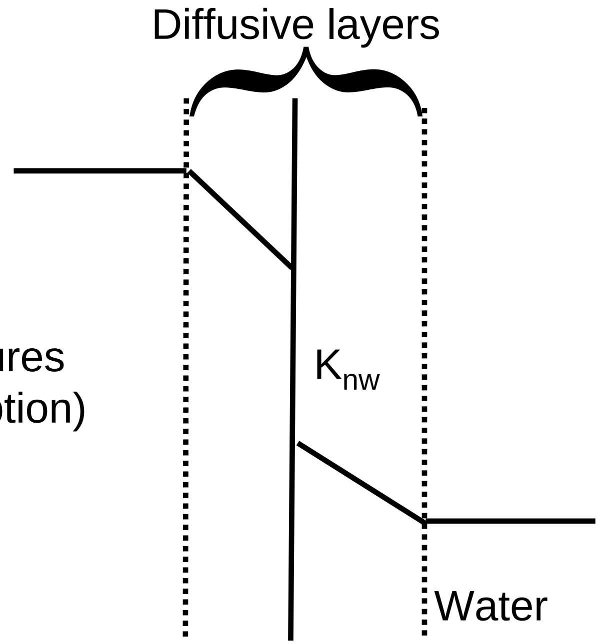


Electroanalysis/ -chemistry
Dr. Holger Krohn
Dr. Bernd Wermeckes

Fields of Research: Process-Oriented Environmental Chemistry

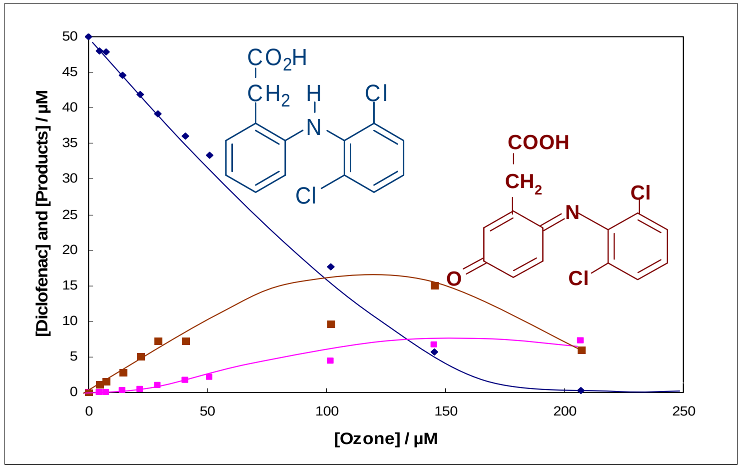
Phase Transfer Processes at Aqueous Interfaces (NN)

- Air
- Liquid mixtures
- Solids (sorption)



