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Chapter SubTitle	
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Abstract

We performed a rational reconstruction of the relationship between biogeochemistry and the study of ecological productive systems. A structural and a functional possibility for building biogeochemical integrated models with optimal complexity have been identified. The conceptual framework was then applied to metals in contaminated areas. Metal mobility results from the interaction (coupling) of environmental entities at a multitude of scales. We classified for the managerial interest the processes involved in metal mobility by their range of scales in "site" specific and "region" specific, and then detailed the processes involving theoretical entities specific to soil science, hydrology, and ecophysiology. In the end, we pointed out some consequences of the coupling between processes of different scales for the risk assessment of contaminated sites.

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Chapter 19
Contributions to the Theoretical Foundations of Integrated Modeling in Biogeochemistry and Their Application in Contaminated Areas

V. Iordache, R. Lăcătuşu, D. Scrădeanu, M. Onete, S. Ion, I. Cobzaru, A. Neagoe, F. Bodescu, D. Jianu, and D. Purice

19.1 Introduction

This chapter is a continuation and development of the ideas introduced in a review of integrated modeling in metals biogeochemistry (2009). We attempt here to make operational steps toward the research direction identified there. Two types of integrated models have been identified in the mentioned review: models integrating biological and abiotic processes, and models integrating processes of the same type (biological or abiotic) occurring at different scales.

Integrated modeling efforts are not specific only to metals biogeochemistry, but also to all other areas characterizing from different perspectives the planetary productive systems (ecological, socioeconomic, or socioecological). One can

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E. Kothe and A. Varma (eds.), *Bio-Geo-Interactions in Metal Contaminated Soils*,
Soil Biology, 31, DOI 10.1007/978-3-642-23327-2_19,

even say that integration is underdeveloped in metal biogeochemistry. But fully covering all approaches for integrated modeling in environmental sciences in order to extract lessons to learn is a matter of writing a book, rather than a chapter. However, a screen of several examples from the literature can easily reveal the main trends.

What is at stake is to use knowledge (and models) developed in different disciplines in order to solve more complex problems, cross-cutting the disciplinary fields. There are two strategical trends: one is to react to the existence of many individual models developed disciplinary and to try ad-hoc integrations without paying much attention to relevance of the integrated model for the real coupled processes. The second is more proactive and suppose the development of new research areas conceived from the start as interdisciplinary.

The first (reactive) strategy is illustrated by the platforms/frameworks for linking existing models (reviewed by Argent et al. 2006). An example of software framework for integrating reusable components describing hydrological processes are Branger et al. (2010), one of a software platform for integrating existing models is Kraft et al. (2010), and an example of technical aspects raised by the integration software are illustrated by the work of Schmitz et al. (2011).

For the second, proactive strategy examples are the development of hydropedology and ecohydrology. Lin (2003) is a promoter of the integration between pedology, soil physics, and hydrology within a new disciplinary field hydropedology. His review uniquely points out the problems related to linking data and scale specific to separate disciplines, and is followed by conceptual developments (Lin 2010a, b) aimed at catalyzing the development of the new discipline. No consequences for integrated modeling in practice seem to have been generated by this effort by now, excepting for the estimation of pedotransfer functions (Pachepsky et al. 2006), suggesting that classic hydrological approaches are still dominant (Kohne et al. 2009). But, the accent of Lin and coworkers on data and concepts coherentization is a better strategy than hurrying up for integration of old models within and between disciplines. Following general recommendations for the evolution of hydrology ("cross-disciplinary integration must become a primary characteristic of hydrologic research" – Wagener et al. 2010), ecohydrology is an effervescent field for modeling coupled processes on a realistic base, from basic data, not by integrating previously developed disciplinary models (Hwang et al. 2009). The scale dependence of the studied processes in ecohydrology is in the top of research priorities in this field (Thompson et al. 2011).

The above two examples are bilateral integrations. How far can one go with this trend? Are there conceptual limitations for integrated many disciplines, as many as needed in biogeochemistry for dealing with biological and abiotic processes at large scale? Such limitations have been signaled within each discipline. For instance, besides technical aspects precluding integration and model performance in hydrology (Buytaert et al. 2008; Kavetski and Klark 2011), there are also general conceptual problems and attempts to solve them by alternatives to the current approaches (Schaefli et al. 2011 in hydrology), but have been not systematically characterized for large-scale ecological systems.

The extreme form of integration would be a holistic one (Odum 1995). Even more ambitious is the holistic research and integrated modeling of socioecological systems (Seppelt ~~1993~~). In this line of thinking, there is a recognized need for a holistic, integrated approach in metal biogeochemistry and in ecotoxicology (Matyssek et al. 2006; Breure et al. 2008). But, the accent of the holistic approach is more on the biological part of the ecosystem (methodology of systems identification Pahl-Vostl 1995), and less on the heterogeneity of the abiotic part. Most of the abiotic part of the holistically conceived ecosystems remain unstructured in systems ecology description, and are put under general headings such as biotope, or hydro-geomorphic unit. These abiotic features are characterized in detail by other scientific disciplines, such as geomorphology, soil science, hydrology, and hydrogeology.

In this chapter, we explore the following questions:

1. Is there an optimal level of integration for understanding the biogeochemical role of abiotic and biological objects, larger than the bilateral interdisciplinary integrations exemplified above, but smaller than the holistic integration?
2. If there is such optimal level of integration, to what extent is it practically possible to produce such integrated models?

The ideas introduced here have roots in previously published theoretical work (Lăcătuşu and Iordache 2008; Iordache et al. 2009, 2010a, b; Iordache 2010). They have been developed in the frame of biogeochemical interdisciplinary research programs (Neagoe 2007a, b; Petrescu 2007; Kothe 2009) in order to conceptually support the modeling of effects of local management measures in contaminated sites on processes occurring downstream in the contaminated catchments.

19.2 Basic Characterization of Productive Entities

We first introduce a concept of complex object based on properties following Ryan (2007), as different from the concept of complex object in standard system analysis. The new concept will be used later in describing the general form of a productive entity.

The nested hierarchical spatial partitioning is the most convenient approach in modeling spatial processes. Band et al. (2000) use this for watersheds and include one-dimensional ecosystem models in the patches. Also, Thompson et al. (2011) recently express their confidence in the usefulness of emergent properties in understanding the relationships across processes and scales in catchments. Mathematical modeling in standard systems analyses paradigm requires as a first step systems identification, i.e., the definition of boundary, components, and interactions. For a spatial model, one has to choose a spatial extent (spatial scope) and a granularity (spatial resolution), and the scope is assumed to be the size of the investigation area (Seppelt 2003). Then this is said to be the scale of the modeled object. While in the case of time scale, it is accepted that a model can include slow and fast processes as they are in reality, the system boundary is *defined* by the modeler and associated for spatial models with one scale. This kind of approach leads naturally to nested hierarchies of environmental objects by the simple association of the discretization units of space and to the emergence of *new* and irreducible properties at each hierarchical level in terms of new processes characterizing that level, an idea difficult to accept if the higher level system results exclusively from lower level systems. Such a model can then be regionalized by changing the model parameters and eventually the model structure in function of the spatial location of the discretization unit, and simulating the model in each grid cell. Alternatively, a spatially explicit model, which allows exchange of matter between the spatial units can be built (Seppelt 2003). In both cases, no explicit coupling between entities of the same or of different scales is conceptualized. This single scale raster cell is assumed to represent an ecosystem and the aggregated cells a landscape.

Ryan (2007) notices that using emergent hierarchies to give account for emergence is circular and propose to define emergence by the extent (scope) of the system whose emergent properties are observed. This spatial extent can be wider or narrower depending on the scale of observation. Instead of starting the individuation of the object by delineating the boundaries of the system, one starts with the set of properties and finds the scales of observation at which those properties emerge. Then the complex entity is characterized by a multitude of scales of observation, its boundaries being the reunion of the boundaries of the subentities characterized by properties observable at certain scales. This view developed from general physics perspective is convergent with the idea that at least some environmental objects are multiscale not only in time, but also in space (developmental systems, Iordache et al. 2011). From this perspective, a model “flattened” at a single scale is always a stiff system *sensu* Seppelt (2003). The variability in space of the state variables within the classic space–time boundaries of the system may reflect the ontologic diversity of its subsystems, and ignoring this is simply not realistic enough for scientific purposes. The main advantage of this concept of complex object is that allows an objective, independent from the researcher, allocation of spatial scales to the environmental entity. The ontological structure of the system is ensured and not sacrificed from the start in order to reduce the dimensionality of the model.

