Ekotoxikologie vodních ekosystémů

Osud látek a biodostupnost

Osud látek ve vodních ekosystémech ovlivní:

- Vlastnosti chemických látek
- Vlastnosti vodního prostředí
- Biotické i abiotické interakce
- Pohyb a míchání vody (…podzemní!!!)
- Kyslíkové a redox poměry na lokalitě
- pH
- Světlo (fotolýza, autotrofní biodegradace
- Sorpce (obsah org. Látek, jílo/min. komplexy, HK

Properties of a chemicals in environmental/hydro chemistry

- Molecular structure
- Molecular weight
- Water solubility and precipitation (a)
- Vapor pressure
- Henry's law constant
- Octanol-water partition coefficient (b)
- Sorption constants for soiLs, sediments, or atmospheric particle ©
- Acid or base dissociation constant (a)
- Complexation constants (a)
- Electron transfer (redox) constant (a,b)
- Polymerization constants (a)
- Diffusion coefficients
- Light absorption spectrum and quantums yield
- Bioconcentration factor (a,b)
- Biodegradation or biotransformalion constant (b)
- Hydrolysis constants (b)
- Particle size (for solids)

(a) Both equilibrium and rate constants are important.

(b) Primarily used for organic chemicals.

© Primarily used for inorganic chemicals.

Properties of the aquatic environment important in predicting the fate and transport of a chemical

Physical properties

- Surface area
- Flow, extent of mixing, and bottom scouring
- Sedimentation rate
- Solar irradiation (at surface) and irradiance as function of wavelength and water body depth

Chemical properties

- Temperature
- pH
- Eh* (for several redox couples, including oxygen)
- Suspended solids (nature and concentration)
- Hardness, salinity, ionic strength
- Concentration of major ions
- Concentration of dissolved organic matter
- Bottom sediments (nature, including organic carbon content and redox status)

