Bioaccumulation processes in ecosystems

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Abstract. The fate of environmental pollutants – the various isotopes of elements, and inorganic or organic compounds – is a fundamental aspect of ecology and ecotoxicology, and bioaccumulation is a phenomenon often discussed in this context. Human activities have drastically altered natural concentrations of many substances in the environment and added numerous new chemicals. An understanding of the processes of bioaccumulation is important for several reasons. 1) Bioaccumulation in organisms may enhance the persistence of industrial chemicals in the ecosystem as a whole, since they can be fixed in the tissues of organisms. 2) Stored chemicals are not exposed to direct physical, chemical, or biochemical degradation. 3) Stored chemicals can directly affect an individual's health. 4) Predators of those organisms that have bioaccumulated harmful substances may be endangered by food chain effects. While former theories on the processes of bioaccumulation focused on single aspects that affect the extent of accumulation (such as the trophic level within the food chain or the lipophilicity of the chemical), modern theories are based on compartmental kinetics and the integration of various environmental interactions. Concepts include results from quantitative structure-activity relationships (QSAR), pharmacokinetics, ecophysiology and general biology, molecular genetic aspects and selection, and finally the structure of communities and man-made alterations in them.

Key words. Bioaccumulation; bioconcentration; BCF; pesticides; ecotoxicology; compartment models; QSAR; food chain; atrazine; lindane; DDT; DDE; PCB; heavy metals; plants; earthworms; birds.

1. Introduction

The process of bioaccumulation is often discussed in the context of man-made environmental pollution. But it should also be studied as a result of evolutionary processes and interactions between organisms and chemicals that have led to the storage or metabolic separation of nutritional elements or compounds. While for ions, and more generally for hydrophilic compounds, specialized uptake or avoidance mechanisms are widespread, lipophilic compounds often invade cells passively, and avoidance mechanisms have been poorly developed in the course of evolution.

Understanding the process of bioaccumulation is important for several reasons. Bioaccumulation in organisms may enhance the persistence of industrial chemicals in the ecosystem as a whole, since they are fixed in the tissues of organisms, rather than being exposed to direct physical, chemical, or biochemical degradation. In times of starvation, the release of stored chemicals into the blood system can directly affect an individual's health. Finally, predators of those organisms that have bioaccumulated harmful substances face food chain effects.

While former theories focused on single factors that were thought to determine the extent of bioaccumulation, such as trophic levels in the food web or lipophilicity of the chemical, more recent theories combine models of various environmental interactions. In this paper, I will focus on some concepts that have been elaborated for lipophilic organic chemicals and inorganic pollutants in aqueous and terrestrial environments. After some general remarks about the usage of the term bioaccumulation, the history of concepts, the physico-chemical properties of xenobiotics in the context of the QSAR theory, and a

short outline of the compartmental concept, the problem will be discussed for three major topics: 1) Bioaccumulation of heavy metals by plants, 2) bioaccumulation in terrestrial food chains, and 3) bioaccumulation in the aquatic environment.

2. Definitions of bioaccumulation

The term 'bioaccumulation' is used in two ways: a) to describe a dynamic process of passive or active uptake and concentration of an element or a compound within an organism; b) in a static sense, meaning a currently high concentration as the result of previous accumulation processes. Similarly, the term 'bioconcentration', which is sometimes used synonymously, sometimes indicates the direct uptake of chemicals from the environment into the organism (through plant roots, fish gills etc.) rather than from ingested food. If the use of the term 'bioconcentration' is thus confined to the direct uptake, then the food chain uptake is mostly termed 'biomagnification' or 'biological magnification'. Using a compartmental approach, all input (or inlet) and output (or outlet) mechanisms are treated in a similar way. Distinguishing between bioconcentration sensu stricto, and biological magnification, is sometimes highly artificial[56, 69]. I will therefore use the two terms synonymously throughout this review (discussions on the terms have been presented many times[17, 40, 56]).

Bioaccumulation in the static sense can be quantified in terms of concentrations (on a mass base), e.g., µg chemical per kg living biomass, per kg dry mass, or per kg fat, and so on. For practical purposes, the use of dimension-

less relative figures is widespread and based on the concentration in the ambient water or ingested food. These dimensionless figures are usually called 'bioaccumulation factors' or more frequently bioconcentration factors and abbreviated as BCF. BCF can be defined and measured under steady state conditions (after an input-output equilibrium has been established) and will then correspond to the static bioaccumulation concept. Or it can be defined and measured as a function of time, depending on actual input-output rates and the metabolic activities. In the first case, BCF will be identified by the subscript 's' ('BCF_s' for 'steady state BCF'), in the second case it will be written as a function of time, i.e. as 'BCF (t)'.

Different types of BCF calculations are in use. Concentration figures in organisms and tissues can be based on fresh mass (wet weight), on dry mass (dry weight), or for lipophilic compounds also on fat mass. The concentration in water is usually given in mass per volume (e.g., µg chemical per liter), which is comparable to the µg chemical per kg biomass unit as used for living organisms, since the specific density of tissues is close to one. Relative units, such as 'ppm', 'ppb', and 'ppt', should only be used if they have been clearly defined with respect to the calculations. For chemical reaction mechanisms, the preferred units in water and body fluids are molar units.

Special problems occur with the use of the terms in terrestrial systems. The concentration of a heavy metal or an organic pollutant in the soil environment can either be related to dry soil, to wet soil (fresh soil), or to the aqueous phase of the soil, which is actually the subsystem of the soil that acts as the immediate source for the uptake by plant roots. However, the concentrations of a given pollutant in the soil water may vary to a great extent according to the actual water saturation, redox potential, and pH. A simple bioaccumulation or bioconcentration factor can therefore not be calculated for chemical transfer for exchange from soil to plant or from soil to earthworm compartments.

3. A brief history of concepts

Food chain approach

Early models of bioaccumulation in food webs and ecosystems were derived from residue samples and more or less realistic reconstructions of food chains within communities. An early scheme for DDT bioaccumulation, by Woodwell, is redrawn in figure 1, left (omitting the concentration figures originally included). In this scheme, several species from the East Coast of North America are arranged in such a way that they become part of a food web approximately following increasing concentration figures. The concentration figures used were based on earlier and more critical presentation of data by Woodwell, Wurster and Isaacson[96] published in
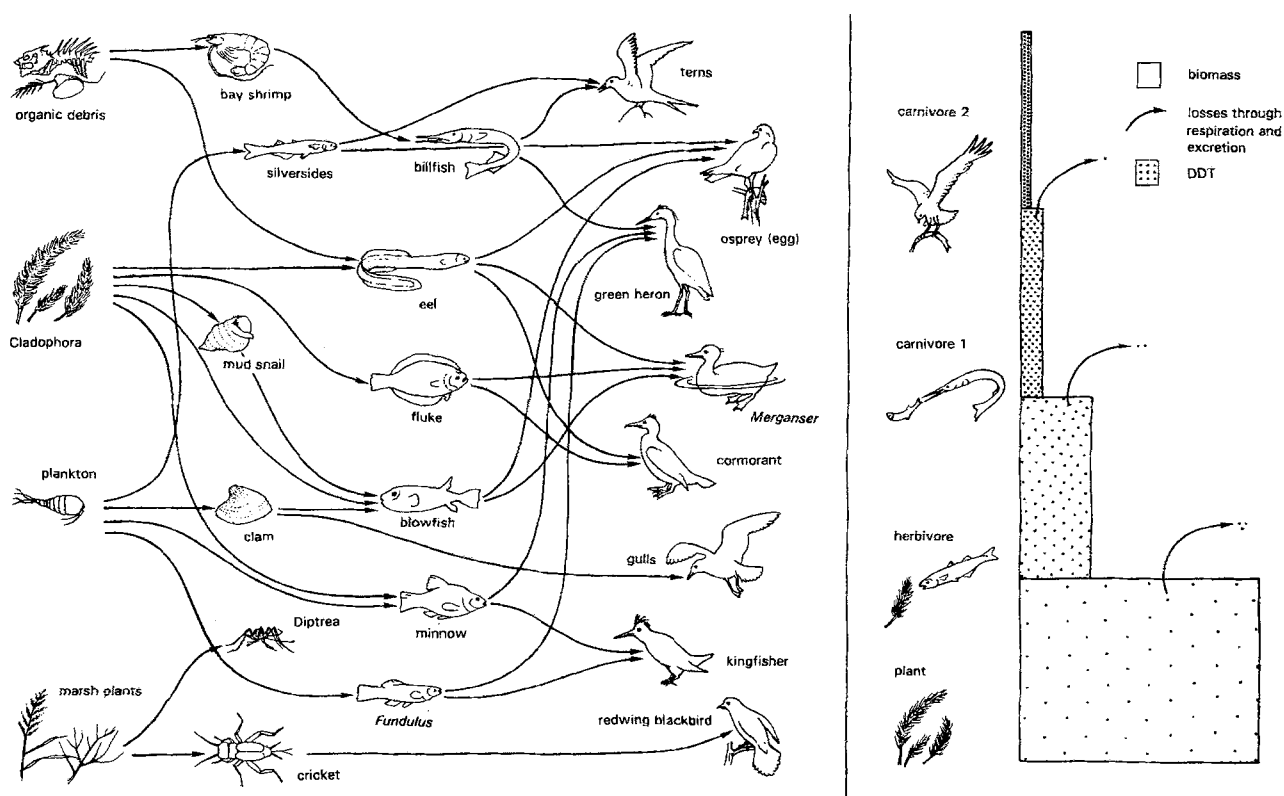

Figure 1. *Left*: Traditional concept of DDT bioaccumulation in a food web in Eastern USA. For comment on erroneous assumptions see text. *Right*: The even more abstract representation on the right suggested a food chain bioaccumulation parallel to the energy pyramid, and was extracted from the figure on the left. Both representations adapted from Woodwell[95], omitting concentration figures.

page 956,   figure 1:   read 'Diptera', not 'Diptrea'.