We assume that a procedure for producing a model of a complex entity such as above involves three steps. Step 1: define extratheoretical objects at scales xi, step 2: measure/observe properties at scales xi, step 3: define/model complex multiscale theoretical environmental object at scales xi by lawful connection between measured/observed properties.

Now we can introduce a concept of productive entity developed elsewhere based on a reconstruction of Darwin’s “Origin of species,” the first book dealing implicitly with the ecological (nature’s) productivity (simplified from Iordache 2010). A productive entity ”*i*” is a system of the following form:

(P_i, I_i, G_i, I_j, G_j, M_i^{rel}, M_j^{rel}, S, M^{ob}) where properties which should be characterized using an observation model, theoretically independent from the structural model S, are:

P_i, a property or a set of properties describing the biological production of the entity *i*, with *i* from 1 to *n*, where *n* is the populations size and $n \geq 2$ (biomass, or number of descendants)

I_i, a set of observable properties at space–time scales smaller than the maximal scale of the organism *i* (parts, genes, etc.)

G_i, a set of properties observable at the maximal scale of the organism

I_j, sets of observable properties at space–time scales smaller than the maximal scale of the organisms *j*, with *j* from 1 to *n* excepting for *i*

G_j, sets of properties observable at the maximal scale of the organisms *j*, with *j* from 1 to *n* excepting for *i*

M_i^{rel}, a set of relational properties between the organism *i* and its environment (the "subjective" environment of the organism *i* characterized from the perspective of the scientific observer)

M_j^{rel}, sets of relational properties between the organism *j* and their environment, with *j* from 1 to *n* excepting for *i*, the "subjective" environment of each organism from the perspective of the scientific observer

M^{ob}, intrinsic and relational properties (different from M^{rel}) of the environment, the "objective" environment of the organisms from the perspective of the scientific observer

S is the structure of the system of properties described above. S is characterizable by a structural model decomposable into a production law L expressed by an unknown mathematical function (submodel, "subjectivistic model" in Iordache et al. 2009) of the form $P_i = L\ (I_i, G_i, I_j, G_i, M_i^{rel}, M_j^{rel})$ and one or many coupled structural models of environmental entities characterized by the properties M_i^{rel}, M_j^{rel} and M^{ob} ("objectivistic models" in Iordache et al. 2009). For productive objects without competition the production law reduces to $P_i = L\ (I_i, G_i, M_i^{rel})$. The coupling between production submodels and objectivistic models occurs at the level of M^{rel}. The coupling between productive submodels takes place at the level of P and M^{rel} (P or a property structurally linked to P – I or G – in a productive submodel is M^{rel} in another productive submodel).

The potential unit of selection is a system (P_i, I_i, G_i, M_i^{rel}, S) describing the development of the organisms (developmental system, DS, Iordache et al. 2011, as an extension of the homonymous concept of Oyama, e.g., Oyama et al. 2000). For selection to occur, the following conditions should be fulfilled.

The condition of finite lifetime: the lifetime of the potential units of selection is finite.

The condition of coupling: M_i^{rel} and M_j^{rel} are not decoupled in space–time (i.e., with independent dynamic) at the existence time scale of the units of selection (i.e., either these properties characterize environmental objects which from the perspective of the observer – by M^{ob} – are the same for all organisms, or are characterize parts of a complex environmental object, which are in causal relation at the existence time scale of the units of selection).

The condition of scarcity: to have scarcity in the productive object (for the reason of space we will not develop this here; in short, it is a condition linked to the functional relationship between P and M^{rel} such as to have "struggle for existence").

The condition of variability: to have variability of the values of I_i and/or G_i and/or M_i^{rel} in such a way that P_i would be different (i.e., the fitness would be different). This condition is needed for sorting the units of selection by P_i. AU6

In the absence of the conditions for selection and by eliminating the condition the $n \geq 2$ one has the general structure of a productive object. The relevance of this structure for the biogeochemistry of metals comes from the fact that metals are in this abstract model both at the level of I properties (internal resources or toxicants for the organism), at the level of M^{rel} properties (external resources or potential toxicants for the organism), and at the level of M^{ob} properties (part of the structure of the objective environment linking the organisms, where transport takes place).

This model of productive objects implicit in the "Origin of species" cannot be studied operationally as a whole because of its extreme complexity. But Darwin work (in the interpretation associated with the reconstructed model) puts the bases for a research program of biology. The multiscale system of coupled productive systems in the ecosphere can be studied only by disciplinary fragmentation and discretization. Current systems biology tries, for instance, only to relate I and G properties, while biogeochemistry works in investigating the circulation of elements only with G, M^{rel} and M^{ob} properties. Other environmental disciplines such as hydrology focus only on some of the M^{ob} properties, or on some of the G, M^{rel} and M^{ob} properties in the case of more integrated developments such as ecohydrology. The way of discretizing the physical space, which includes the productive object controls the solution to the "ontology" problem much studied by computer scientist from the database and knowledge base design perspectives (Sui and Maggio 1999; Pundt and Bishr 2002), and the way of representing the real productive system model is linked to the problem of relational data bases in GIS (Cova et al. 2002). The discretization in space–time for research purposes is needed both for well delimited objects and for fields (e.g., mobile masses), although it is appropriate for describing the environmental reality only in the first case. In the case of fields, the partitioning into discrete pieces is needed for accommodating the finite computing environment (Bian 2007, a source nicely reviewing the object-oriented representation of environmental phenomena).

The scales of the productive entity are the space–time scopes and the minimal associated resolutions at which the properties can be observed. Lifetime is the scope in time of an entity, whether biotic or abiotic. Characterizing the entity only by properties (without reference to scales) is not enough for meaningful individuation of the productive entity. Modeling the productive systems makes physical sense only within its range of ST scales, so the relevant mathematical properties of the model are only those characterized within these scales. A productive entity is multiscale by its different properties. The maximal such scale is *the* scale of this complex object. The same ideas apply to other complex objects. For instance, *the scale of an organism* is the scope of the physical space–time needed by an individual to develop its lifecycle, a function of both the size of the organism and its

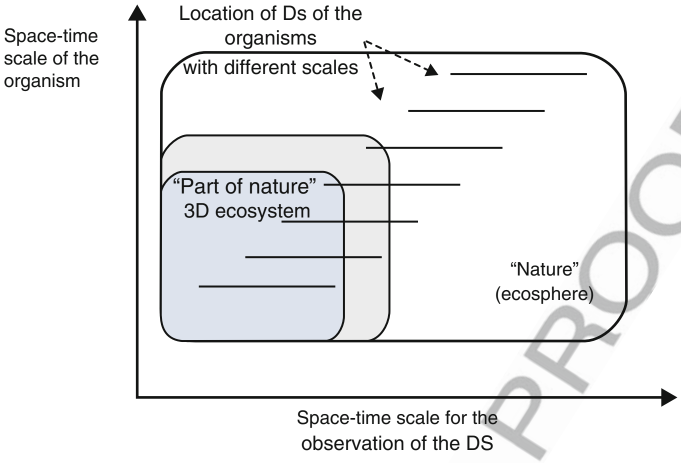

Fig. 19.1 Relationships between three-dimensional (3D) ecosystems in space (or “parts of nature” in Darwinian terms) and the space–time scale of organisms and of their developmental systems (DSs). The point is that always some parts of the DSs will be out 3D physical space delineated by convention as ecosystem for management reasons. The DSs in this situation at one ecosystem scale (hierarchical level) are apparent structural emergent properties at higher level in the hierarchy of ecosystems. See Iordache et al. (2011) for other representations supporting the same idea

mobility in space, and the minimal resolution needed to observe the characteristic processes of the lifecycle (Iordache et al. 2010). It can be dynamic along the lifecycle length.

Due to the multiscale character of the DS, the discretization of the physical space of the ecosphere in nested three-dimensional units (nested hierarchies of ecosystems) will always cut the continuum of scales in such a way that some of the DS will have parts outside the ecosystem (Fig. 19.1). In Iordache et al. (2011), we have analyzed this situation working only with the biological objects from the DS and demonstrated that the obtained hierarchy of ecosystems is not a true one (with true emergent properties at each level), but a pseudo-hierarchy, with new structural subsystems at each pseudohierachical level not arising from the interaction of the parts, and with the possibility to cut the hierarchies across scales on subjective grounds (according to human interests).