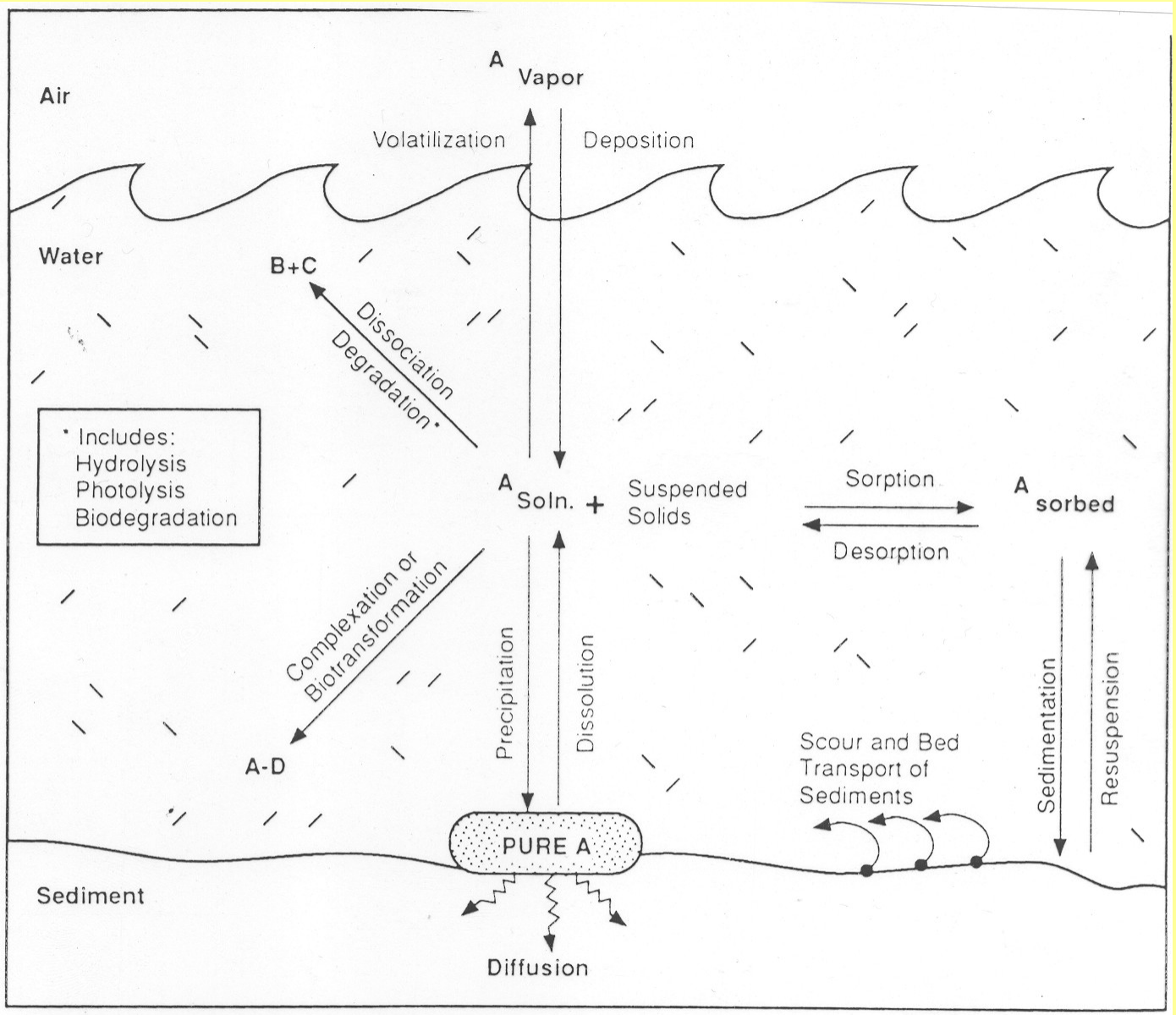
Biological properties

- Microbiological populations and activity
- Trophic status
- Nutrient concentrations

*Eh = value which «presents potential of redox reactions.

Faktory ovlivňující biodostupnost

- Forma toxikantu
- Dostupnost formy do organismu
  - Komplexaxe/dekomplexace
  - Adsopce/ desorpce
  - pH
  - Konc. Org. látek
  - Konc. Organic/ minerálních částic
  - Teplota okolí a v organismu
  - Způsob příjmu (kůže, respirace, s potravou, membránový přenos)



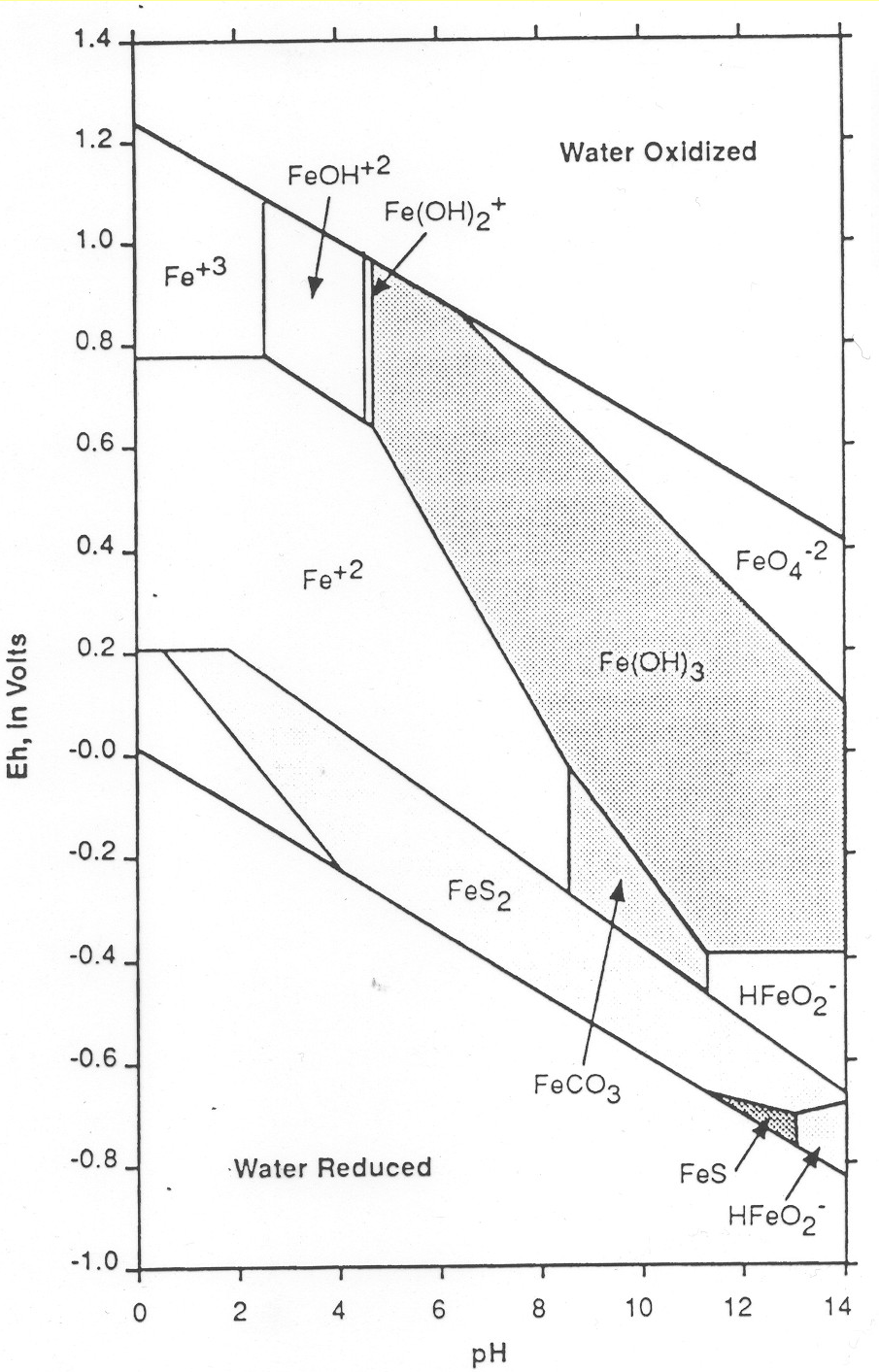
Note. Symbols B and C represent degradation products of chemical A, and symbol D represents a ligand that complexes with (or adds to) A.