Science. It was, however, the idealized and popular scheme by Woodwell[95] from figure 1 (published in *Scientific American*) that got numerous citations in many textbooks in the following years, despite the fact that it had obvious biological fallacies and information omissions:

1. In the original data set, Woodwell et al.[96] included important information about the origin and validity of the data. For example, field samples had been collected at quite different times; some biological samples were dead at the time of sampling, others alive; in some cases, the study was based on adult individuals, in others on single tissues, or even on the yolk of the egg stage only (as in some bird samples).

2. The 'food web' suggests many astonishing biological relationships, such as eels feeding upon algae of the Cladophora group and on organic débris, geese feeding on eels, and terns feeding on billfish. There was no explanation given that could explain these rather unusual food relationships.

3. Those data that best fitted a 10:1 ratio of biological magnification (in an analogous way to energy flow, see below) were compiled in the scheme of figure 1, right, to 'exemplify' a bioaccumulation rule along a food chain. This latter diagram should focus on the most important issue, i.e. the increase in concentrations of DDT by a factor of approximately 100 between water and the first food step, and of 10 between subsequent food steps. The basic idea behind this form of explanation was the correlation of bioaccumulation with energy flow analyses, as found by Odum[53], Teal[83], and others during the preceding one and a half decade. These ecologists had found that energy flow per unit area in aquatic environments decreased by two orders of magnitude from solar light to primary producers, and approximately one order of magnitude in subsequent food steps.

The mechanism of lipophilic pesticide bioaccumulation in aquatic environments is no longer considered to be primarily the result of food chain effects, at least not in aquatic communities and for trophic levels below mammals and birds. Besides biological and other misinterpretations, the model also neglected the direct pesticide uptake from water, the strong affinity to fat content, and the various transfer constants under equilibrium or nonequilibrium conditions. Nevertheless, it did focus on the importance of the food chain transfer coefficients, and in many terrestrial food chains the transfer of pesticides through ingested food is indeed of great importance. Although its explanatory value was poor (and partly wrong), the figure became very popular and made the problem of contamination within communities well known. It also helped people to understand that there could be high residue concentrations in sea birds and sea mammals compared to their aquatic food items, and that harmful effects, such as the thinning of eggshells due to high DDT concentrations were alarming, and contributed to the decline in wild populations of those species.

In the early 1970s, first experimental results indicated the fast uptake of some organic and inorganic chemicals into organisms even in the absence of food[64]. In addition to the lipophilicity approach (see below), a second one, the compartmental approach, was introduced through pharmacokinetics[6]. By using radioactive tracers, more information was found on uptake and elimination rates, food chain transfers and the relationship between lipophilicity and storage of xenobiotics in fat tissues[67-69]. Multicompartmental concepts have finally stimulated detailed uptake and elimination research of environmental pollutants in fish organs[25], as well as the first fundamental multicompartmental approaches in pharmacological studies[15].

Lipophilicity approach

In contrast to the ecology-based food chain approach, a chemistry-based model came into general use among those scholars who emphasized the correlation between bioaccumulation and the lipophilicity of a compound. Lipophilicity is the tendency of a substance to be attracted primarily by non-polar, usually organic solvents, in contrast to hydrophilic substances, which are attracted by polar solvents such as water. As a measurement unit of lipophilicity, most often the partition coefficient between water and n-octanol is taken and designated as P_{ow} or K_{ow} (or $K_{o/w}$). The relationship between the steady state bioconcentration factor (BCF_s) and K_{ow} has been found many times to follow a logarithmic regression of the form:

$$\log BCF_s = a \times \log K_{ow} + b.$$

Regression models of this kind have been published for various organisms, especially from aquatic environments. Tables or figures for fish covering between 8 and 122 individuals points (n), have been compiled by various authors[3, 12, 34, 42, 49, 55, 73, 88]. There are similar tables for molluscs (n = 14–34)[22, 31, 54], for microorganisms (n = 14)[5] and for sediment analyses (n = 10)[33]. The n-octanol/water partition coefficient (log K_{ow}) is generally inversely correlated with the water-solubility. Therefore, there is also a correlation between BCF_s and the water-solubility of chemical compounds (both on a log basis), as shown in figure 2 for teleost fishes. It should be emphasized that published graphs of this kind sometimes include data that were not empirically found, but estimated from previously found correlations.

Using independently found data, it has been emphasized in more recent times that the increase in bioconcentration does not follow a straight line. Beyond log K_{ow} values of 6–8 and log BCF_s values of 6–7, a slower increase or even a decrease is observed. The best-fit, however, is still a matter of debate, as is the underlying theory explaining this phenomenon[50].

The extension of the bioconcentration vs lipophilicity relationship to other characteristics of molecules, such as steric configuration, extended the explanatory basis of
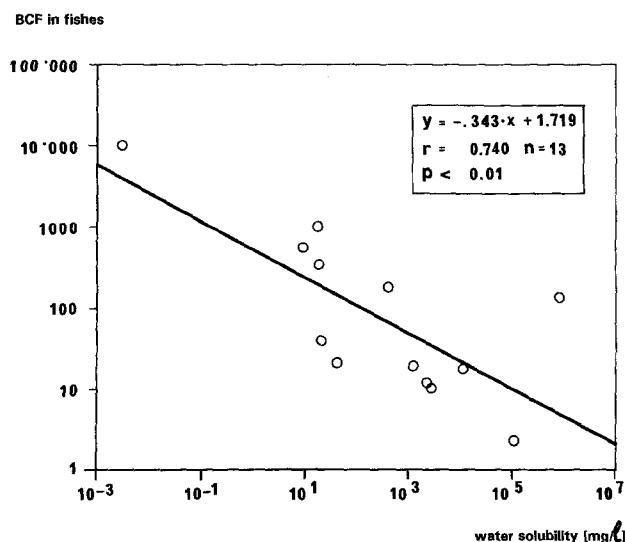
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page 957, line 16/17: omit 'geese feeding on eels', Woodwell depicted a merganser (a fish-eating duck, not a goose), which may well feed upon small eels. Questionable food relationships are rather those starting from the four food items at the very left side of the diagram and leading to the next trophic level.

BCF in fishes

Figure 2. Correlation between the water solubility of organic compounds and the steady-state bioconcentration factor (BCF_s) in teleost fish species (the correlation is usually even better for correlation of BCF_s vs n-octanol/water partition coefficient), as an example of a QSAR. From a historical perspective, this relationship has been used as a counter-approach to the food chain concept for some time. From Streit[73].

bioaccumulation and different kinds of toxic effects to a variety of types of chemicals, including hydrophilic substances. It also allows a distinction to be made between different groups of chemicals. A more detailed overview of these aspects, today unified under the concept of QSAR, will be given in section 4.

Ecophysiological and compartmental approach

Bioaccumulation is basically the result of local chemical bonds that overcome the dissipation tendency of the chemical. In a closed local system, a thermodynamic equilibrium will eventually be reached, in which the association and dissociation rates are equal. Nevertheless, also under non-equilibrium conditions, e.g. when substances are continuously added or subtracted, a steady state may be accomplished.

The structure of ecosystems with respect to environmental pollutants can be described by a complex of subunits or subsystems, each usually separated from the others by some distance and often also by physical barriers like membranes. The amount of a substance at a given location is said to constitute a compartment. But even within a given location, different forms of a substance (such as a form occurring either in free solution in the blood plasma or bound to albumins) represent different compartments. Compartments are therefore basically idealized stores of substances[10]. Physically, compartments can be as far from each other as are the atmospheric pollutants in the clouds over the sea and a plant community somewhere on the continent that will be affected through wet deposition from fog and rainfall. They can also be as close as those between two separate organelles within a cell or between dissolved and adsorbed molecules in a suspension.

For environment/organism interactions, membranes and various kinds of cuticular structures are the most important barriers that separate individuals from the environment. Together with general aspects of ecophysiology (such as ingestion rates, respiration mode and so on), they control the chemodynamics in the biota. As a general rule, those epithelial areas that are used for ion uptake or for ionic regulation, for uptake of dissolved oxygen or release of carbon dioxide and ammonia, allow to a certain extent the passage of other substances. Ambient substances can enter, and previously stored substances can leave the body again.

For *plants*, it is of basic importance that there should be intimate contact between their root cell membranes (or symbiotic fungal cells) and the ambient water environment in the soil or (for aquatic plants) in the sea, the lake, or the river. Those substances that are easily translocated will be distributed in the whole plant; those that are bound to structural parts will remain in the root section of the plant. Shoot parts are generally well protected from contamination from the air, but lipophilic compounds (and certain small inorganic molecules) can, to a certain degree, pass the cuticle surface. In aquatic species, (semi)permeable membrane structures may be permeable for various kinds of substances, both to lipophilic organic compounds and to heavy metals. Hydrophilic compounds up to a certain molecule size can pass if they are electrically neutral.