Two important consequences result from this discussion with respect to the need for integrated modeling. The first one is that there is no need to study the function of the whole three-dimensionally delimited ecosystem in order to understand the role of a population of certain organisms in that ecosystem. This is important when at stake is to understand the role of a service production unit (Luck et al. 2003), and not all the mechanisms supporting the biogeochemical services provided by the ecosystem. A simpler, with minimal complexity, homomorphic model can be built according to the structure of the DSs of those organisms [see, for example, ectomycorrhizal fungi in Iordache et al. (2011), and arbuscular mycorrhizal fungi in Neagoe et al. (2011b)]. The second is that it makes little sense to study the circulation of one element (e.g., a heavy metal) in the DSs identified by the homomorphic model separately from the circulation of other elements playing the role of resources or toxicants (e.g., in the case of plants from the circulation of nitrogen or phosphorus), because all of them influence the productivity of the DSs. Based on these ideas in Neagoe et al. (2011b), a concept of biogeochemical role of organisms has been proposed, and a concept of integrated biogeochemistry. In other chapters of this book, (Neagoe et al. 2011a; Jianu et al. 2011) the role of abiotic objects (organic matter, minerals) is investigated in the same framework.

Next in this chapter we further develop these ideas by looking at two aspects. In part X.3, we look at the way of coupling biological and abiotic objects resulted from the discretization in space–time of the productive objects at multiple scales. At stake here is how to produce a homomorphic model of a productive object with the general form introduced above [note that in Iordache et al. (2011), we limited the methodology of homomorphic model construction to the biological compartments without taking into detailed analyses the abiotic objects]. In part X.4, we synthesize from the literature the processes of different scales occurring in two common types of management units in contaminated areas, sites (from smallest scale environmental process up to 10^5 m^2) and regions (processes from 10^5 to 10^{10} m^2). In the same part, we screen the ontological assumptions of soil science and of catchment hydrology, and the possibilities of coupling between theoretical objects of these disciplines and selected groups of organisms. In the end of the chapter (part X.5), we extract several applied consequences of this theoretical framework for the risk assessment of contaminated areas.

19.3 Theoretical Framework for Coupling Environmental Entities in Order to Characterize Scale-Specific Processes in Productive Entities

Once one has discretized the multiscale productive system into environmental objects with well-defined positions in space–time (either specific to the observation model, or to disciplinary theories independent of the observation model), its reconstruction depends on how the interactions (the coupling mechanisms) between the environmental objects are conceptualized.

A *coupling mechanism* is the process of interaction between at least two entities explaining a pattern observed in one or all entities (for example, either in the entity with smaller substance turnover rate – distribution pattern of metals in soil as a result of the interaction with atmosphere, or in the entity with larger turnover rate: in distribution pattern of metals in organisms as a result of the interaction with soil). A coupling mechanism suppose the existence of at least two scales of observation: that of each entity involved in coupling, and that of the complex entity resulted from coupling. A coupling mechanism in nature takes place by an exchange of substance and energy between the coupled entities, i.e., is a causal mechanism. However, there is no need for a speak in terms of bottom-up and top-down causation, as the multiscale nature of the complex systems does not entail necessarily true hierarchies of systems (Iordache et al. 2011).

The *scale of coupling* is the scale of the coupling mechanism, is implicitly the *scale of the process*, and is the space–time scope and minimal resolution at which the interactions of two subentities with the same or different scales of a complex system can be observed. The ontological condition for coupling, and implicitly for the complex entity, is the existence of a causal relation (a process) between the coupled entities at the scale of coupling. Not everything is coupled to everything because of the limited lifetime of the entities and the fact that causal connections occur in time. Processes cannot interact, only distinct entities by processes. A *pattern* is the distribution of a measurable variable in space or in time within the scope of the coupling between two entities, and is caused by this coupling. Resolution is the minimal fragmentation of the scope at which a variable should be measured in order to observe the pattern.

The *scales of the external entities with value* (EV, characterized by M^{rel} properties in the general model of productive entities) for an organism are the scales of coupling between an organism and other abiotic or biotic entities with positive or negative value for it. The scale of the organism is the maximal scale at which one should estimate the objective (from the observer perspective) distribution in space–time of the entities with values for an organism. Figure 19.2 shows a general representation of a pseudohierarchy of environmental entities.

The *scale-specific mechanisms of metals mobility* are the coupling mechanisms between environmental entities involving fluxes of metals and causing the generation of patterns in the space–time distribution of metals. Within this framework, it does not make sense to speak of scale-specific processes of metal mobility in general, but only within multiscale entities, when we are looking for explanations

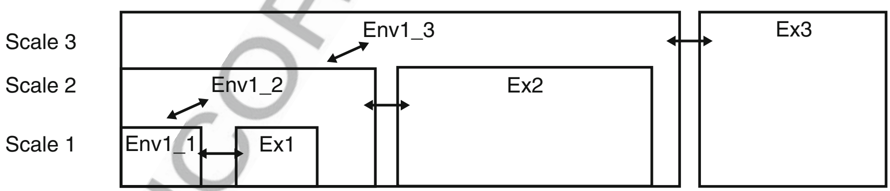

Fig. 19.2 General representation of a pseudohierarchy of environmental entities (Env) showing the coupling mechanism with external entities (acronym Ex, *continuous arrows*) at each scale, which generate scale-specific patterns, and implicitly the partial decoupling (*dashed arrows*) of the larger scale patterns from smaller scale mechanisms and associated patterns. The environmental systems Env1 from scales 1 to 3 (e.g., soils, biological systems, hydro-systems, ecosystems, socioeconomic systems) are not a true hierarchy of nested systems, as usually approached in a systems analyses context, but only a pseudohierarchy including in their structure new entities at each scale (usually conceptualized as external driving "forces", or forcing functions in a nested hierarchy paradigm). In order to observe the complex environmental entity Env-Ex, one needs a scope of observation larger than the scope associated with the scale of Env or of Ex taken separately

of a mechanismic type. The fact that such processes are reported in the literature separately by discipline means only that disciplinary knowledge is waiting for integration.

Conceptualizing coupling mechanisms is trivial in abstract terms, but is far from trivial when one works with entities defined and characterized in scientific disciplines with different traditions. This is the case of biogeochemistry. In this case, conceptualizing the coupling involves a translation between the entities assumed in each discipline in terms of scopes and generally accepted (transdisciplinary) measurable properties. The first problem in modeling the coupling mechanisms or in upscaling and downscaling is to conceptualize relationships between entities developed under different scientific paradigms. The external entities represented in Fig. 19.1 may not be of the same type or may be even complex systems (think at the influence of bedrock geochemistry on the patterns of metals in soil, in comparison with metal patterns generated by solid phase inputs from industry, by atmospheric phase inputs from industry, or by atmospheric inputs modulated by different vegetation roughness covering the soil). The external entities may be from the perspective of the observer of a larger scale than the coupling scale (think, for instance, at the coupling between a mycorrhizal fungi and a plant).

The patterns in one entity resulted by the coupling with external entities at the coupling scale is dependent to some extent also on smaller scale processes occurring in the entity manifesting that (target) pattern. In this sense, there is a partial internal decoupling of the target scale pattern from smaller scale internal processes due to the external coupling at the target scale.

By *role* of a variable in the mobility of elements, we understand the causal influence of a variable in a coupling mechanism in producing the outcome of a process involving it. The *role* of a subsystem of the coupled entities (characterized by a variable) is specific to the coupling scale. The fluxes resulted from this role at the coupling scale propagate to larger or smaller scales (these effects at distance could eventually be labeled as indirect roles). Neagoe et al. (2011a) explore the role of organic carbon in the mobility of metals, and Jianu et al. (2011) characterize the role of mineralogy.

One important use of the above framework, and actually the research problem which pushed us to its development, is in modeling the effects of local processes at large distance in space–time (Fig. 19.3). From the existence of large distance effects, it results that an indirect role of a variable in metal mobility can be not only across scales, but also at the same scale if the effect is localized at distance in space–time.