Figure 1. Schematic representation of some transport and transformation phenomena important for a chemical in an aquatic environment.

Table 5. Measured values of soil or sediment sorption constants for selected organic chemicals

Nonaromatic chemicals		Aromatic chemicals			
Chemical	log K_{oc}	Chemical	log K_{oc}	Chemical	log K_{oc}
Acrolein	0.70	Acetophenone	1.54	Glyphosate	3.42
Aldrin	4.30	Acridine	4.11	Hexachlorobenzene	3.59
Bromacil	1.86	Alachlor	2.28	Leptophos	3.97
Chlordane	5.15	Ametryn	2.59	Linuron	2.91
Crotoxyphos	2.23	2-Aminoanthracene	4.45	Methazole	3.42
Cycloate	2.54	6-Aminochrysene	5.16	Methoxychlor	4.90
2,4-D	1.23	Anthracene	4.78 (4.41)	2-Methoxy-3,5,6-trichloropyridine	2.96
DBCP	2.11	Aroclor 1254	6.25	9-Methylanthracene	4.81
Diallate	3.28	Asulam	2.48	3-Methylcholanthrene	6.09
cis-1,3-Dichloropropene	1.36	Atrazine	2.17	2-Methylnaphthalene	3.93
trans-1,3-Dichloropropene	1.41	Benzene	1.92	Methyl parathion	3.33
Dieldrin	3.82	Benzo[*a*]anthracene	6.24	Metobromuron	1.78
Dinoseb	2.09	Benzo[*a*]pyrene	6.74	Metribuzin	1.98
Disulfoton	3.25	2,2′-Biquinoline	4.02	Monolinuron	2.30
Endrin	3.56	Carbaryl	2.36	Monuron	2.00
EPTC	2.38	Carbofuran	1.45	Naphthalene	3.55 (3.11)
Ethion	4.19	Carbophenothion	4.66	1-Naphthol	2.72
Ethylene dibromide	1.64	Chlorbromuron	2.66	Napropamide	2.83
Heptachlor	4.00	Chloroneb	3.06	Neburon	3.36
Ipazine	3.22	Chloroxuron	3.51	Nitrapyrin	2.62
Lindane	2.96 (3.03)	Chlorpyrifos	4.13	Norfluorazon	3.28
Malathion	3.17	Chlorpyrifos-methyl	3.52	Oxadiazon	3.51
Methomyl	2.20	Chlorthiamid	2.03	2,2′,4,4′,5,5′-PCB	6.08
Methyl isothiocyanate	0.78	Chrysene	5.77	2,2′,4,5,5′-PCB	4.63
Monuron	2.20	Cyanazine	2.30	Parathion	3.93
Pebulate	2.80	DDD	5.38	Phenanthrene	4.36
Pentachlorophenol	2.95	DDE	5.17	Phenol	1.43
Phorate	3.51	DDT	5.48 (5.38)	Prometon	2.54
Picloram	1.17	13*H*-Dibenzo[*a*,*i*]carbazole	6.02	Prometryn	2.91
2,4,5-T	1.87	Dibenzothiophene	4.05	Pronamide	2.30
Tebuthiuron	2.79	Dibenzo[*a*,*h*]anthracene	6.23	Propachlor	2.42
Terbacil	1.71 (1.58)	Dicamba	0.27	Propazine	2.20
Toxaphene	3.00	Dichlobenil	2.27	Propham	1.71
Triallate	3.35	Diflubenzuron	3.83	Pyrazon	2.08
		7,12-Dimethylbenz[*a*]anthracene	5.35	Pyrene	4.92
		Dipropetryn	3.07	Pyroxychlor	3.48
		Diuron	2.60 (2.47)	Simazine	2.01
		Fenuron	1.43	Terbutryn	2.85
		Fluometuron	2.24	Tetracene	5.81
		Fluoranthene	5.31	3,5,6-Trichloro-2-pyridinol	2.11
		Fluorene	4.01	Trietazine	2.78
				Trifluralin	4.14

Source: Lyman and Loreti, 1987 (values compiled from several sources).



Shaded areas are stability regions for solids; predominant dissolved species are shown in unshaded areas. Activity of sulfur species = 96 mg/l as SO_4^{-2}. CO_2 species = 1,000 mg/l as HCO_3^{-}, and total dissolved iron activity = 0.0056 mg/l.

Source: Hem (1970)

Fields of stability for **solid and dissolved forms of iron** as a function of Eh and pH at 25°C and 1 atmosphere (Courtesy, 1990)