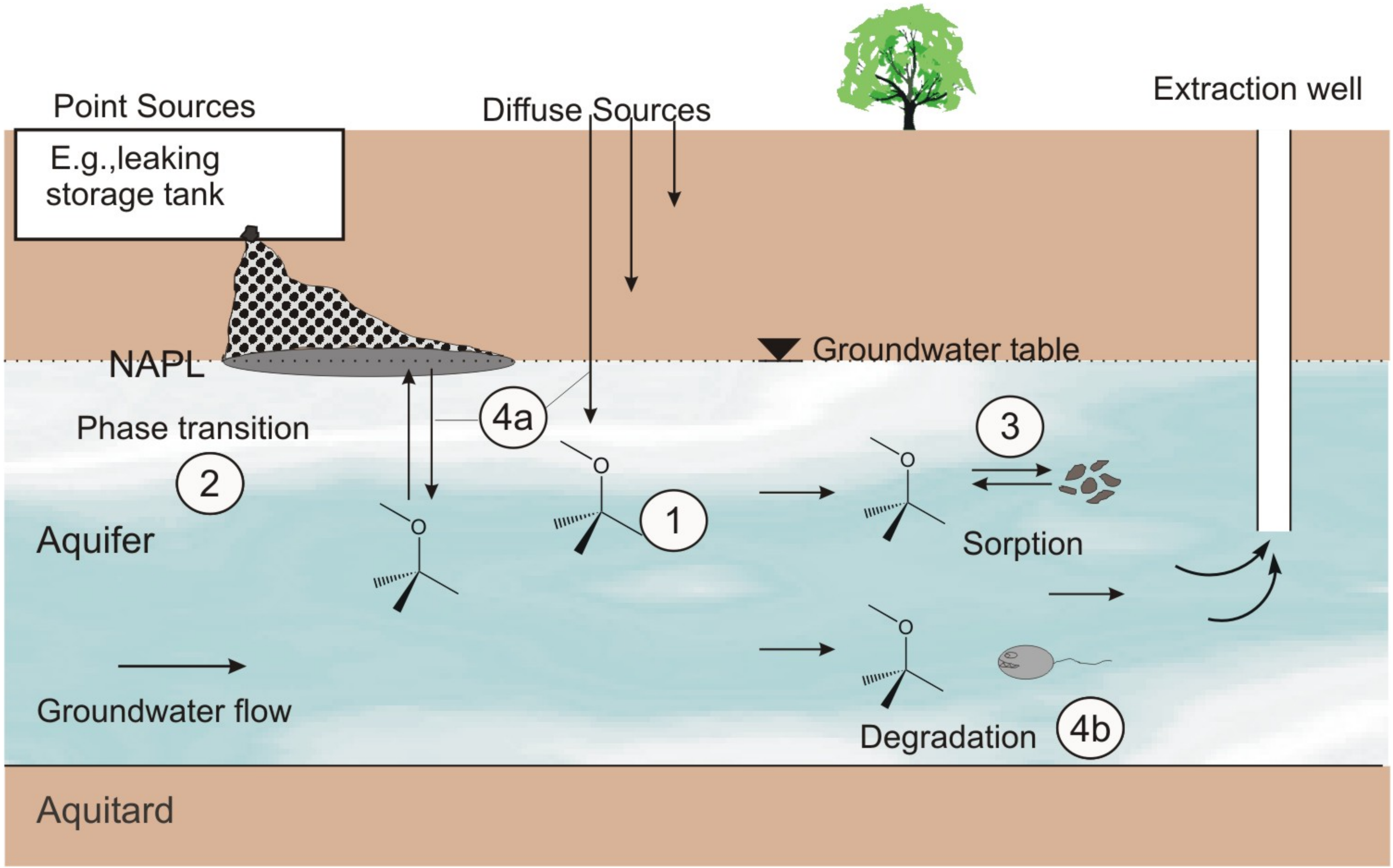
- Fundamental mechanisms, e.g., of sorption
- Equilibrium partitioning (incl. modelling)
- Kinetics of phase transfer

Advanced Oxidation Processes (Dr. Myint Myint Sein)