In many *animal* groups, such as fishes, amphibian larvae and many invertebrates, these permeable areas are basically at the gill/environment interface. Those animals that are descendents of originally land-living predecessors, such as aquatic beetles and spiders, birds and mammals, usually have well-protected skin areas rather than permeable membranes in direct contact with the ambient water. Their bodies will therefore usually not take up dissolved chemicals by direct diffusion, except for those substances that can pass intact skin structures. Among animals in terrestrial habitats there is also a range from rather permeable skin structures, like those of earthworms, to rather impermeable ones, for example in diplopods. As well as the epidermal structure, the size of the organism is an important aspect. Larger organisms, or organisms with low exchange rates between their bodies and water solutes outside their bodies (e.g., many reptiles), show very low turnover rates of water (cf. Streit[71] for a compilation of water turnover rates) and therefore probably also of dissolved substances.

4. Chemical structure, interactions, and kinetics

Not all chemical elements (or isotopes) and chemical compounds are subject to bioaccumulation, and among those that are, the extent of bioaccumulation varies considerably. On the one hand, the differences are the result of variable membrane passage capabilities due to different electrical charges, particle diameters, and chemical

interactions. On the other hand, bioaccumulation rates differ owing to variable binding constants of substances to living substrates, especially binding to different kinds of molecular structures in organisms. The complex relationship between chemical structure and biological effects can be studied on the basis of purely physico-chemical principles or from a more statistical viewpoint, such as by (quantitative) structure-activity relationships (SAR and QSAR).

QSAR

Statistical analyses between classes of chemical substances and organisms are the basis of the empirical 'quantitative structure-activity relationships' or QSAR, a tool originally used in pharmacology and toxicology, but in more recent times also in ecotoxicology. Although the term and acronym themselves go back only a few decades, statistical studies and correlations between the molecular organization of chemicals and their response in organisms were already being carried out towards the end of the 19th century. Comparison of the toxicity of alcohols and ethers suggested that 'the more soluble they are, the less toxic they are' (Richet). Meyer and Overton clearly showed in 1899 that the fat-water partition coefficients correlated with the narcotic action of simple organic compounds[52].

After these empirical studies, more systematic considerations started with Hammett[28], who proposed a numerical constant (σ_x) to assign electronic effects of substitution on an aromatic ring, an index used later by Ormerod[58] to predict chemical behavior, such as hydrolysis. (A survey of Hammett substituent constants has been given recently by Hansch et al.[29]). Hansen[30] used this index to predict a biological-toxicological, and therefore much more complex phenomenon, namely the toxicity of different compounds to mosquito larvae. Steric effects, which can occur in non-aromatic molecules, were taken into account only by applying a steric parameter, E_s (by Taft[82]). This parameter was used, for example, to correlate inhibition of fly brain cholinesterase[21].

In the early 1960s, the concepts of Hammett and Taft were combined by Hansch and co-workers to derive a hydrophobic parameter for substituents that would be related more closely to biological activities. 'Log P', or the octanol-water partition coefficient, became the most widely used descriptor in quantitative structure-activity relationships. The correlation between these calculated log P (or 'log K_{ow}' as used throughout this paper) values and experimentally determined partition coefficients was actually very good.

The most generalized formulation of the combined observations of all these studies led to the concept of the 'linear free-energy relationship' (LFER). This concept implies that the effect of substituents is based on the strength of interactions between a drug and a receptor and is an additive combination of hydrophobic, electronic, steric, and dispersive factors[29].
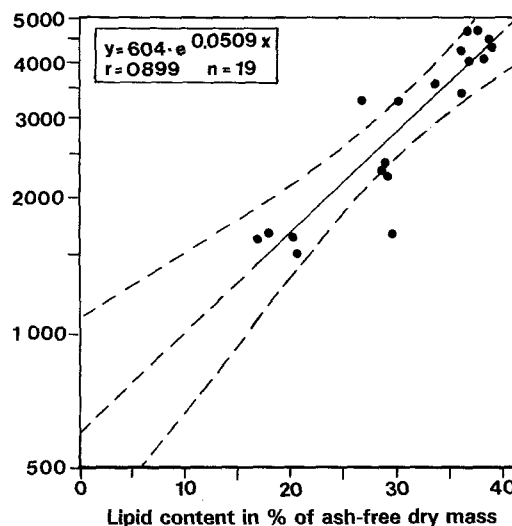
Bioconcentration factor

Figure 3. Another example of a QSAR: Steady state bioconcentration factor (BCF$_s$) of lindane, a lipophilic organochlorine compound, in freshwater diatom algae as a function of the algal lipid content. From Trautmann and Streit[85].

For a long time, only the lipophilicity approach was used as an explanatory basis of bioaccumulation concepts in ecological studies (see also fig. 3). But other QSAR aspects are important, such as steric effects[57]. Kinetic interactions and time delays of complex system behavior can only be explained by including QSAR in a compartmental approach to the chemical-organism interactions studied.

It should be emphasized at this point that all QSAR represent basically empirical relationships. For example, thermodynamic considerations indicate that a unique log BCF/log K_{ow} relationship cannot exist, since enthalpy changes vary for different classes of chemical substances. Within a given class (e.g., the 209 PCB congeners), the relationship is much better than for the sum of all organic compounds. Furthermore, the interactions of different parameters in the natural environment also influence water solubility, partition coefficient, and bioaccumulation[86].

The physico-chemical basis of interactions

In the following we will first focus on elements (light and heavy metals), then on organic compounds.

Metals in environments and organisms are mostly found in the form of metal complexes with different types of organic or inorganic binding partners (ligands). They differ according to ligand preferences and are characterized as either 'A metal cations', 'B metal cations', or 'borderline cations' (i.e., those with characteristics lying between A and B). Whereas 'heavy metals' as a group do not show any common characteristics concerning bioaccumulation processes that would separate them from the light metals[51,80], the A and B subcategories provide information about preferred ligands and potential local

accumulation forms[76]. These subcategories are based, however, on earlier models, primarily on Pearson's[59] hard-soft concept of the electronic shell.

In type A metal cations, the electron sheaths are not readily deformed under the influence of electronic fields, as produced by adjacent charged ions. They form complexes preferentially with fluoride ions and ligands which have oxygen as the donor atom. If a potential complexing agent contains only N or S as ligand atoms, it will not coordinate with type A cations with any appreciable stability. Typical examples of this metal group are alkaline and earth alkaline metals, as well as Al^{3+}, Ga^{3+}, Sc^{3+}, Y^{3+}, Zr^{4+}, Hf^{4+}, Cr^{3+}, and Fe^{3+}. They will usually bind to bony structures, such as Ca^{2+} or Sr^{2+} isotopes, not to SH-groups of proteins, as do some representatives of type B and borderline metals.

Type B metal cations have a more deformable electron sheath and are therefore more strongly polarizable than type A metals. They coordinate preferentially with ligands containing sulfur, nitrogen, or iodine as donor atoms. Together with S^{2-} or HS^-, type B metals form insoluble sulfides in the abiotic environment and strong complexes with proteins (such as metallothionein within organisms). Typical examples of this group are Ag^+, Au^+, Hg^{2+}, and Tl^{3+}. Borderline metals include different cations of a) Co^{2+}, Ni^{2+}, and Pb^{2+} (which are closer to type A), and b) Cd^{2+}, Cu^+, and Tl^+ (which are closer to type B).

Some metal-ligand complexes are lipophilic and can easily accumulate in the fatty or oily tissues of organisms. Examples are metal alkyls and metal aryls, e.g., triphenyltin[19] or methyltin[97]. Alkylation can occur during normal metabolism and biomethylation and has been reported for Ge, Sn, As, Se, Te, Pd, Pt, Au, Hg, Tl, and possibly Pb.

Pure *organic compounds* may exhibit characteristics that either act in favor of high BCF values, or favor rather equal distributions between compartments. Factors enhancing high BCF figures are:

1) lipophilicity,
2) low water solubility,
3) low molecular charge and degree of ionization,
4) small size of the molecule,
5) low biodegradability.

(1) and (2) are directly related to each other in a physicochemical sense, in that non-ionic molecules are most easily dissolved in a similar solvent (such as fat or oil) and least in a polar solvent (such as water). (3) and (4) have to do with the passage through biological membranes. Beyond a relative molecular mass of 500–1000 and/or a molecule diameter of about 1 nm, the passage capability is substantially reduced. (5) describes biochemical features that co-determine the extent of bioaccumulation; degradation rates will become notable where they approach the level of uptake or elimination rates.

Metabolism (or biotransformation) and excretion mechanisms act as counterreactions to bioaccumulation. Or-

ganic compounds can be metabolized in such a way that water solubility and urinary excretion increase, whereby the toxicity is often diminished. A counter example to the latter, however, is the transformation of parathion into paraoxon, which is more toxic, or of heptachlor into its epoxide. The basic biochemical transformation steps are similar in microorganisms, plants, and animals, and comprise essentially oxidation, reduction, hydrolysis and conjugation reactions. Plants often exhibit relatively slow, but more complete transformations and will store metabolized compounds or their conjugates in the cytoplasm or within vacuoles. Animals will usually rather excrete part of the pesticide (or its conjugate or degradation product).