19.4 Scale-Specific Processes in Metal Biogeochemistry

In order to build models with the general structure presented in Fig. 19.3, a first step is to have an idea about the scale specific to various processes involving environmental entities. Based on a literature review and our own expertise, Tables 19.1 and

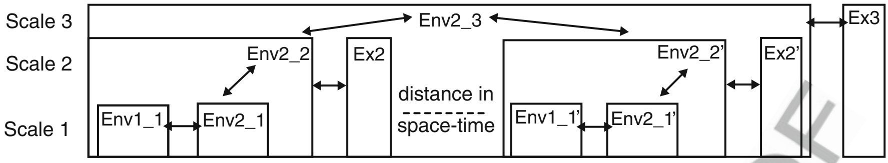

Fig. 19.3 General representation of the structure of a model in an integrated approach in order to assess the effects of local processes involving metals at one space–time location on other local processes at large distance in space–time (designate by '). Env1_1 can be a tailing-dam or a mining dump or a polluted soil, or a complex soil-vegetation entity. Env2 (scale 1–3) can be hydro-systems, Ex2 can be geomorphological, pedologic and microclimatic entities in the landscape, Ex3 geologic and regional climatic features of a larger catchment, and the model could attempt to predict the effects of local phyto-remediation of a contaminated site in the slope area of a small catchment on late and distant bioaccumulation of metals in crops in an agricultural floodplain site. The coupling at the same scale and between scales is based on variables characterizing the coupled entities. Successive up-scaling and downscaling of some variables are needed in order to predict ST large-distance effects of local changes

19.2 show a synthesis of the site (from smallest scale environmental process up to 10^5 m^2) and region (10^5–10^{10} m^2) specific processes of metal mobility by various pathways. The larger literature body supporting this synthesis is not presented here for reasons of space, but some aspects will be detailed in part X.5.

These processes generate patterns in metal distribution at different scales, and what we have to do is to separate by modeling and in situ observation the patterns generate by the processes of interest from the patterns generated by other processes. For instance, the contamination of the floodplain in the vicinity of a smelter can occur both by hydrological processes and by atmospheric deposition, and we have to separate the effect of sedimentation during floods from the effect of particles deposition.

From a different perspective, because multiscale experiments are a useful strategy in designing the remediation of sites contaminated with metals we performed, we also underlined the specific processes which can be investigated by such experiments at each scale (Table 19.3).

In the sense of this chapter, biogeochemistry is interdisciplinary and deals with the mobility of elements in three-dimensional (physical) volumes (sites, regions, etc.) hosting complex systems formed by coupled entities fully or partially located in that physical volume. Such clearly delineated in space entities are management units providing local resources and services and having large distance effects on the local resources and services production in other sites. The processes specific to this approach result from the multiple coupling between entities occurring in a three-dimensional physical space volume. Each simple couple of entities support phase specific, multiphase abiotic or biological processes. Thus, what is specific to interdisciplinary biogeochemistry is the complexity of the processes, and not the scale. We define then a scale-specific process in metal biogeochemistry as the complex process resulting from the multiple coupling of the entities involved in processes occurring at a certain scale in a three-dimensional physical space.

t1.1 **Table 19.1** Site-specific processes involved in metals mobility

	Scale	Transport pathway of metals	Mechanism
t1.2	Scale	Transport pathway of metals	Mechanism
t1.3	Part of soil column 10^{-8} to 10^{-4} m^2	Various	Chemical and microbiological weathering
t1.4	Part of soil column 10^{-4} m^3	Biological	Microbiological direct and indirect (by organic carbon) immobilization/mobilization for hydrological fluxes
t1.5	Rhizosphere	Biological	Microbiological direct and indirect (by organic carbon) immobilization/mobilization for plants
t1.6	Soil column 10^{-8} to 10^{0} m^2	Hydrological	Diffusion and dispersion
t1.7	Soil column 10^{0} m^2	Various	Other biological weathering (by plants, invertebrates)
t1.8	Soil column 10^{0} m^2	Hydrological	Colloidal transport
t1.9	Soil column 10^{0} m^2	Hydrological	Soluble transport
t1.10	Soil column 10^{0} m^2	Hydrological	Soluble complexes transport
t1.11	Soil column 10^{0} m^2	Hydrological	Preferential flow (vertical)
t1.12	Soil column 10^{0} m^2	Biological	Bioaccumulation in soil invertebrates with low mobility
t1.13	Bioaccumulation area 10^{-2} to 10^{4} m^2	Biological	Plant uptake (bioaccumulation in plants)
t1.14	Field 10^3–10^4 m^2	Hydrological	Unsaturated (preferential) flow (to groundwater)
t1.15	Slope area 10^2–10^4 m^2	Hydrological	Infiltration excess overland flow (dissolved and particulate)
t1.16	Slope area 10^3–10^5 m^2	Hydrological	Retention in and remobilization from transversal buffer zones
t1.17	Bioaccumulation area 10^3–10^5 m^2	Biological	Bioaccumulation in mobile epigeous invertebrates
t1.18	Large slope area 10^3–10^6 m^2	Hydrological	Saturation excess overland flow (dissolved and particulate)
t1.19	Large slope area 10^4–10^8 m^2	Hydrological	Subsurface storm flow (lateral flow)

t1.20 Shaded areas indicate processes crossing the site-region scale boundary

The complexity *of the model* can further increase by coupling besides processes at the same scale, also processes between scales. This is the most interesting case (coupling both at the same and between scales, Fig. 19.2), because this provides an operational approach for studying the effects of local management actions in space–time at large distance.

In order to make operational this general framework for contaminated sites management, one needs to compare the ontologies of soil science, hydrology, and population ecology to identify scale-specific patterns of metals distribution reported in each discipline, and to infer the coupling mechanisms between disciplinary entities in the cases where one or more variables explicitly or implicitly common are reported to be involved in the generation of the patterns. Fully following these steps is beyond the objective of this text, but we will illustrate the approach in the next chapter.

Table 19.2 Region specific processes involved in metals mobility t2.1

Scale	Transport pathway of metals	Mechanism	
			t2.2
Region 10^4–10^{10} m^2	Hydrological	Groundwater flow in different types of aquifers	t2.3
Region 10^4–10^8 m^2	Atmospheric	Dry and wet deposition from local sources	t2.4
Bioaccumulation area 10^4–10^8 m^2	Biological	Bioaccumulation in mammals and in nonmigratory birds	t2.5
1st order catchment 10^5–10^6 m^2	Hydrological	Retention in and remobilization from transversal buffer zones	t2.6
2nd–6th order catchment 10^6–10^8 m^2	Hydrological	Interactions between types of hydrological flows	t2.7
Region of 10^6–10^7 m^2	Various	Soil catena formation	t2.8
Large order catchment 10^7–10^9	Hydrological	Retention in and remobilization from longitudinal buffer zones (floodplains)	t2.9
Region of 10^6–10^7 m^2	Atmospheric	Volatilization	t2.10
Bioaccumulation area 10^5–10^{12} m^2	Biological	Bioaccumulation in migratory birds	t2.11
Region 10^8–10^{11} m^2	Various	Zonal soil formation	t2.12
Region 10^9–10^{12} m^2	Atmospheric	Dry and wet deposition from distant sources	t2.13

Shaded areas indicate processes crossing the upper scale boundary of regions t2.14

Table 19.3 Processes involved in metals mobility investigated in experiments at different scales t3.1

Name of the system and usual scales	Environmental complex system studied at these scales	Processes, fluxes, effects studied/control variables	
			t3.2
Pot 10^{-2} m^2	Soil + plants	Exploration by root, bioaccumulation/ microorganisms, organic carbon, level and spatial structure of amendments	t3.3
Lysimeter 10^{-1} to 10^0 m^2	Soil + plants + small-scale hydro-system	Same as in pots + leaching, internal redistribution, net outputs/same as in pots + soil structure, hydraulic conductivity, humidity, redox potential on profile	t3.4
Plot 4×10^0–10^2 m^2	Soil + plants + larger scale hydro-system + other organisms	Same as in pots + effects of heterogeneity in space, margin effects, other processes due to external entities (consumers, runoff, etc.)/same as in pots + variables for external entities	t3.5