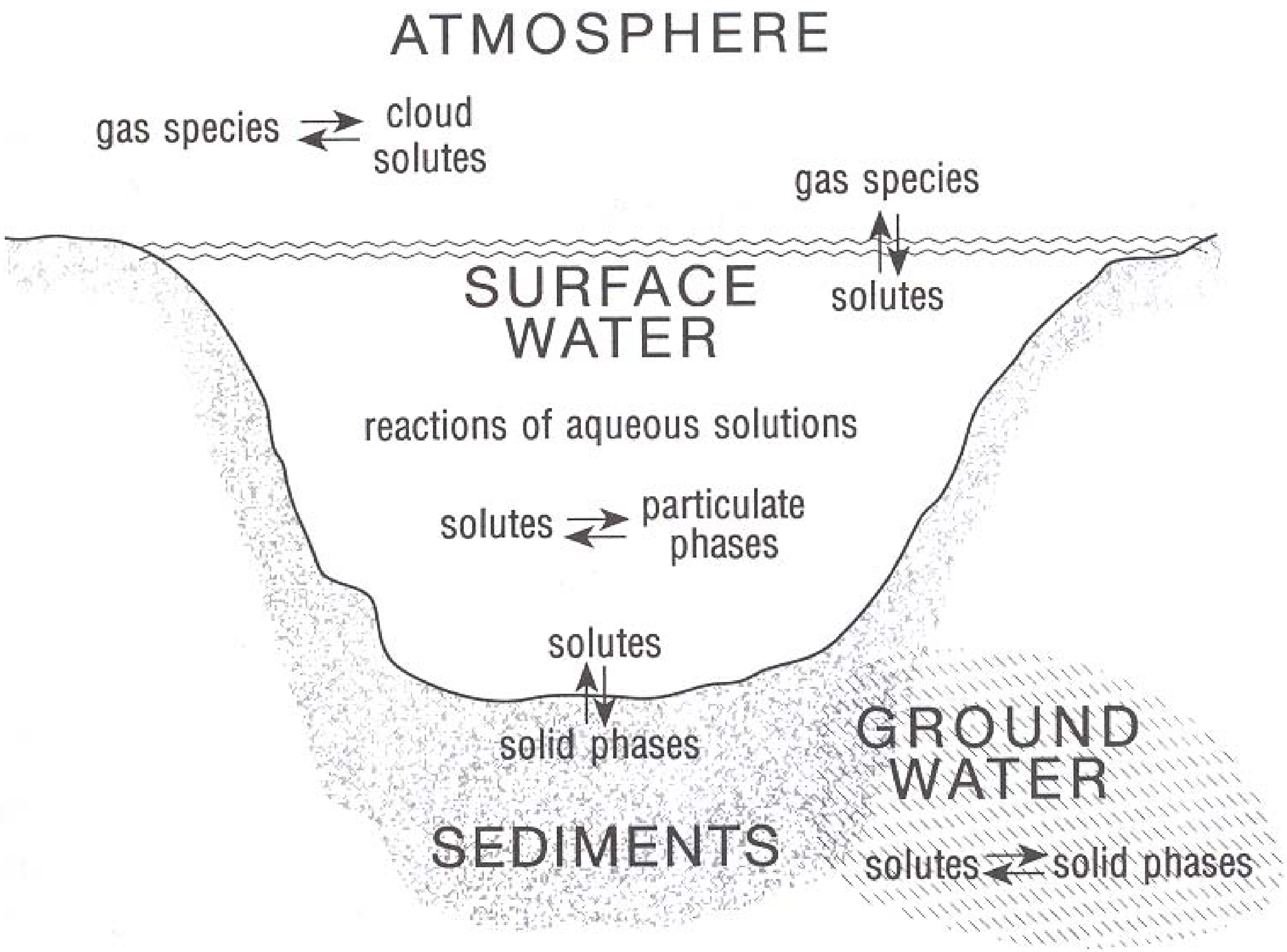


- Fundamental concepts in advanced oxidation processes such as peroxone, Fenton and nonthermal plasmas
- Kinetics, product formation and reaction mechanisms in the removal of micropollutants from raw and wastewater
- Formation of oxidation byproducts