The problem of the rate constants

Important structural system characteristics of bioaccumulation processes are the rate constants. They can be defined for the physical transport of substances from one locality to another (e.g., moving water with solutes in the soil or in the xylem of plants) and to processes like reversible or irreversible binding. If all rate constants were very high, thermodynamic equilibria could easily explain all observed bioconcentration phenomena. However, non-equilibrium conditions resulting from slow physical transport and/or chemical reactions often dominate in ecological systems. Unidirectional mass transport can occur in atmospheric winds and precipitation and in water bulk flows (as solute transport in the xylem and also phloem of higher plants as well as blood or hemolymph circulation in many animal groups). Another unidirectional transport mechanism, important for cell membranes, is active transport, a mechanism under metabolic control.

Non-directional transport and other physico-chemical reactions that all have specific reaction rates include diffusion, precipitation, ion exchange and complex formation. Compared to other processes in nature, such as water bulk flow in ecosystems or within plants, and the blood circulation system of animals, some chemical and biochemical reactions that are important for the fate of environmental pollutants are slow (such as degradation of DDT), whereas others are fast, such as complexation of metals by different kinds of ligands and protein binding by xenobiotics. While in the first case physical transport models will be of great importance, thermodynamical equilibrium models often provide the appropriate basis for an estimation of the distribution of various chemical species in a small-scale reaction compartment. Nevertheless, reaction rates differ substantially for different reaction types:

Complexation constants for metals and natural ligands show a large variability. In hydrated metal species of, e.g., the type $M(H_2O)_6^{2+}$, the loss of a water molecule in exchange for a ligand molecule ('L') is usually the rate-determining step for complex formation. Exchange rates covering the range between 0.1 and 10^9 per second are

found for metal cations like Li^+, Na^+, Rb^+, Cs^+, Ca^{2+}, Sr^{2+}, Ba^{2+}, Cu^{2+}, Cr^{2+}, Cd^{2+}, and Hg^{2+} (cf. [80]). Organic xenobiotics within organisms are formed as solutes in free solution or bound to certain structures, for example to special receptor sites, as in an enzyme-substrate complex (important for substances acting as pharmaceuticals), or to plasma or tissue proteins forming reversible aggregates. This latter association is not very specific and is generally known as protein binding. The adsorbed organic molecules are in equilibrium with the solutes in the ambient water phase. In vertebrate circulatory systems, it is the albumin fraction that provides many kinds of binding sites, involving hydrophobic and ionic interactions as well as hydrogen bridges. The fraction of the molecules of a given organic compound that are bound will not be able to pass biological membranes, and thus not get into subcellular structures responsible for biotransformation (i.e., these molecules become less available for the target receptors). The exchange rate between the liquid phase and the adsorbate is a rather fast organic reaction with a typical half-life time of 20 ms [20]. This high rate explains fast and effective reversible binding both during bioaccumulation and elimination processes, e.g., at the blood passage through gills.

5. Compartments and kinetic modelling

Chemicals in ecosystems are always more or less concentrated in some subsystems (or compartments) and are exchanged between subsystems at specific transfer rates. In a very general sense, the interactions between chemicals and major ecosystem substructures can be simply expressed in a diagram (fig. 4, top). In the following, some structural features of the biota subsystems are discussed.

For complex biosystems, the bioaccumulation theory is based on concepts similar to pharmacokinetics [63]. Although long-term exposure of organisms to environmental contaminants is qualitatively different from short-term drug-administration, the underlying concepts are nevertheless similar and can be transferred from one situation to the other. Early studies about distribution and elimination of organic compounds, e.g., diethyl ether [26] or ethanol [93], were already carried out some decades ago. The term 'pharmacokinetics', however, was introduced into the scientific literature only on the publication of Dost's book in 1953 in German [16], and came into wider use in English-speaking countries in the 1960s. Other important books on the topic include those by Atkins [2] and Wagner [89]. In the 1970s, compartmental theory came into general use in ecological turnover studies with organisms (e.g. [39,66]) and was soon applied for the study of the bioaccumulation of pesticides [9,25,32,41,67,78].

Compartments can be formulated on an abstract basis from the kinetics of uptake and elimination. Although compartments are basically defined as idealized stores,
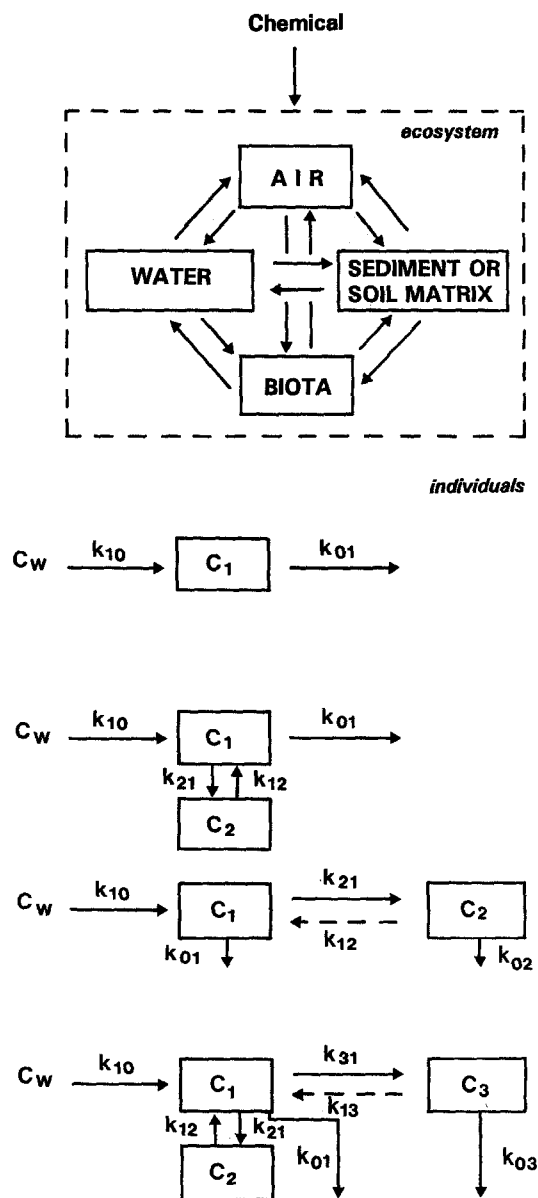

Figure 4. *Top*: General subsystem concept of mass transfer in ecosystems, including the aspect of chemical dissipation and concentration. *Below*: General compartmental concept of bioaccumulation in individuals, representing one- to three-compartmental systems, including one-way excretory metabolic pools in models III and IV; the environmental compartment in these representations is considered to be compartment zero. Notation of the fluxes is adapted from those used by mathematics and physicists, i.e., the first index of the constant rate (k_{ij}) refers to the destination compartment (i), the second to the source compartment (j).

realistic modelling involves the correlation to physical or biological structures and functions, such as metabolic pools or physically-defined fractions. These models will then allow physiological (or ecophysiological) interpretations of the observed kinetics in an animal, a plant, or another environmental subsystem. For lipophilic chemicals, physical sub-systems within organisms will usually include the fat mass of the body.

The most simple model is a one-compartment model according to the uppermost version (model I) in figure 4

(lower part). The rate constant (or rate coefficient) for the input mass flow is usually designated as k_1 or k_{in}; the rate constant of the output mass flow from compartment 1 is k_2 or k_{out}. In more complex system structures, it is convenient to characterize each transfer rate by a double index: Ecologists often use the notation k_{ij} for the transfer rate from element i to element j; the more common usage in compartment theory, however, is the notation k_{ji} (e.g.[1,10,13,14]). Whereas the first version seems more logical at first sight, in that the index letters are written in the order of the elemental transfer, the second corresponds formally to the matrix notation (with i being the row number and j the column number) and is thus more consistent with generalized m × n compartment models. In multi-compartment models with more than one inlet or outlet constant, the single constants are usually called fractional rate constants.

The second model is a two-compartmental model: C_1 represents the concentration in compartment 1, e.g., the whole body except for a high-concentration compartment C_2. The latter may represent the fat store (for lipophilic compounds) or a metal-binding protein (such as metallothionein in animals) or complexing acid (such as citric acid in plants). The third model has no store compartment, but instead a metabolic compartment, where the chemical is transformed into an excretory product (usually a more hydrophilic compound). Since this transformation is enzymatically controlled and practically unidirectional, the backward reaction can be neglected. The fourth model, finally, combines the model versions II and III.

BCF_s values, as explained above on a phenomenological basis, can now be defined for the various compartmental structures (the subscript 's' indicating steady state conditions):

$BCF_s = (C_1/C_w)_s$ for model I,
$BCF_s = (p_1 \times C_1 + p_2 \times C_2)_s/C_w$ for models II through IV (p_i indicating volume or mass fraction of whole reference size).