19.5 Contributions to a Comparative Ontology of Environmental Sciences

19.5.1 Soil Science

From soil science, we refer here only to aspects related to soil classification and mapping. Soils are described for their classification by soil profiles, so the scale of observation is that of a soil column of the order of 1 m^2. The concept of soil column refers to a three-dimensional physical object organized in horizons and having one or more properties, with no equivalent in other scientific disciplines (e.g., gleyc, vermic). These properties are derived from a combination of characteristics indicating soil-forming processes (European Commission 2005). The characteristics comprise single observable or measurable variables. Their relation to the properties is to a consistent extent tacit knowledge of the soil expert (Scull 2009), and for this reason difficult to include in an explicit knowledge base useful for integrated interdisciplinary modeling. Moreover, there are country specific classification schemes, the official classification scheme of the International Union of Soil Science serving only for comparing national soil classification systems (European Commission 2005). It is not explicit in soil science theory if a soil unit mapped at a small map scale is composed (in a systemic sense) of the soil units mapped at a larger map scale in the same area. One cannot identify emergent properties of the soil type mapped at smaller scale compared to the soil types mapped in the same area at larger scale. In a review paper, Scull (2009) goes up to stating that "the soil landscape is continuous and is not composed of distinct individual soil types." Soil classification is in this view only a way to summing up the information obtained about soil columns, the "pedons" sharply represented would not have a strong ontological status as a spatial object.

If this is the case, then what is real in the case of soil? First of all, of course, the soil layer as an integral object extending in space. Another possibility, pursued to some extent in soil science, is to interpret soil as an ecosystem. In this case, the minimal scale ecosystems could be a soil column hosting plants, and larger scale soil ecosystems would go up to the surface needed for supporting a population of large-scale soil organisms (e.g., mobile animals). This approach would work well for biological properties of the soil, and can lead to soil pseudohierarchies with biological apparently emerging properties (actually resulting from the coupling of the soil parts with organisms of different scales). But predicting soil abiotic properties would much more effective by assuming a continuous distribution of these properties in space. Soil columns, such as organisms, seem to be unique and classified only methodologically in the same type; the real entities are soil columns, not the types of soil columns. A better prediction of soil abiotic properties can be done either by refining the soil classification procedure (Qi et al. 2006), or by attempting to detect the space–time distribution patterns of abiotic properties at various scales. Patterns of measurable characteristics (pedochemical, geochemical) can be observed by grid sampling or other sampling methods. In this approach, soil is treated as physical entity, not as an ecosystem.

The patterns of metal distribution in soil reflect internal processes (resulted from coupling between internal entities) and external processes (resulted from coupling of soil with external entities). The coupling of soil with external entities leads to apparent soil pseudohierarchies (Fig. 19.1) with patterns of abiotic parameters as apparently emerging properties. It is interesting to note that the soil manifest separate biotic and abiotic pseudohierarchies. This leads us to the theoretical hypotheses that the pseudohierarchy concept is but one way to reduce the complexity of the environment, more complicated and appropriate that nested hierarchies, but no more than a concept. Studying its mathematical properties is a research direction.

Internal redistribution processes in soil will be discussed in Neagoe et al. (2011a) and Jianu et al. (2011) in terms of the role of organic carbon and mineralogy in the mobility of metals in soil. These internal processes influence the hydrological export of metals, the export by wind and the biological export.

External coupling processes of soil involves the interaction with atmosphere (liquid, particulate and colloidal phases; wet and dry deposition), with hydrosystems (liquid, particulate and colloidal phases (deposition and resuspension), and with organisms (input by organic matter, output by bioaccumulation processes). In terrestrial contaminated areas, the soil has a key role for the investigation of the patterns resulted from external coupling because its turnover time is much lower than that of the biological, hydrological, and atmospheric entities, but higher enough to allow the detection of patterns as a result of these interactions at the scale of human observation. Soil is a more reactive entity than bedrock, for instance, with much higher reactive surfaces because of its fragmentary structure. The reactive inorganic parts in the soil are minerals and organic carbon, whose importance is underlined by their use in soil classification. The soil as physical multiphase entity (solid, liquid, and gaseous) links entities with value for plants and for soil organisms, and provides variables also in hydro-system model (for vertical and runoff flows, etc.). The internal (within soil) distribution of variables is a key for understanding the coupling between plants, soil organisms, and hydro-systems.

The scale of the externally patterns differs with the coupling mechanism: solid waste deposition, bedrock weathering, differential deposition of atmospheric pollutants around industrial sources (gradients and barrier effects), and differential sedimentation from surface hydrological fluxes (lateral and longitudinal buffer zones). Other soil characteristics are controlled by topography, climate, etc., with their different scale of coupling.

Rodriguez et al. (2008) studied the patterns of metal distribution in agricultural soils. They found that the heavy metal concentration is influenced by bedrock composition and dynamics at all the spatial scales, while human activities had a clear effect only at the short- and medium-range scale of variation. There were differences between metals: Cu, Pb, and Zn (and secondary Cd) were associated with agricultural practices (at the short-range scale of variation), whereas Hg variation at the short and medium scale of variation was related to atmospheric deposition (Rodriguez et al. 2008). The multiscale structure of metals in soils is studied also by Xiaoni et al. (2010), who found scale-dependent variability of metals reflecting the existence of pollution hot spots. Lăcătuşu and coworkers extensively studied the distribution of microelements in Romanian soils not only at small resolution on large surfaces, but also at large resolution in contaminated areas (Răuţă et al. 1995; Lăcătuşu et al. 1996). In certain areas, a natural high background of metal concentration due to geologic bed led to important ecotoxicological and human health problems (Lăcătuşu et al. 1993). The distribution patterns of element concentration studied by Galan et al. (2008) have been controlled by the lithology and geochemistry nature of bedrock and by the occurrence of metallogenic belts in the studied. However, not always the natural background in mining areas leads to large concentrations of metals in the soil because of the differences between deep and surface geochemistry (Lăcatusu et al. 2009); review of the geochemical background concepts and of their application is provided by Galuszka (2007). Meirvenne and Meklit (2010) analyzed a data set of 14,674 copper and 12,441 cadmium observations in the topsoil of more the 10,000 km^2 area and identified regional patterns and potential causes (smelters of effects of First World War). However, they eliminated outliers, not being interested in small-scale patterns of distribution (Meklit et al. 2009). By now, we have given examples of patterns only for total metals. The problem is complicated by the factors controlling the availability of metals, such as soil humidity, organic carbon, pH, porosity (Keur and Iversen 2006; Scrădeanu et al. 2010a, b). We will not develop these aspects here, but one should consider also these patterns of distribution when evaluating the mobility of metals at site and region scale.

AU8 AU9

19.5.2 Hydrology

From this disciplinary field, we refer here only on some aspects of surface hydrology, mainly catchment hydrology. The entities assumed in hydrology are hydrosystems, thus entities restricted to the aquatic phases, considered separated from their solid environment, which however controls water movements. The concept of hydro-system includes implicitly external ontological assumptions by the relations of the water with entities determining the types of flows at different scales. In the area of hydrology the distribution across scales of the processes is well documented (Bloeschl and Sivapalan 1995; Bloeschl 2001). Clear is also the fact that in the water quality modeling currently there are no models operating at multiple space–time scales, the integration of processes occurring at different scale being possible only by including separate models in common GIS-type platform (Srivastava et al. 2007). This is due to the coupling between processes of different scale generating nonlinearities in the system (Beven 2006). In this context, integrating the knowledge about processes occurring at different scales and places is a priority in hydrology (Bloeschl 2006). However, this cannot be done restricting the integration only to hydrological processes, because the hydrologic processes

AU10

"emergent" at different scales are controlled by new types of not hydrological entities occurring at those scales (slope areas, geomorphological patterns, geological structures, etc.). Relationships with external biological entities are assumed also by their influence on water flow or chemical parameters (for instance, by microorganisms clogging of pores, or consumption of chemical substances, or vegetation influence of water distribution in soil by evapotranspiration, or of preferential flow in former roots spaces, or increase of the roughness of the surfaces over which the water flows). The study of such coupled ecological–hydrological processes generated an entire research subfield, the ecohydrology (Manfreda et al. 2010).