Fields of Research:
Process-Oriented Environmental Chemistry

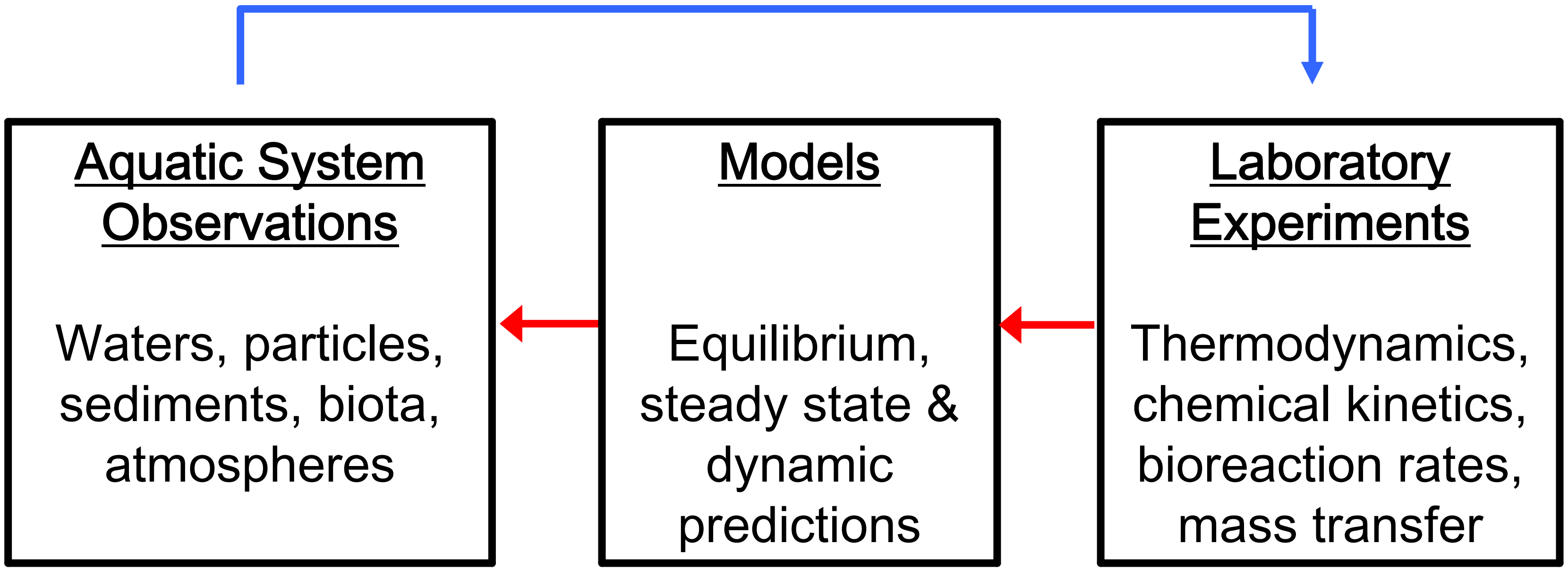


What is Water Chemistry?



Source: Stumm&Morgan, Wiley, 1996

What is Water Chemistry?



Source: Stumm&Morgan, Wiley, 1996

Why is Water Chemistry an Important Issue in the Master Course?

1. Chemistry of water (including dissolved or particulate substances) is the backbone of aquatic ecosystems and biogeochemical cycles
2. Chemistry of water governs the behavior of pollutants in aqueous systems
3. Understanding of water chemistry is a prerequisite for the appropriate use of technical processes for water treatment and purification

Aims of the Lecture

- Qualitative and quantitative understanding of processes dominating natural aquatic systems
- Fundamentals for evaluation of the fate of pollutants in natural and technical systems
- Realisation of (necessary) simplifications and plausibility control of assumptions and results
- This is NOT an introduction to water treatment!

Required Background

- Physical Chemistry:
  Thermodynamics, chemical equilibrium
- Organic Chemistry:
  Functional groups, Reaction mechanisms
- Water Chemistry:
  - Ions in aqueous solution (Acid/base, Dissolution, Complexation)
  - Redox chemistry
  - Fundamentals of phase transfer (sorption, air-water)

Organisation

- Lecture and Tutorial
  Wednesday 8^{15}-10^{00}, MG 272,
  Wednesday, 14^{15}-16^{00}, MG272
- Formation of groups á 4-5 students for problem discussion and presentation,
- Each group presents in the tutorial on Wednesday their solution to a specified problem in a problem set handed out in the course. Their approach will be discussed. It is NOT the primary goal to show the correct result but to learn how to tackle such problems. When forming groups you should try to incorporate people with different levels of expertise and **each group should encompass one of the students who have started here with the Master course**. By doing so, all of you will benefit most.

Course Contents

Subject	Date
Introduction/Concepts/Organization/Literature search, data retrieval	**15.10.**
Essentials in Equilibrium aquatic chemistry	**22.10.**
Essentials in Kinetics in aquatic systems	**29.10.**
Linear Free Energy Relationships	**05.11.**
Aquatic Chemistry of Surfaces and Colloids	**12.11.**
Advanced Sorption	**19.11.**
Transformation reactions: Substitution and Elimination	**26.11.**
Photochemistry	**03.12.**
	10.12.
Mile Stone I: Concept	**17.12.**
	07.01.
Mile Stone II: Relevant Processes	**14.01.**
	21.01.
Case Study Presentation and Discussion	**28.01.**
Case Study Presentation and Discussion	**04.02.**

Organisation II

- 2nd half of term:
  Case Studies
  Deadlines for coursework before milestones, discussion during contact meetings with advisors (milestones).
  Presentations of major findings during last two lectures
  Preliminary topic list:
  1. Cyanide spill Danube (Dirk Steinmann)
  2. Oil spill Exxon Valdez (Dirk Steinmann)
  3. Drinking water pollution by chlorinated solvents: Woburn case (Alexandra Jarocki)
  4. Drinking water pollution: hexavalent chromium/Erin Brockovich (Alexandra Jarocki)