In the first case, the relationship between BCF_s and the rate constants is given by:

$BCF_s = k_{10}/k_{01}$ (model I)

whereas the relationships for models II through IV are much more complicated. It should be mentioned that metabolized products are usually not included in calculations of BCF_s values. Besides, when mass fractions in compartment models are used (as in the above definitions of BCF_s in models II through IV), they should not be based on mass units in metabolic systems, since the molar mass of the metabolic reaction product is usually not identical to that of the original compound. Suitable units are moles per volumes or mass.

6. Three case studies

Uptake and accumulation by higher plants

Lipophilic compounds can enter a terrestrial plant over the entire surface area of root and shoot parts. In the shoot, an inlet path is provided by diffusion through the wax layer of the leaf. In the root area, many lipophilic substances, like traditional insecticides, cannot pass the plasmalemma. They are transported only within the cell walls from cell to cell by apoplasmatic transport[44,45]. They will predominantly remain in the root area and be translocated only partly. Herbicides, on the other hand, can pass the plasmalemma by means of a mostly active, energy consuming process. The translocation within the plant occurs primarily through the xylem, to a minor extent through the phloem backwards from the leaves. PCBs seem to be actively taken up by some food plants, but uptake intensity varies for different plant species. TCDD is not usually actively taken up either by leaves or by root cells, as was found on the occasion of the Seveso accident in 1976. According to experimental results, the final concentration found within plants is approximately the same as in the soil environment[74]. Phthalic acid esters are probably taken up primarily via the gas phase[90]. Some *metals* are taken up by plants predominantly at the apical root region, others are taken up over the entire root surface. When metal uptake by roots is high and the concentration in the soil is low, metal uptake will often be limited by diffusion. Where diffusion rates are low compared to uptake rates, a metal ion depletion zone adjacent to the root surface will occur. The roots would therefore rapidly deplete the soil around their surface of metal ions, if the roots had not the capacity of continuous growth. Metal uptake (and more generally nutrient supply) depend on both the uptake capacity of the root (and mycorrhizal fungi) and the growth characteristics of the root system. The uptake of metal ions by epidermal and cortex cells seems to be by active transport, at least in some cases, for example for K^+ and Na^+ and some anions (Cl^-, SO_4^{2-}, NO_3^-). Whether transport into the xylem is passive or active is a problem still to be resolved, especially for other metal cations[80]. In the xylem, heavy metals will usually only be transported if special chelates are formed, e.g., by citrate. A general overview of metal speciation in the soil system and uptake mechanisms by plants is summarized in figure 5 (according to Streit and Stumm[80]).

Some ions can pass leaf surfaces, a fact sometimes agronomically used by foliar applications of nutrients. In such cases, metal movement into the plant seems to involve diffusion through the cuticle and uptake by leaf cells. Foliar deposition from anthropogenic aerosols has been reported to occur to a great extent, but the extent and the mechanism of lead uptake by the plant leaf are a matter of debate. The volatile selenium species, dimethyl selenide, biomethylated by microorganisms, may be taken up by terrestrial plants and thereafter as-
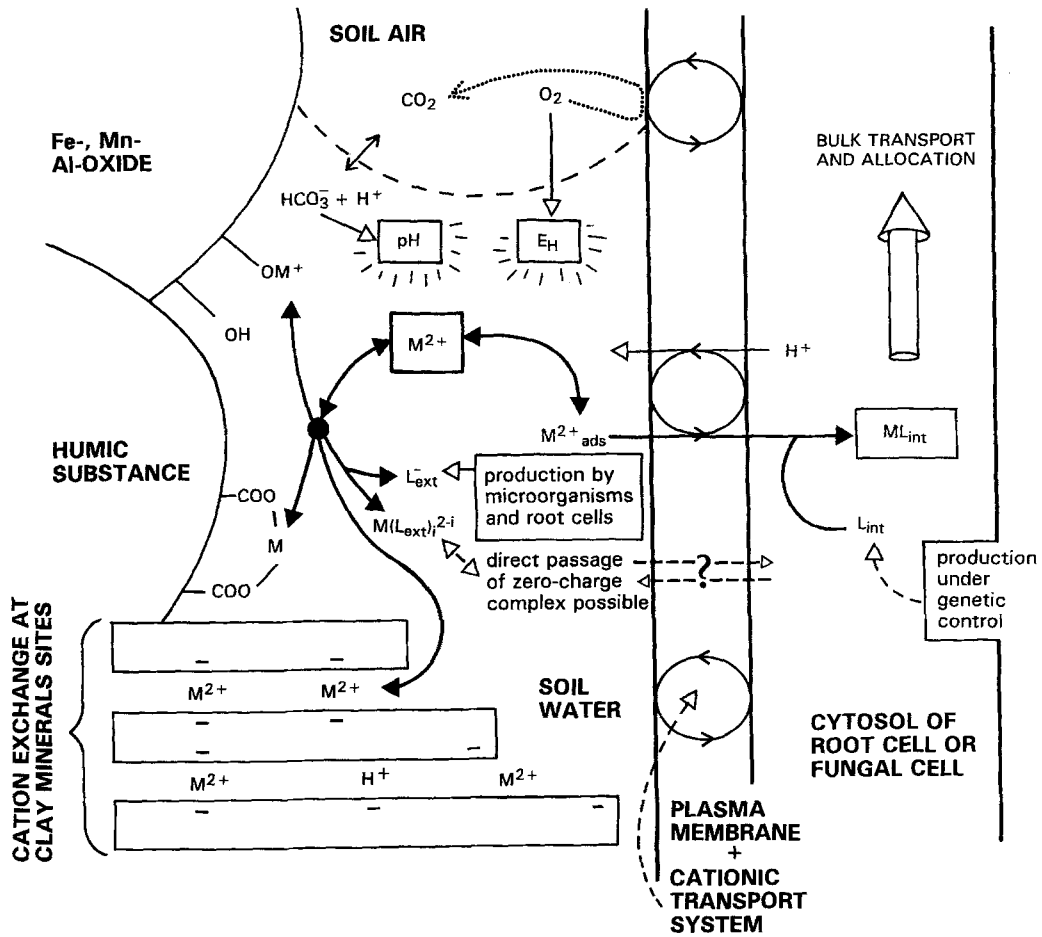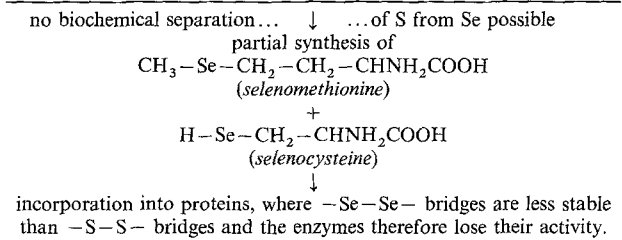
Figure 5. Metal uptake in higher plants: Metal speciation in soil solution and on soil surfaces, and root metal ion uptake, assuming a divalent metal cation (M^{2+}) and a monovalent soluble external ligand (L_{ext}). Uptake rate into the cell and binding to internal ligands (L_{int}) is deter-

mined (in a given individual) by the number of metal ions bound to receptor sites on membrane transport molecules, e.g., metal ion ATPases. From Streit and Stumm[80].
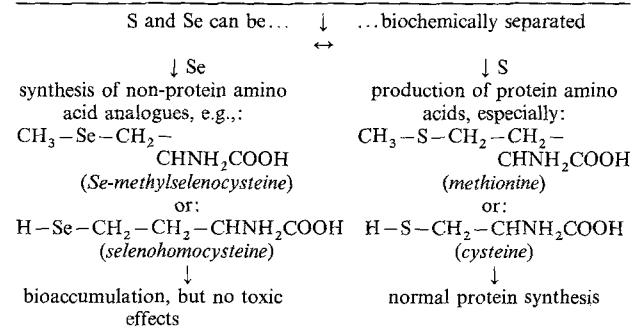
similated[80] (table): whereas normal plants cannot differentiate between sulfur and selenium, adapted plants can, and these plants sequester selenium compounds to become bioaccumulated as amino acid analogues.

Bioaccumulation in plants is usually expressed as metal mass per unit mass of plant dry material. The calculation of BCF values is possible on the basis of soil dry mass, but is not usual. Absolute bioaccumulation figures can be compared for different plant species, which has often been done for plants from sites that are naturally rich in certain metals. Some species or ecotypes can accumulate certain metals considerably more strongly than other plant species in the same locality, often by a factor between 10 and 1000 and have therefore been called 'hyperaccumulators'. These plants often grow in environments where the fraction of available metal ions in the soil is high. For nickel hyperaccumulators which concentrate up to several 10000 ppm (= several %) on a dry mass basis, citric and malic acids are considered to be the complexing ligands which allow these high concentrations to develop in the leaves of those plants, like the New Caledonian tree *Sebertia acuminata*[62, 65]. Hyperaccumulation of chromium has been found in the form of the

Adaptation and bioaccumulation of selenium in plants, according to Streit and Stumm[80].

I: Normal plants, grown in presence of Se

no biochemical separation... ↓ ...of S from Se possible
partial synthesis of
$CH_3-Se-CH_2-CH_2-CHNH_2COOH$
(*selenomethionine*)
+
$H-Se-CH_2-CHNH_2COOH$
(*selenocysteine*)
↓
incorporation into proteins, where $-Se-Se-$ bridges are less stable than $-S-S-$ bridges and the enzymes therefore lose their activity.