The sources concerning metal mobility by hydrologic fluxes are numerous, and it cannot be our purpose here to fully cover this body of knowledge, but only give some examples. A hot area in hydrology is the influence of upstream on downstream processes, the fluvial connectivity, especially because of its jurisdictional consequences under water quality regulations (Caruso and Haynes 2010). At catchment level, there is a coupling between upstream and downstream elements in terms of fluxes, there is a partial and decreasing with increasing stream order coupling, but in terms of patterns of distribution in space–time there is not a simply observable coupling. Alexander et al. (2007) found, for instance, that first-order headwaters contribute approximately 70% of the mean-annual water volume and 65% of the nitrogen flux in second-order streams. Their contributions to mean water volume and nitrogen flux decline only marginally to about 55 and 40% in fourth- and higher-order rivers that include navigable waters and their tributaries (Alexander et al. 2007). As for patterns, Saunders et al. (2004) found a decoupling of upland and stream inorganic nutrient patterns at base-flow conditions independent of the season. The longitudinal pattern of the total copper distributions in a large system reflected the balance of flushing, sources, and losses (Chadwick et al. 2004). From an applied perspective, metals dispersal at large catchment scale is a hot problem in the light of Water Framework Directive (Bird et al. 2010). Freeman et al. (2007), also, point out the key ecological role played by headwater streams on downstream processes, in terms of water-mediated transport of substance and energy.

Many factors influence the transit time of elements from upstream to downstream parts of the catchment: intra-catchment topographic variability, catchment area, path length, and slope gradient the aspect of the land surface, factors that influence the local energy budget (latitude of the study site, the ratio between direct and diffuse solar radiation, prevailing winds, and shading due to distant topography) (McGuire and McDonnell 2006; Broxton et al. 2009). A key role in the transit is played by the riparian area. Understanding of the co-occurrence of hot spots and moments for contaminants in riparian systems is essential for designing the management strategies of pollutant removal at the catchment scale (Vidon et al. 2010). At the other extreme of the range of scales, the daily patterns of elements distribution in water are controlled by temperature and the activity of organisms (Tercier-Waeber et al. 2009). For instance, the diel cycle of Fe is controlled by photoreduction and reoxidation processes (Gammons et al. 2005) inducing a diel cycle of other toxicologically important elements. Daily temperature-dependent adsorption onto actively precipitating hydrous Fe and Al oxides can occur, because the adsorption of metal cations onto oxide surfaces is endothermic (Chapin et al. 2007). In a multiscale study of catchments impacted by mining (monthly, daily, and bi-hourly), Nagorski et al. (2003) observed that monthly changes were dominated by snowmelt and precipitation dynamics, that on the daily scale, post-rain surges in some solute and particulate concentrations were similar to those of early spring runoff flushing characteristics on the monthly scale, and on the bi-hourly scale, a diel cycling for pH, dissolved oxygen, water temperature, dissolved inorganic carbon, total suspended sediment, and some total recoverable metals occurred. They found that short-term (daily and bi-hourly) variations of some geochemical parameters covered large proportions of the variations found on a much longer term (monthly) time scale (Nagorski et al. 2003). A review of remote in situ voltammetric techniques to characterize the biogeochemical cycling of trace metals in aquatic systems is made by Tercier-Waeber and Taillefert (2008). Micro multiscale studies of parameters such as porosity (Stockdale et al. 2009) in sediments and soils with appropriate micro-scale technologies (Viollier et al. 2003) are essential for understanding the mechanisms supporting the mobility and bioaccumulation of metals beyond a black-box approach.

In what concerns the groundwater, most of the leachate contamination plumes do not exceed the width of the landfill (Christensen et al. 2001). Metal transport in groundwater at large scale is increased as the sediment permeability increased, and the groundwater pH decreased (Simpson et al. 2004). Acidic groundwater (pH from 3 to 3.5) transported high concentrations of Pb, Cd, Zn, Cu, and Fe at a former battery recycling plant (Lee and Saunders 2003). Seepage of acidic groundwater at the base of tailing dams is common (Lottermoser and Ashley 2005).

The small watershed approach is a valuable tool for understanding the transport and cycling of metals (review in Driscoll et al. 1994, with case studies for Pb, U, Pb, and Al). The biogeochemical controls on metal behavior in aqueous environments involve complex linkages of biological (mainly microbiological) and geochemical processes occurring at microscopic and macroscopic scales (Warren and Haack 2001). Seasonal and spatial variations in metal concentrations and pH were found in a stream at a restored copper mine site (Bambic et al. 2006). Mechanistic studies of the interactions between groundwater and surface water fluxes of metals are, however, very few. Fritz and Arntzen (2007) study the flux of uranium in the hyporheic zone and found an important influence of the river level by changing the groundwater discharge and by dilution of the uranium in groundwater. The discharge of contaminant from groundwater by seepage areas was spatially variable depending on river valley morphology, and in some cases a dilution by uncontaminated groundwater occurred at the seepage point (Fryar et al. 2000).

19.5.3 *Ecophysiology*

The general ontological status of organisms and the case of ectomycorrhizal fungi have been characterized elsewhere (Iordache et al. 2011). Here, we point out the situation of three types of organisms with larger scale: plants, carabids, and birds. We investigate the possibility of characterizing an apparently simple process, the bioaccumulation of metals. These organisms have been selected as representative for the complexity of this problem (estimating the role of organisms in the circulation of metals). What is at stake is how to model the bioaccumulation of metals in such organisms and the toxicological (at individual level) and ecotoxicological (at population level) effects and how to build integrated transport – bioaccumulation models for metals. In order to do this, one needs basic information concerning the scale (in the sense introduced above) of the organisms, and that of the populations (their location in space–time).

Although for plants their scale seems to be very easy to characterize, the situation is not as straightforward as it seems to be. The bioaccumulation from the soil takes from the volume occupied by the roots systems, so one needs to have knowledge about this volume, the heterogeneity of metals distribution in this volume and the root growth strategy. Only the heterogeneity occurring at the scale of the plant affects plant uptake and the leaching of trace elements (Robinson et al. 2006). Very often such detailed information for the species occurring in contaminated sites is not available, so field observations are needed. Deeply penetrating roots such those of trees complicate the problem ~~by making necessary the estimation of metals distribution in the full soil profile.~~ But an even more complicated situation is that of the clonal plants, and this is the case that we want to develop here in order to illustrate the difficulty of computing even apparently simple bioaccumulation factors.

Almost all plants have modular structure (Harper 1977; White 1989). Plants with vegetative spread (clonals) grow realizing sets of shoot or roots units named ramets. Every ramet can survive alone once established in the proper habitat. The modularity combines the transport of recourses among ramets allowing plant to survive in more places in the same time (Oborny 1994; Oborny et al. 2000). It is considered that the ability of connected ramets is their specialization for the usage of local abundant resources, permitting the plants to have great flexibility in adjusting their relative abilities in usage of different resources. Producing different units of shoots and roots, the plants (clonal individuals, synonym with genets) allocate different ratio of biomass for light acquisition for photosynthesis versus water and mineral resources acquisition (Stuefer 1997). From the physiologic point of view, clonal plant acts systemic, the resources are transported from parts of the plant living in resources-rich area to parts of the plant living in resources-poor area. This specialization is based on clonal integration named "labor division" (Charpentier and Stuefer 1999). Clonal plants consists of possible interconnected (via stolons or rhizomes) and repetitive units (ramets). Clonal plants have two reproductive strategies: sexual reproduction via seeds, and clonal propagation via the development of vegetative offshoots from the parents (Canullo and Falinska 2003).

Isozyme analysis of perennial stoloniferous *Glechoma hederacea* (Widdén et al. 1994) in Sweden collected from natural population showed that one genotype might cover 20 m length and 10 m width surface. At *Hylocomium splendens*, the isozyme electrophoresis could identify 25 genotypes among total 75 ramets; most genets (clonal individuals) occurred in one plot (10 cm $\times$ 10 cm), two genets occurred in more than one plot inside of every site (10 m $\times$ 10 m) and four genets occurred in more than one site (separated by 500–1,000 m). The conclusion is that one genet might occupy a surface bigger than 1 km^2. The physiological integration is another problem, but at least in the case of tree clonal plants this can occur over very large areas. Anyway, for clonal plants what is characteristic is that the integration is at the scale larger than that of separately observed ramets.