Literature

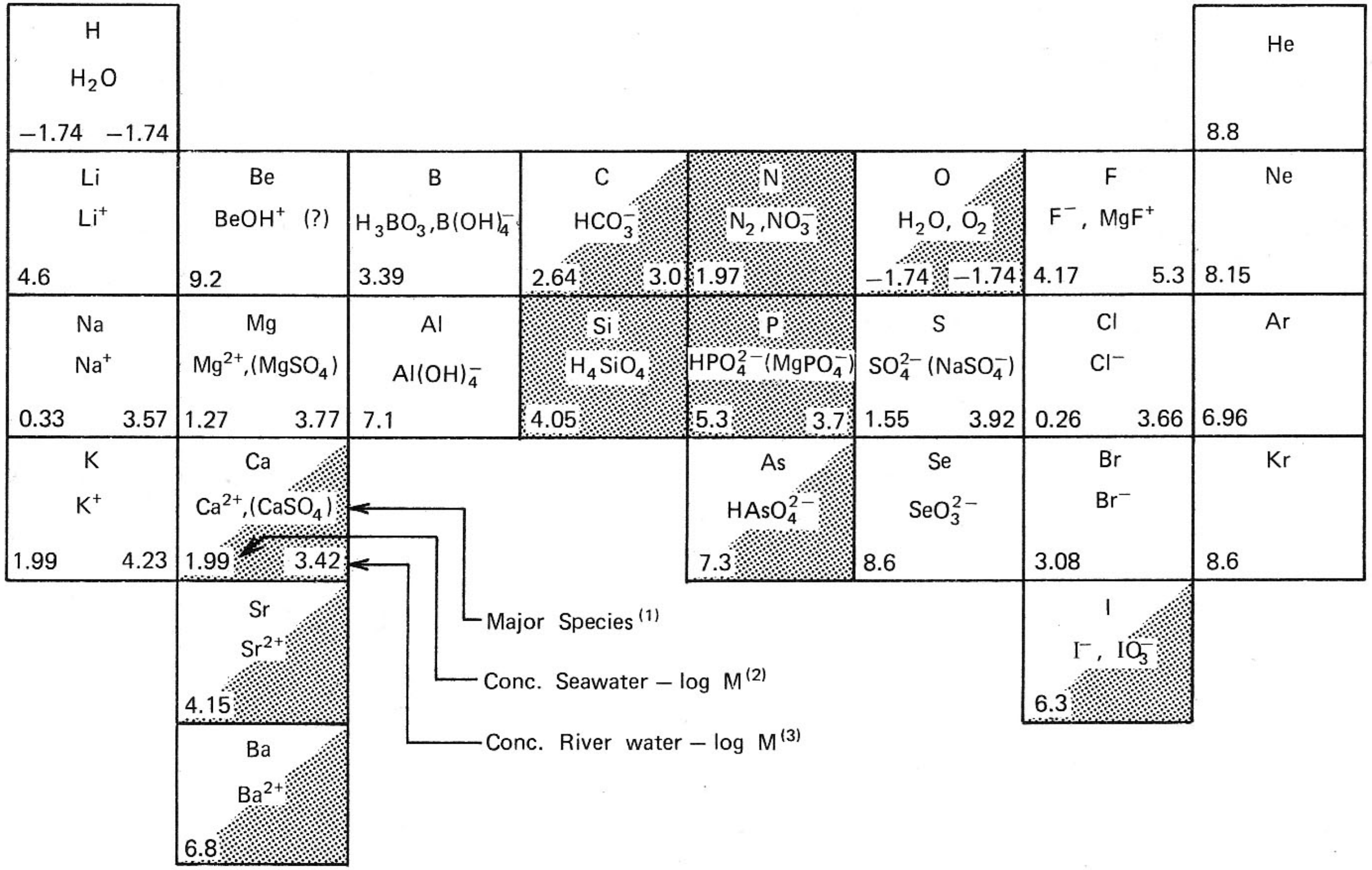
- Jensen, J. N., 2003: A Problem-solving Approach to Aquatic Chemistry, Wiley, NY
- Benjamin, M.M., 2002: Water Chemistry, McGraw-Hill, New York,
- Stumm, W. and J.J. Morgan, 1996: Aquatic Chemistry, Wiley, NY
- Schwarzenbach, R.P., Gschwend, P.M. and D. Imboden, 2003: Environmental Organic Chemistry, Wiley, NY