II: Adapted plants, grown in presence of Se

S and Se can be... ↓ ...biochemically separated	
↓ Se	↓ S
synthesis of non-protein amino acid analogues, e.g.,:	production of protein amino acids, especially:
$CH_3-Se-CH_2-$	$CH_3-S-CH_2-CH_2-$
$CHNH_2COOH$	$CHNH_2COOH$
(*Se-methylselenocysteine*)	(*methionine*)
or:	or:
$H-Se-CH_2-CH_2-CHNH_2COOH$	$H-S-CH_2-CHNH_2COOH$
(*selenohomocysteine*)	(*cysteine*)
↓	↓
bioaccumulation, but no toxic effects	normal protein synthesis

trioxalatechromate(III), e.g., in *Leptospermum scoparium*, accumulating up to 2% or 20000 ppm[38].

Bioaccumulation in terrestrial food chains

Plants are only one of the sources for contamination in subsequent food chains. Other sources come from the physical environment directly, for example from ambient soil, water, and atmosphere. Some uptake and bioaccumulation characteristics for metals and lipophilic compounds will be summarized in the following:

Metals can enter soil-living animals not only from ingested food, but to some extent also through the entire epithelial surface, as for example in earthworms[72]. In terms of biomass, earthworms are often the dominating part of the invertebrate fauna and an important food source in the food chains, e.g. for birds. Steady state concentration figures for heavy metals in worms were found to correlate with available concentrations in the soil, as with plants, although the earthworm skin has not the primary function of nutrient uptake, as have plant roots. Thus, steady state bioconcentrations are increased with increasing levels of available metal ions in the soil, as is shown with copper in figure 6. In experiments it is often difficult to distinguish between metals taken up through the epidermis and metals taken up by ingestion.

The various metals differ in accumulation behavior, which in part has to do with their different physiological function[77]. Overall copper concentration seems to be well controlled within the earthworm body, whereas cadmium and probably also lead are accumulated much more strongly and not readily released again[72,77].

µg/g in earthworm

$$y = 11.38 \times x^{0.47}$$
$$r = 0.906, \quad p = 0.001$$
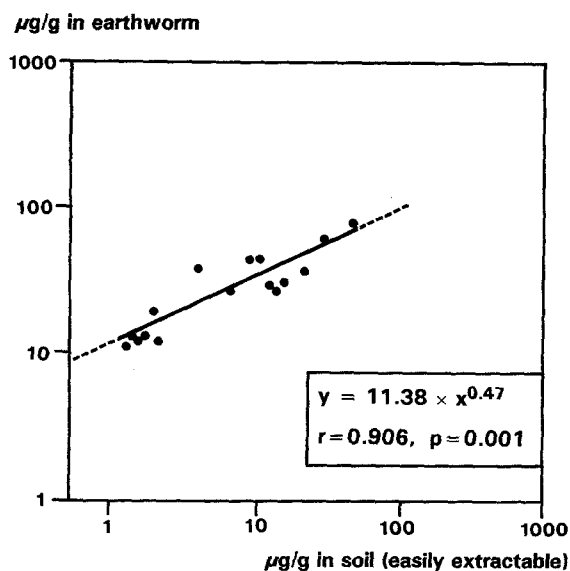
µg/g in soil (easily extractable)

Figure 6. Copper concentration in various earthworm genera, as found from experiments and field observations. While correlations between internal copper in worms to total copper in soils are weak, correlations are highly significant when based on the 'easily extractable' copper fraction in the soil (as defined by extraction with 2.5% acetic acid or with DTPA). Modified from Streit[72].

Uptake and elimination of heavy metals have also been studied in many other terrestrial animals, such as blackbirds, that feed predominantly on earthworms[92].

Lipophilic compounds. Lipophilic compounds can enter soil organisms by food ingestion as well as by skin permeation. In species that have developed thick cuticular structures, such as many dry-resistent arthropods, the input path through the gut content is the more important one. In soft-body organisms, such as earthworms, a direct uptake over the entire surface is possible and highly likely, at least as an additional uptake path to absorption within the gut system; results on bioaccumulation with earthworms resemble relationships found for aquatic organisms and depend on the concentration in the soil solution[87]. Primary consumers feeding directly upon plants, such as phytophagous insects, will receive their burden of xenobiotics on the one hand from the plant tissue, on the other hand, at least in certain cases, from atmospheric depositions. Primary consumers as well as detritivores are the basis for many food chain bioaccumulation processes in terrestrial ecosystems.

Many areas that are now free from usage of persistent pesticides or open application of PCBs still show considerable contamination in higher trophic levels. This is easily revealed by residue studies in field populations, even in forest ecosystems. In Central Europe, we can still detect many PCBs, HCH isomers, and DDT metabolites in the biota today, nearly 20 years after prohibition, for example, of DDT. Results similar to those from North America (e.g., from studies on starlings in the USA[8]) show that PCBs and DDE are still the predominant contamination compounds of the persistent organochloride type (DDE is a metabolization product of the once widely-used DDT).

In contrast to aquatic communities, we do not find a kinetic equilibrium with the ambient water system or any other medium in birds, mammals, and many other terrestrial animals. The renal or biliary excretions are very low for persistent lipophilic organochlorines. Thus, we find an internal distribution equilibrium between fat tissue on the one hand, and aqueous phases as well as adsorptive sites (such as albumins) on the other. If fat depletion occurs as a consequence of starvation or metabolic switch, large amounts of stored chemicals may be set free and become potentially hazardous in the remainder of the body. Developing eggs, which are rich in fat, also become highly contaminated. Further contamination of the developing juvenile and the adult bird will depend very much on the food source.

In a survey of a Central European oak wood system[94], the concentrations of 15 organochlorine chemicals (PCBs and pesticides) were measured in a food chain system during the breeding period: Oak leaves (*Quercus robur*), various caterpillar species, and the Great Tit (*Parus major*). During the breeding period, Great Tits feed mainly on insects, such as the caterpillars studied. During other periods of the year the birds mainly eat various kinds of
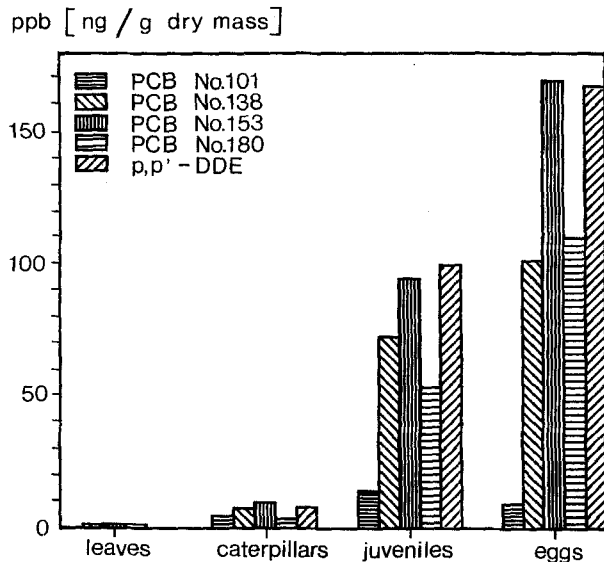
ppb $\left[\, \mathrm{ng} \, / \, \mathrm{g} \;\; \mathrm{dry} \; \mathrm{mass} \,\right]$

Figure 7. Bioconcentration of PCBs and a DDT metabolite (all organochlorine compounds) in the food chain oak leaf – caterpillar – Great Tit (*Parus major*). Figures represent ng substance per g dry mass (i.e., ppb [dry mass based]). Eggs from bird samples had higher concentrations than the juveniles due to the result of the dilution effect in the growing biomass. From Winter and Streit[94].

plant material. The concentrations of PCB 153 (2,2', 4,4', 5,5'-hexachlorobiphenyl, the most abundant in this study) were found to be as follows: in leaf material ca. 1 ng/g, in caterpillars 10 ng/g, and in birds' eggs 170 ng/g on an average and on a dry mass basis. The contamination of the caterpillars was therefore about 10 times higher than that of the plants; this corresponded with the different fat content of caterpillar vs leaf material. The birds' eggs, however, received their organochlorine burden from the mother bird and showed much higher concentrations. The concentrations in the developing juveniles reflected more and more the burden of the insect diet during the period of feeding by the adults, so that concentrations became slightly reduced again. A summary of the results is given in figure 7.

Bioaccumulation in the aquatic environment

In principle, *heavy metal* uptake and bioaccumulation in the aquatic environment are similar to the situation in the soil for plants and soil-living animals. Heavy metal concentrations in algae and aquatic animals are typically several orders of magnitude higher than the concentration in the ambient water[74]. Aquatic algae usually take up metals via the formation of coordination complexes with specialized transport ligands in their outer membranes, and metal uptake is determined by the interplay between redox, complexation, or oxide dissolution reactions of metals in seawater and ligand-exchange reactions at these sites[81]. Some metals are heavily chelated by organic ligands in seawater, and their biological availability is determined by the concentrations of free metal ions or kinetically labile inorganic chemical species (e.g., copper and zinc). Considerable differences exist between taxonomic groups of algae in their requirements and bioaccumulation of nutrient and non-nutrient metal cations. The kinetics of adsorption and uptake of Cu(II) by *Chlamydomonas*, for example, have been found to occur as a fast pseudo-adsorption equilibrium with the surface, followed by slow diffusion-controlled uptake into the inside of the cell[98].