The morphological plasticity in plants is very important, and in clonal ones even more important. In natural patchy heterogeneous environment, the plasticity in growth form may increase the probability that ramets are placed in the more favorable microhabitats within such environment. In *Carex flacca,* the depth of the shoot below soil surface may vary between 0.2 and 5 m, and rhizome length is separated in three classes: $<$ 5 mm (0), 5–49 mm (5) and $\geq$ 50 mm (50). This evidences that stolon internode and rhizome (“spacer”) lengths may be extremely variable. Tamm et al. (2002) highlighted the ramet lifespan (years) of many species (Table 19.4) and their vegetative mobility (mm/year) in natural wooded meadows. For example, *Fragaria vesca* has 2 years max ramet lifespan with 465 mm/year max vegetative mobility for stolons and 6 years max ramet lifespan with 15 mm/year max vegetative mobility for rhizomes. *Rubus caesius* has 2 years max ramet lifespan for stolons and rhizomes with 595 mm/year max vegetative mobility for stolons and 40 mm/year max vegetative mobility for rhizomes. The internodes that separate the individual clonal units often prove highly responsive to environmental conditions (Oborny 1994).

The “foraging” rule is that the plant tend to “escape” from adverse conditions and to “remain” in favorable ones. Metal heterogeneity in soil may provide such adverse conditions. The plant morphology responds to site quality, meaning the environmental variability induced morphological variability within clone, and this reduced the degree of intraclonal competition. Spatial and temporal effect cannot be separated, thus, proper characterization of the environment exactly on the scale of clonal growth is of special importance. Spatial patterning of plant populations and the relative roles in intra- and inter-specific interactions play an important role in plant adaptation, species interactions (Silvertown and Charlesworth 2001) and community dynamics (Morin 2005). The availability of resources often changes considerably over a broad spatial distance and at different time scale. Clonal species are more likely to explore environmental heterogeneity than nonclonal plants species due to their spatial distribution and the longevity of the genet. Storage of resources is very common phenomenon in clonal plants. Experiencing temporal and/or spatial heterogeneous environments, the resource storage may serve

Table 19.4 Maximum vegetative mobility (mm/year) of some clonal plants from natural wooded meadows (according to Tamm et al. 2002) t4.1

Species/life span	1	2	3	4	5	6	7	8	9	t4.2
Achillea millefolium	202									t4.3
Aegopodium podagraria					645					t4.4
Agrostis stolonifera	135									t4.5
Anemone ranunculoides	32									t4.6
Arrhenatherum elatius	16									t4.7
Brachypodium pinnatum	129									t4.8
Briza media				161						t4.9
Calamagrostis epigeios		275								t4.10
Carex tomentosa		190								t4.11
Festuca arundinacea			90							t4.12
Festuca pratensis					130					t4.13
Festuca rubra		260								t4.14
Filipendula vulgaris						19				t4.15
Galium mollugo	263									t4.16
Galium verum	190									t4.17
Geum rivale								25		t4.18
Helianthemum nummularium	210									t4.19
Hypericum maculatum	152									t4.20
Hypochaeris maculata							12			t4.21
Leucanthemum vulgare			83							t4.22
Lotus corniculatus		70								t4.23
Medicago lupulina		30								t4.24
Melica nutans	136									t4.25
Pimpinella saxifraga						13				t4.26
Plantago lanceolata									4	t4.27
Plantago media			3							t4.28
Poa angustifolia		190								t4.29
Polygala amarella	75									t4.30
Polygonatum odoratum	48									t4.31
Potentilla erecta					10					t4.32
Primula veris							6			t4.33
Prunella vulgaris	144									t4.34
Ranunculus acris		10								t4.35
Stachys sylvatica	350									t4.36
Trifolium pratense			30							t4.37
Veronica chamaedrys	578									t4.38
Veronica officinalis	160									t4.39
Vicia cracca	300									t4.40
Vicia sepium	420									t4.41
Viola mirabilis			72							t4.42

1–9 are the maximum ramet life spans of the species (years). The soil surface and volume relevant for bioaccumulation of metals are constantly increasing each year with species and environmental dependent rates t4.43

ecological functions in similar ways to temporal and spatial heterogeneity, which are partially different from nonclonal species (Suzuki and Stuefer 1999).

Almost 400 plant taxa are classified as heavy metal hyperaccumulators, part of which is clonal. Studies have been developed in the last years regarding population gene flow patterns and the structure of genetic diversity. *Arabidopsis halleri*, a close wild relative of *A. thaliana*, is a clonal insect-pollinated herb tolerant to heavy metals (Zn, Pb, Cd) and a hyperaccumulator of Zn and Cd. Clonal spread occur only at short distance (<1 m). Metallicolous populations occurring in polluted areas are of particular interest. The contaminated site act like an island in noncontaminated areas with a very high heavy metals concentration in the soil, meaning there are very strong ecological constrains. *Arabidopsis halleri* (Brassicaceae) is used as a model species because is closely related to *A. thaliana* for which a vast array of genomic tools and molecular markers is available (Van Rossum et al. 2004).

Clonal spread was reported to be higher under harsh ecological conditions (Falińska 1998). Heavy metals significantly decreased the performance of *Potentilla anserina* (Saikkonen et al. 1998) measured as number of ramets, total vegetative biomass, and number of flowers, limiting the growth of the species. Hyperaccumulator plants have greater requirements for the metal of interest is given to the fact that hyperaccumulator plants allocate more roots into soil patches containing potentially phytotoxic metal concentration (Liu et al. 2010). Metal concentration (Zn or Cd) affected both root and shoot biomass in *Sedum alfredii*. The experimental studies showed that when the same amount of Zn/Cd was provided heterogeneously rather than homogenously, the plants allocated approximately 90% of root biomass to metal rich patches.

We will explore now the problem of assessing the bioaccumulation in mobile organisms, namely in carabids and birds. Carabids are epigeous invertebrate able to inspect favorable and unfavorable microhabitats. Knowledge about their habitat preferences, a mapping of the habitats at their scale and knowledge about their movement and feeding patterns is needed. The situation is complicated when the species have flying capabilities.

Carabids are mobile organisms as adults and less mobile, even immobile in immature stages. Their mobility is determined by extrinsic factors (abiotic and biotic conditions) and intrinsic factors (fiziological state, age, etc.). Their movement increases almost linearly with temperature and starvation (Raworth and Choi 2001). The movement pattern is randomized in a favorable environment and with a precise direction in unfavorable conditions (Lys an Nentwig 1991). At flying species, the fly occurs only for young individuals (Meijer 1974). Observations about carabids movement are mainly done on populations, not on individuals. The surface covered by a population range from 1 ha to several square km. The home range of a population may change with the time of observation, as the species are freely moving (Loreau and Nolf 1993). It is not clear the scale of a carabid (i.e., its foraging area). One can make an idea about this by looking at change of the location in time. Using radio-transmitters mounting on large carabids, Riecken and Raths (1996) found that in 12 h an individual of *Carabus coriaceus* moved 51.25 m, and in 17 days 191.1 m. This technique is limited to species with large individuals.

A *Pterostichus cupreus* moved in 1 month 250 m (Thiele 1977). In other cases, the distance varied between meters to tenths of meters in a day (Lys and Nentwig 1991; Joyce et al. 1999). But a starved *Calosoma sycophanta* moved 3.7 km in 3 days (Thiele 1977). From this information, one can conclude that modeling or even computing a realistic bioaccumulation factor of metals in contaminated areas for carabids is practically impossible with the current knowledge about their ecology. The risk assessment in case of such species can be made based on structural differences between the contaminated and not contaminated landscapes, and not on a description of their role in metals mobility (which is not to say that this does not exist, but only that we are not ready to understand it because basic population ecology is not characterized with enough accuracy).

In the end of this part, we assess the possibility to model the bioaccumulation in birds. There is in the literature a cellular automata model for assessing the bioaccumulation of metals in birds (Cormont et al. 2005), suggesting that this might be feasible. From our research of the communities in mining areas (Ampoi and Geoagiu river catchments, Romania) and from the literature, we established the list of the present or potential species in contaminated areas (not exhaustive, but large enough to give an idea about the problem), and then inspected the literature for the scale of these organisms. Results are presented in Table 19.5 (spatial scales of individual organisms, not of populations).