Concentration Scales

- ***Molarity,* M *(unit: mol L-1):***
The ***number of moles*** of a specific species ***per liter*** of solution
- ***Molality, m (unit: mol kg-1):***
The ***number of moles*** of a specific species ***per kilogram*** of solvent. Unlike molarity, units of molality are ***independent*** on changes in ***temperature, pressure and/or composition***. Molality is therefore frequently used in situations involving seawater.
- ***Mass concentration (unit: g L-1):***
The ***mass*** of a specific species ***per volume*** of solution.
- ***Formality,* F *(unit: formula weights L-1):***
The number of ***formula weights per liter*** of solution.
- ***Normality,* N *(unit: equivalents L-1):***
The ***number of equivalents*** (e.g., acid, base, charge, or redox-active species) ***per liter*** of solution. N is also known as ***equivalent concentration***. Note that the normality ***depends on the type of reaction*** considered!
- ***Mole fraction, x (dimensionless):***
The ***fractional concentration of a specific species*** computed, based on the knowledge of the ***numbers of moles of all of the species*** present. The mole fraction concentration scale can be used equally well for gases, liquids, and solids. It is important to note that for any given phase, when all concentrations are expressed as mole fractions, the sum of all mole fractions must equal 1. If the number of moles of a species ***i*** in a given phase is denoted ***ni***, then

$$x_i = \frac{n_i}{\sum_i n_i}$$

Important Elements in the Aquatic Chemistry of Natural Systems



Shaded areas: Elements, whose concentration in aquatic systems is influenced by biota

Table 13.1: Major Ions in Selected Water Bodies[1]

(ion concentrations in meq/L)

	Great Lakes[2]	Lake Tahoe	Ganges River	Colorado River	Mississippi River	Dead Sea
$[Na^+]$	0.28	0.27	0.28	4.13	0.93	1519
$[K^+]$	0.03	0.04	0.06	0.13	0.08	193
$[Ca^{2+}]$	1.50	0.47	1.10	4.14	2.03	788
$[Mg^{2+}]$	0.59	0.21	0.40	1.98	0.93	3453
Sum of cations	2.39	0.98	1.84	10.37	3.97	5954
$[SO_4^{2-}]$	0.38	0.05	0.06	1.71	0.52	11
$[Cl^-]$	0.37	0.05	0.16	7.61	1.52	5859
$[HCO_3^-]$	1.65	0.66	1.70	2.21	2.03	4
Sum of anions	2.40	0.76	1.93	11.53	4.08	5874
TDS (mg/L)	176	64	149	694	280	309,040

1. Source: United Nations Environment Programme's Global Environment Monitoring System Freshwater Quality Programme (UNEP GEMS/WATER
2. Average values for the Laurentian Great Lakes (Superior, Michigan, Huron, Erie, and Ontario)