Experimental studies on the uptake of *lipophilic organic compounds* in animals usually reveal a hyperbolic function, resulting from direct uptake from the aqueous phase and steady state conditions. Characteristic accumulation and elimination curves are shown in figure 8 for the herbicide atrazine in freshwater leeches. The elimination often follows a two-phase pattern characteristic for many xenobiotics[48]. In fishes, elimination is possible via the gills, the kidney, and biliary excretion (leaving the body through the end gut). Whereas a fast exchange rate is observable for elimination through the gills, the slower excretion rates by the two other paths are based on metabolism leading to more water-soluble compounds, such as the glucuronide and sulfuric acid derivatives[24, 47] (fig. 9).
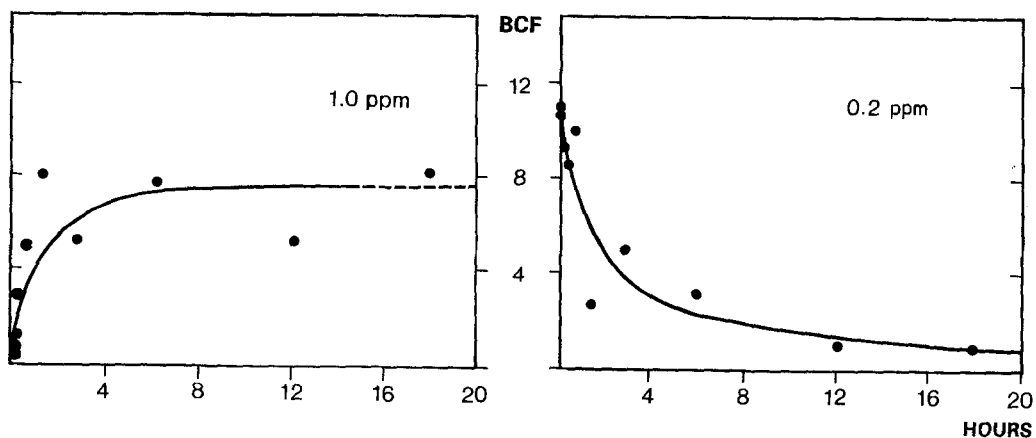

Figure 8. *Left*: Increase of BCF for the herbicide atrazine by direct bioaccumulation from the ambient water in the leech *Glossiphonia complanata*. *Right*: Decrease of BCF from *Glossiphonia complanata*. Absolute initial BCF is higher than in the uptake experiment, because the lower experimental concentration in the water phase (0.2 ppb vs 2 ppm) resulted in higher BCF_s values, as shown by the sorption isotherm principle in fig. 10. Both figures from Streit and Schwörbel[78] and Streit[75].

page 965, caption, figure 8:　　in column 2 read '. . . (0.2 vs. 1.0 ppm) . . .', as printed also within the figure.
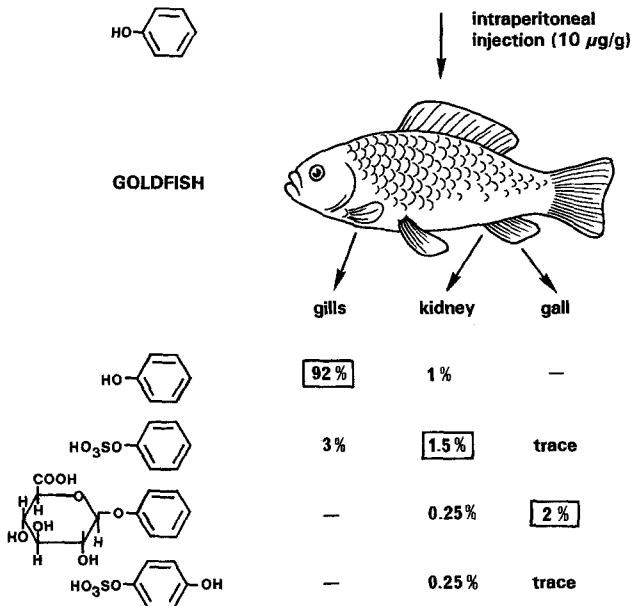
Figure 9. Metabolism and elimination of phenol in the goldfish, four hours after intraperitoneal application (10 μg/g). In mass balance studies of fish individuals, elimination occurs primarily via the gill passage, only to a low percentage via kidney or biliary excretion after partial metabolization. From Nagel[47].

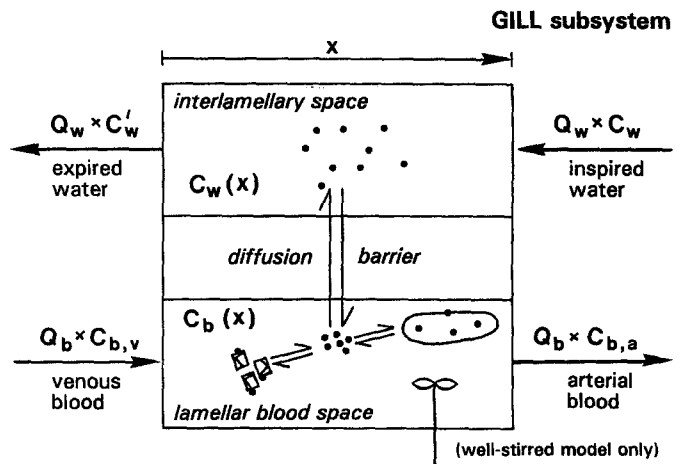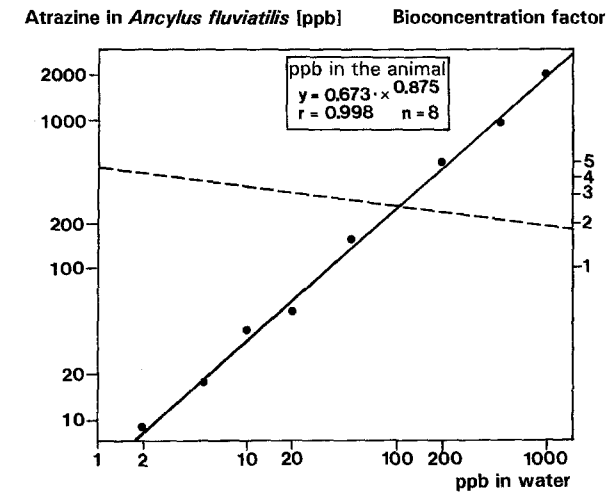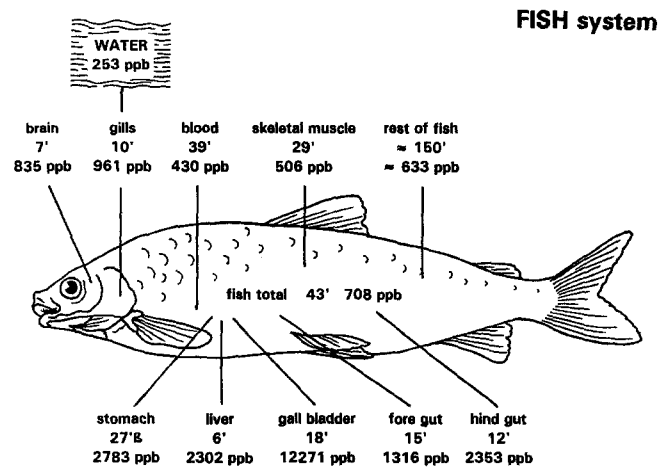**Atrazine in *Ancylus fluviatilis* [ppb]   Bioconcentration factor**

Figure 10. An example of a sorption isotherm: The concentration of the herbicide atrazine in freshwater limpets is a double-linear function of the concentration in the ambient water. The left ordinate and the continuous line indicate absolute concentrations within the animal (on a fresh mass basis), the right ordinate and the broken line indicate the steady state bioconcentration factor (BCF_s). From Streit[67].

BCF values are higher for low concentrations in the ambient water than for high concentrations. The underlying principle is a sorption isotherm, which can be approximated for lipophilic storage over a wide range of concentrations by using a Freundlich adsorption isotherm[67−69] (fig. 10).

Compartmentalization has been studied primarily in teleost fish species. An example of atrazine uptake by a 5 cm long fish is represented in figure 11, top[25, 73]. The same concentration as in the ambient water (253 ppb or

ca 1 μmol/l in this experiment) was found in the gills only 10 min after the transfer from clean into contaminated water, and even sooner in some inner organs, like the liver (6 min). Due to the high fat content of the liver, this organ accumulates chemicals from the blood stream very rapidly, and these will eventually reach higher concentrations than in the gills or the blood itself. The highest concentrations in this study were reached in the gall bladder, possibly as a result of the biliary metabolization and excretion process. The study, despite relatively high experimental concentrations, illustrates well the fast uptake kinetics of lipophilic contaminants through gill surfaces.

