

## State of the art

After the failure of the heavily subsidized attempts to do produce holistic models of ecological systems in the 1970s in the frame of the International Biological Program, the financing of such research program went down to reasonable dimensions, despite the widespread recognition of the existence of a hierarchy of ecological systems, from local to global level, whose functional modelling is a desirable research objective (Loijen 1998). The idea to do such costly modelling revived recently under the heading of "modelling the socio-ecological systems", but still the possibility of successful implementation of this research agenda is debated: the holistic approaches have failed in the past, and the reductionistic ones are said to not reflect the true characteristics of the systems. At this general level, the idea of this project is to implement a new strategy for modelling hierarchically organized ecological systems, coupling holistic and mechanistic approaches. The complex systems such as the ecological ones are characterised by an intrinsic principle of uncertainty (Jorgensen and Svirezhev 2004, Stanciulescu 2005). Because there are no precise solutions for complexly organized systems, there is no single method for their study. It isn't quite "anything goes", but we cannot tell what might work without trying it. Taking into consideration also the non-linearity of the complex systems and their real, non-stochastic, indeterminacy (due to biological evolution, for instance), one can say, from a philosophy of science standpoint, that there cannot be a final mathematical model of such systems: models of the functioning of ecosystems will evolve (in an evolutionary epistemology sense). Our strategy is to not look for a single comprehensive model, whose epistemic "mutations" and evolution are very costly, and consequently difficult to accept by the scientific community, but to produce a maximally coherent portfolio of models with a modular structure, most appropriate for a high rate of epistemic evolution occurring by piecemeal changes at the level of the modules and of the relations between them. By now the models belonging to the potential "modules" have evolved independently, disciplinary, without explicit concern about their relationships with other disciplinary developed models. To give substance to this strategy, the project deals with modelling biogeochemical cycling of metals occurring in hierarchically organized ecological systems. That this is a basic research priority is proved by a comprehensive analyses of the bioaccumulation models coupled with ecotoxicological models done in the frame of a previous ESF project (\*\*\*, 2003). In order to do describe the metals' circulation there is a need to develop food-web models (modifying and extending their structure), especially models describing natural, complete terrestrial ecosystems (\*\*\*, 2003). Starting from the conclusions of this ESF project we performed a review of the state of the art concerning the mathematical modelling of the cycling and effect of metals at landscape level (Iordache and Stelian 2007). The general conclusions were: 1. Current models applicable at landscape scale describe mainly the abiotic side of the processes, the best example being reactive transport models. However, there are many opportunities for interdisciplinary transfer of ideas profitable for the field of mathematical modelling in biogeochemistry and ecotoxicology. 2. The limits related to modelling the involvement of the organisms cannot be surpassed at the current state of biological knowledge, despite the efforts in the systems biology field. 3. With respect to the development of the scientific knowledge in biogeochemistry and ecotoxicology the potential of modelling is underused, because the modelling efforts are focused mainly on the side rapidly relevant for socio-economic systems. 4. There is an important opportunity to use populations of similar contaminated and, eventually, bioremediated sites (seen as in situ experimental areas) for testing biogeochemistry hypotheses with modelling tools (i.e. to build some kind of "long term contaminated ecological research" network). The difficulty which blocked the refinement of this kind of models for in situ cases is related to the large heterogeneity of the control parameters, the distribution in space, as well as to the large number of relationships between the control parameters for each metal. In these conditions, to set up mathematical relations between the control parameters of metals mobility and their mobility proved to be not yet feasible in situ. It may be that the development of new mathematical tools, more adapted to biological phenomena, would contribute to changing the landscape of models in this area. For instance, Schryver et al. (2006) use non-linear analyses with artificial neural networks with good results to describe the relationships between groundwater contamination with metals and the structure of bacterial communities as measured by molecular markers. Beside neural networks, another new tool is the Multivariate Adaptive Regression Splines (MARS). It has been used for instance for predicting the denitrification rate based on data sets at European scale (Pinay et al 2007). These mathematical tools could be applied in order to describe relationships between parameters describing metals biogeochemistry at the explanandum (higher hierarchical) level, on the one side, and its control parameters at the explanans (lower hierarchical) level. Once the analyses are performed, one would have a holistic phenomenological description of the relationships in mathematical forms at site scale. One limitation of this approach is to uncover mathematical laws with 1 member of the reference class (the studied site). This limitation can be surpassed only by studying a population of sites across gradients. Another limitation of the holistic approach is that the discovered mathematical laws will give no indication about the mechanisms supporting them. This indication can be provided only by a mechanistic (bottom-up) approach. By now reductionism has created unwarranted biases in certain mathematical models and experimental designs. Mechanistic models may incorporate unnecessary lower level details that compromise verisimilitude and predictive success. However, without this approach one cannot have an image on the involved mechanisms, and thus on the possibilities of controlling the metals' mobility. Therefore one can proceed this way, having in mind that the mechanistic frame has to be re-verified after each step of upgrading and prediction. Our idea is to develop (bottom-up) mechanistic models of metals' behaviour under the (top-down) constraint of the results of the holistic modelling (figure 1).

Figure 1 Overall structure of the modelling approach. The main focus from the mechanistic perspective will be on the difficulty of allocating values to the parameters under high field heterogeneity. The heterogeneity of the real systems at a certain hierarchical level cannot be predicted based on principles (Dungan et al. 2002). The heterogeneity problem can be dealt with by empirical research for delineating in situ the elementary units of models application (systems

identification) and using a portfolio of models covering the diversity of the elementary units. Different processes require different space-time scale of the elementary units and models' development. Programming in GIS can then be used for upscaling the models' results from the elementary units of application to the site and for linking the results of the models with different space-time scale (Iordache and Bodescu 2005). The upscaling problem is linked to some extent to the reduction of the ontological levels problem, and can be solved partially by recognizing the irreducibility of ecological levels of organization, such as elementary ecosystems and landscapes (contaminated lands are usually at these levels). Then each level can be approached by specific model(s). The remaining part of the upscaling problem, within a certain level, directly reflects the heterogeneity problem. In this context, the general objectives of a research program in this area can be: 1. To uncover mathematical laws describing the mobility and effects of metals at contaminated landscape level. 2. To develop coupled top-down and bottom-up models of key processes of metals biogeochemistry and effects in a population of contaminated landscapes. This project should be seen as one step in such a long-term research program.