Source: Jensen, Wiley, 2003

Speciation in Aquatic Systems

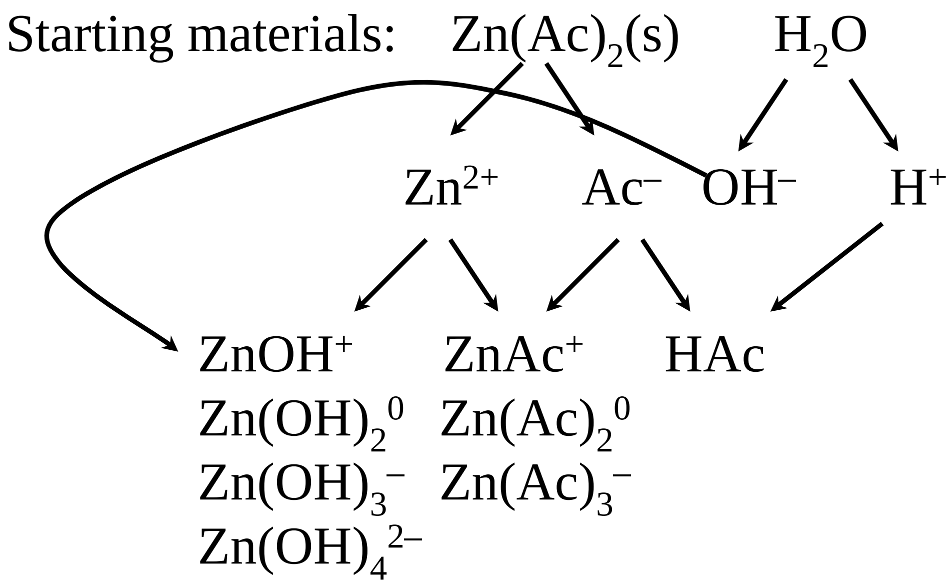


Figure 6.3: Species List Diagram for the $Zn(Ac)_2(s)/H_2O$ System

Source: Jensen, Wiley, 2003

Hydrological Cycle - Pollutants

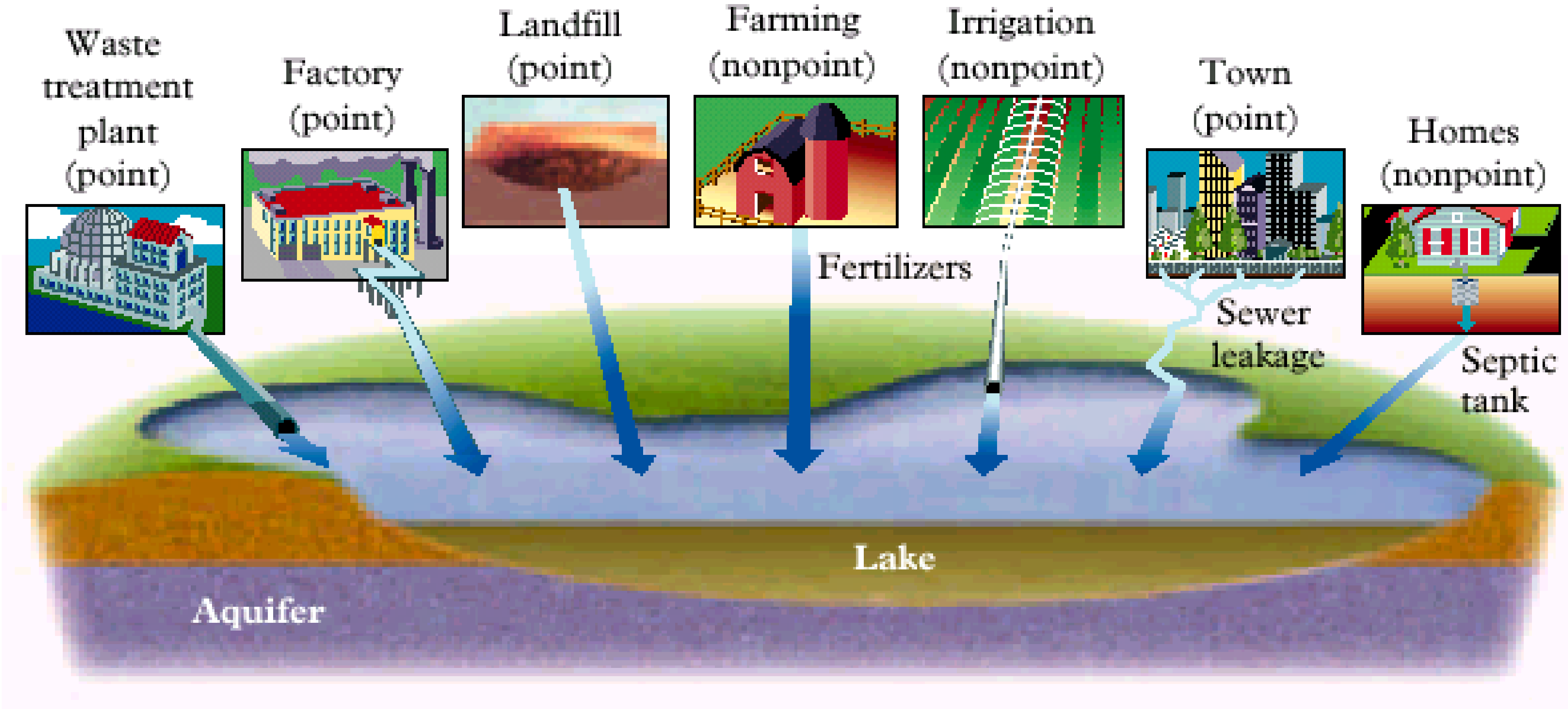


Figure 13.15 Point and nonpoint sources of pollution.

Hydrological Cycle – Pollutants II