FISH system

GILL subsystem

Figure 11. *Top:* Fish system. Uptake of atrazine by teleost fish, showing experimental results found for 5 cm long whitefish (*Coregonus*). Ambient water concentration of atrazine was 253 μg/l (ppb). Indicated are a) the time in minutes for organs to reach the ambient concentration, and b) the final steady state concentrations. The uptake path was predominantly via the gill. From Gunkel and Streit[25] and Streit[73], altered. *Bottom:* Gill subsystem. Schematic representation of the gills' mass transfer system across the epithelial diffusion barrier, including possible interactions of chemicals with albumin and blood cells in the secondary lamellar blood space. Adapted from Streit et al.[79]. Calculations were performed based on two different types of models: a counter-current model on the one hand, assuming a space dependent distribution of the compound along the lamellar longitudinal axis, and an arterial well-stirred model with a well-mixed lamellar blood compartment on the other hand.

The importance of the gills as exchange organs has since been intensively studied with respect to gas molecules by Piiper and Scheid[61], and with respect to xenobiotic exchange by other authors[7,57]. Further, models for chemical exchanges and diffusional barriers were discussed[4,23]. The outline of a detailed model of the gill subsystem and the protein binding of organic pollutants in fish is shown in figure 11, bottom[79]. We could show that the highly efficient transfer of xenobiotics from ambient water into the fish system is essentially based on the presence of blood proteins, such as albumins. (Independently, a similar model from a slightly different approach was developed by other authors[18], and was submitted for publication in the same month). A general multi-input-output linear system theory of bioaccumulation, with special reference to the fish gill system, has also been devised[63].

More complex aspects of chemodynamics include food chain relationships, but so far only preliminary theoretical studies have been presented. An example of a compartmental approach to food chain bioaccumulation in aquatic environments for different organic compounds was proposed by Thomann[84].

7. Populations, biosphere and technosphere

Communities do not consist of chemically and reproductively isolated individuals, but of *populations*, that exhibit a continuity of generations and that may show physiological as well as genetic adaptations to environmental stress, for example with respect to genotype composition. Community changes can result from environmental pollution, in that sensitive species may become sparse or extinct, and new and insensitive colonizers fill ecological niches. Increasing population densities, which result in functional importance for ecosystems, are encountered in an increasing number of introduced species, e.g., in many freshwater systems throughout the world. Some recent anthropogenic introductions include, for example, the zebra mussel (*Dreissena*) and the clam *Corbicula* in North America and Europe, and the amphipods *Gammarus tigrinus* and *Corophium curvispinum* in the river Rhine[75]. For many introduced species either a general tolerance for moderately polluted conditions was found, or even specialized enzymatic insensitivity. As an example, the immigrant *Gammarus tigrinus* is more tolerant against organophosphates than the endemic species, *G. pulex* and *G. fossarum*, in the Rhine river system[37]. Such experimental results are in agreement with current observations of steady faunal changes.

Environmental scenarios of pollutions allow us to evaluate current models and theories of chemical stress and bioaccumulation, as well as constantly to improve them for more general use. An unexpected large-scale 'contamination experiment' occurred in November 1986 near Basel in Switzerland, when a high level of chemical pollution was caused by the accidental release of agrochemi-

cals, including organophosphate insecticides, into the river Rhine. The pollutants were observed to flow downstream at a speed of roughly 100 km per day, and reached the Netherlands about two weeks later. Dilution, longitudinal dispersion, abiotic hydrolysis, oxidation by singlet oxygen, and biological transformations were probably the dominant processes that determined the time-course of the change of concentration of the organophosphate load. Model calculations based on these physico-chemical processes coincided with concentration measurements at different localities of the river, as exemplified for disulfoton in figure 12, top[91]. Data from this accident were used for realistical model calculations of sublethal and lethal effects (Streit and Kuhn, in preparation), as well as to model general bioaccumulation scenarios for lipophilic compounds in large rivers. Assuming a Gaussian type curve, the bioaccumulation of a lipophilic substance (which behaves similarly to, e.g.,
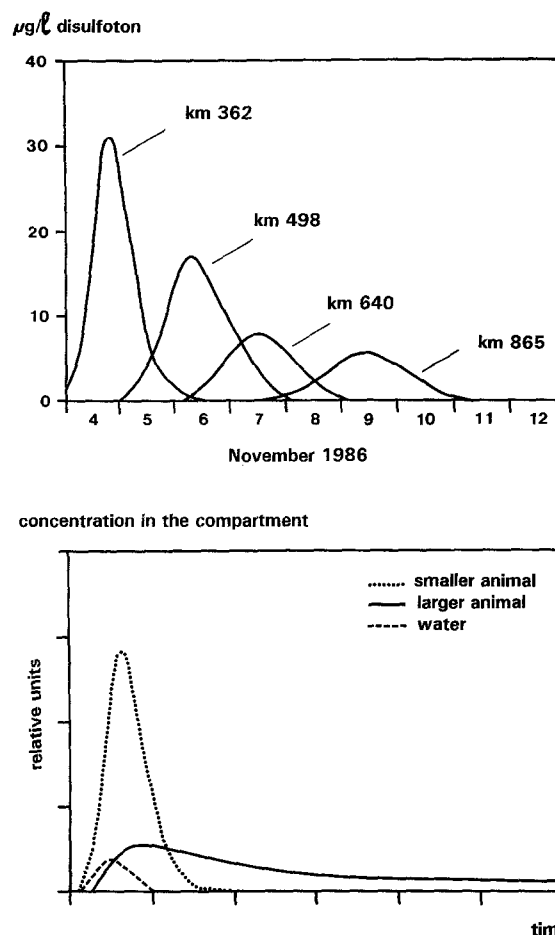

Figure 12. *Top:* Model calculations of concentrations for the organophosphate disulfoton in the river Rhine after an accident near Basel in 1986. The model includes transport rates, dilution und hydrolyzation rates and fits observed data at different localities (indicated by offical km figures). Modified from Wanner et al.[91]. *Bottom:* Computer models indicating bioaccumulation figures in model organisms. The parameters are based on a compound with a lipophilicity similar to that of lindane; time units represent approximately day units; BCF (t) units roughly represent the value of 10 each (unpublished results).

lindane) would result in concentration time-courses like those in figure 12, bottom. BCF will increase and decrease fast in small animals of 2 mm length, like small crustacean species, but slower in slightly larger animals of 2 cm length, like larval fish. Measurements made some time after the time of maximum concentration in the water could erroneously be interpreted as a pure food chain effect, assuming that the 'young fish' ate the 'small crustaceans' (their natural food) which would have resulted in a biological magnification in analogy to mechanisms suggested in figure 1. However, the various BCF figures in this model are the result of different input rates of the pesticide from ambient water as a pure result of different body sizes and therefore different kinetics.

The influences of man-made chemicals on ecological communities are complex and are not confined to the bioaccumulation process. Sublethal or lethal effects on individual populations and communities are measurable in the laboratory, but are usually difficult to transfer to field conditions. Communities do not consist of steady state populations with deterministically controlled population sizes, as was generally assumed until the 1970s. Population interactions are more of a stochastical type, including exogenous stochasticity resulting from unpredicted environmental influences, and endogenous stochasticity, resulting from demographic instabilities. Natural population sizes often undergo fluctuations that look similar to chaotic behavior, and make analyses of natural populations under chemical influence as difficult as prognostic statements about future community developments. Population sizes of introduced species often undergo an initial overshoot before decreasing as the result of new prey-predator relationships or competition effects (cf. also Streit[75] for examples from the river Rhine).

Because of the unpredicted and often chaotic behavior of populations (in a mathematical sense), effects of chemicals in moderate concentrations on complex communities may be hard to detect, to prove, and to model. Effects have sometimes been misinterpreted from short-term experiments for two reasons. 1) Implicit complexities (including, for example, all kinds of adsorption processes in the ambient water), were neglected on the laboratory test scale. Such effects may actually result in lower toxic effects in the field. 2) Subtle sublethal effects at the population interaction level were not found in monospecific laboratory tests, so that the toxic effects were underestimated.

There is a scientific as well as an economic need for developing realistic models of bioaccumulation processes as well as for the toxic potential of all technically-produced chemicals. Both the number of registered and industrially produced products and the number of chemical derivatives and of biochemical metabolites in the environment are increasing. Adequate models will help us to understand environmental chemodynamics. The potential impact of new or unknown compounds should ideally be estimated even before the substance has been synthesized, thus saving time and money[11]. A high bioaccumulation potential of a chemical does not necessarily mean a high toxicity potential[43]; thus toxic effects have to be measured separately. Testing bioconcentration factors, degradation, and toxicity for short- and long-term periods is expensive. Costs are usually of the order of tens of thousands of Ecus (corresponding roughly to US-$) per chemical (including only those tests that are absolutely required and specified by the law).

The fact that it is an interdisciplinary topic at the interface of ecology and economics is one impetus encouraging the study of bioaccumulation, especially of organic chemicals. Another comes from general biology and the nature of organisms themselves: the accumulation of inorganic or organic nutrients is a fundamental property of and a prerequisite for life since its origin. Phenomena which developed in natural environments during evolutionary times suddenly face modern chemical constituents of the biosphere, which actually is a physically and chemically altered 'technosphere' today. But life-mechanisms are basically traditional, and evolved millions of years ago in mostly unpolluted environments. The study of interactions between biological entities and environmental pollutions is a fundamental field of biological and ecological concern. It is frequently embedded in debates on ecology vs economy, biology vs technology, and conservation vs growth and production policies.

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