One can notice two important aspects: most of the species are migratory, and the home range of birds potentially present in the contaminated areas varies one hectare to tenths of square kilometers. The species with the smaller home range, which could feed mainly in the contaminated area, are migratory, so they are not exposed continuously to the flux of metals. From these data, it results that in principle a risk assessment for birds based on metals mobility from the contaminated area can be done in principle, but exact knowledge about the migratory routes and/or about the use of habitats in the home range are needed.

19.6 Consequences for Risk Assessment

In the risk assessment of contaminated sites, there is the assumption that the larger the distance from the contaminated sites, the smaller is the contamination. However, as a result of the coupling between of large-scale processes (like atmospheric dispersion or surface water transport) and local scale processes one can have high contamination areas at large distance from the source (Fig. 19.4), so-called "hot spots." As an illustration, we present an inventory of such situations empirically proved in Romania sites studied within national and international projects (Table 19.6).

Although the lifetime of these hot spots can be short (low retention time of metals from geomorphological processes perspective), it is long enough from the perspective of the organisms and humans coupling to the contaminated systems. Finding the hot spot by standard monitoring means is not feasible as a solution

Table 19.5 Spatial scale of several bird species occurring in Romanian contaminated areas (mining dumps, tailing dams)

Taxon	Ph	Trophic niche	Specific spatial scale	Source
Accipiter gentilis	S	Raptor	12–863 ha	Rutz (2006), Squires and Kennedy (2006)
Corvus corax	S	Opportunist	700 ha	Rösner et al. (2005)
Dendrocopos major	S	Insectivorous	4.5–5 ha	Pavlik (1999)
Emberiza citrinella	S	Opportunist	10 ha	Golawski and Dombrowski (2002)
Garrulus glandarius	S	Opportunist	42.5–358.8 ha	Patterson et al. (1991)
Parus caeuleus	S	Insectivorous	11 km	Pinowski (1987)
Parus major	S	Insectivorous	3.3 km	Pinowski (1987)
Passer domesticus	S	Opportunist	59.2 km	Pinowski (1987)
Passer montanus	S	Opportunist	26 km	Pinowski (1987)
Pica pica	S	Opportunist	3–13 ha	Birkhead et al. (1986)
Buteo buteo	PM	Raptor	123–454 ha	Sim et al. (2001), Rodriguez et al. (2010)
Fringilla coelebs	PM	Opportunist	1,000 m from singing territory	Haila et al. (1989)
Fringilla coelebs	PM	Opportunist	27 individuals/ha	Mikkonen (1985)
Sturnus vulgaris	PM	Opportunist	40 ha	Paton et al. (2005)
Turdus merula	PM	Insectivorous	50–400 m from nest	Khokhlova (2009)
Cuculus canorus	M	Insectivorous	32.7–314.6 ha	Vogl (2004)
Lanius collurio	M	Insectivorous	1.5 ha	Golawski and Golawska (2008)
Phoenicurus ochruros	M	Insectivorous	2 ha	Personal estimation Cobzaru
Saxicola torquata	M	Insectivorous	2 ha	Personal estimation Cobzaru
Upupa epops	M	Insectivorous	3 ha	Personal estimation Cobzaru
Anthus trivialis	MD	Insectivorous	1–5 ha	Burton (2007), Moga et al. (2009)
Delichon urbica	MD	Insectivorous	400 from the colony	Personal estimation Cobzaru
Hirundo rustica	MD	Insectivorous	400 from the colony	Snapp (1976)
Phylloscopus trochilus	MD	Insectivorous	1.5 ha	Personal estimation Cobzaru
Sylvia atricapilla	MD	Insectivorous	1.3 ha	Shaeffer and Barkov (2004)
Sylvia curruca	MD	Insectivorous	1.3 ha	Personal estimation Cobzaru

Ph phenology, *S* sedentary, *PM* partial migratory, *M* migratory, *MD* migratory at large distance

because of the high monitoring resolution needed for large areas. The solution developed is to produce models coupled across scales able to identify the probable location of such contaminated areas. The general structure of the modeling approach was introduced in Fig. 19.2. The preliminary phase of contaminated sites risk assessment (aiming at the characterization of pathways of metals to receptors) should include models able to detect distant hotspot if parts of the

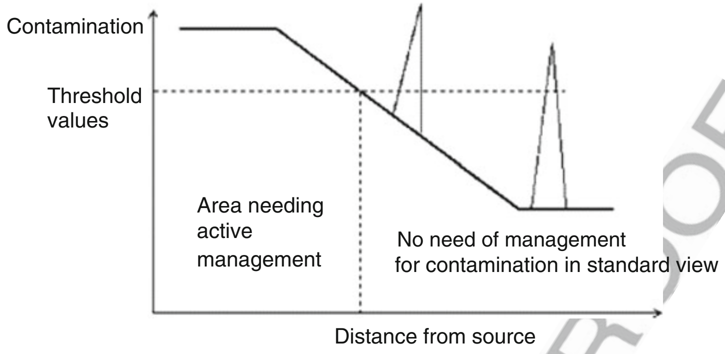

Fig. 19.4 The current assumption in risk assessment and the problem of hot spots at distance

environmental costs are not to be externalized from the eventual remediation project. Starting from this, a new concept of hazard assessment (the first phase of risk assessment) is introduced in another chapter of this book (Jianu et al. 2011).

19.7 Conclusions

Metal biogeochemistry is only one side of the research of productive systems. There is an optimal complexity of the integrated models in metal biogeochemistry. A minimal complex homomorphic model can be built according to the structure of the developmental systems included in the productive entity, allowing for structural integration of several environmental entities. A complementary functional integration results from the observation that it makes little sense to study the circulation of one element (e.g., a heavy metal) in the population of developmental systems (DSs) identified by the homomorphic model separately from the circulation of other elements playing the role of resources or toxicants (e.g., macronutrients), because all of them influence the productivity of the DSs.

Metal mobility results from the interaction (coupling) of environmental entities at a multitude of scales. These interactions generate patterns of metal distribution. The environmental entities are frequently studied within different scientific disciplines, so understanding the coupled biogeochemical processes involved in the mobility of metals is a matter of interdisciplinary research and integrated modeling. There is not a “site” (ecosystem) or “region” (landscape) scale specific for the mobility of metals. This kind of speaking refers only to a simple modularization of the environment for management needs. A scientifically based management should consider the coupling between processes occurring at different scales because of the effects at distance generated by processes at the local scale of the contaminated site.

To answer the questions formulated in the introduction, there is an optimal level of integration for understanding the biogeochemical role of abiotic and biological t6.1 **Table 19.6** Examples of hot spots contaminated with metals in Romania caused by the coupling of processes with different scales

	Source of metals	Large-scale process	Distance to "hot spot"	Local scale process at distance (in "receptor area")		Location in Romania
t6.3				1	2	
t6.4	Batteries factory	Atmospheric dispersion	2–3 km	Forest barrier effect	–	Pantelimon (NEFERAL/ Acumulatorul)
	Smelter		2–5 km	Runoff	Transversal particles buffering	(geomorphology + plants)
t6.5	Ampoi – Zlatna					
	Smelter		2–4 km	Runoff	Longitudinal particles buffering	(geomorphology + plants)
t6.6	Ampoi – Zlatna					
t6.7	Smelter	4–5 km	Runoff	Longitudinal buffering	V. Viilor – Copsa Mica	
t6.8	Mining dump	Surface water transport	12 km	Longitudinal buffering	–	Ampoi – Hg mining dumps to floodplain
t6.9	Mining dump + tailing dams + polluted soil		25–40 km	Longitudinal buffering	–	Ampoi – various sources to floodplain
t6.10	Acid mine drainage		10–15 km	Groundwater recharge in karstic NATURA 2000 area	–	Geoagiu – mine to downstream groundwater Ardeu

objects, and the practical possibility to produce realistic integrated models is still strongly limited by the available knowledge base produced by environmental scientific disciplines.

Acknowledgments This research was done in the Romanian Consortium for the Biogeochemistry of Trace Elements with financing from National University Research Council (CNCSIS) by project 291/2007 MECOTER, from National Center for the Management of Projects (CNMP) by projects 31012/2007 FITORISC, 31043/2007 PECOTOX, 52175/2008 METAGRO, and in the international consortium of the FP7 project UMBRELLA, grant agreement 226870. Special thanks go to the anonymous reviewers for their constructive criticism which improved the quality of the manuscript.

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