

## Objectives

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Â Â Â Â Â Â The key processes which can be feasibly tackled at this moment by math modelling, and are still not satisfactorily tackled in situ, are (Lordache and Stelian 2007, op. cit.): 1) the influence of microorganisms on the fluxes of metals in the saturated zone, 2) the influence of microorganisms on the transfer of metals in the unsaturated zone, 3) the influence of rhizosphere processes on the metals uptake and leaching (including the effects of mycorrhizing fungi), 4) the influence of the vegetation cover on the metals export by run-off, 5) the bioaccumulation in the food chain, 6) the movement of metals by lotic aquatic systems and the transversal and longitudinal buffering of metals fluxes performed by the riparian systems. If these are to be the modules to be dealt with separately by modelling (a task performed by the current disciplinary approaches), the main challenge is how to coherently link such models in a coherent portfolio. The coherence of a portfolio of models developed by the approach described in figure 1 would be assured by: 1) mutual adjustment of the mechanistic and phenomenological models in their development phase, based on the results of their prediction, 2) the partial superposition in time and space of the data sets used for developing the models for different processes, and 3) checking the performance of a model by using its outputs as inputs for other models and verification of the predictions of this second model. From the above processes we will tackle in this project only number 3, and number 5, because of the limited extend of the team. For the same reason within process 5 only bioaccumulation in plants will be tackled

Â Â Â Â Â Â In this context, two objectives of our the project are: 1. To develop macro-, spatially explicit mathematical models about the bioaccumulation of metals in plant and their transfer to surfacewater and groundwater. 2. To develop mezo-, spatially unexplicit mathematical models about the bioaccumulation of metals in plant and their transfer from the topsoil by leaching. The models resulted from the objectives 1 and 2 should be reciprocally checked and coherentized, and this might have been our third objective in the project. However, the picture can be further complicated by taking into consideration the dynamic of the climate systems, in order to simulate the behaviour of the climatically forced ecosystems in terms of metals biogeochemistry. So we decided to have the following form of the third objective of the project: 3. Reciprocal adjustments of the models the simulation of the dynamic of metals mobility in the context of climate changes.

Â Â Â Â Â Â The proposed contributions of the project are: 1. Application of Nonlinear Analysis Methods for Identifying Relationships Between a large set of soil chemical and physico-chemical parameters and 1a) the contamination of the groundwater 1b) the contamination of the flooding water 1c) the bioacumulation of metals in plants. 2. Models for the distribution and dynamic of the key control parameters of metals mobility in soil, as resulted from contribution 1. 3. Models for the dynamic of metals atmospheric deposition at the studied sites. 4. Simulation of the dynamic of atmospheric and hydrological control parameters of metals at the sites in the context of climatic changes. 5. Coherentized portfolio of models descing the biogeochemical processes. 6. Mechanisms explaining the nonlinear relationships between the key control parameters of metals mobility in soil and 1a) the contamination of the groundwater 1b) the contamination of the flooding water 1c) the bioacumulation of metals in plants.

Â Â Â Â Â Â By the first contribution we attempt to phenomenologically characterize the role of the key control parameters of the mobility of the metals. In the second, third and fourth ones we set the conditions for identifying the explanatory mechanisms by modelling the effect of the climatic and hydrological conditions on the key control parameter of metals mobility. This second set of contributions will allow us to extrapolate in space the results of the lysimeters experiments (i.e. the spatially un-explicit models concerning the relationships between set of soil chemical and physico-chemical parameters and 1a) the contamination of the groundwater 1b) the contamination of the flooding water 1c) the bioaccumulation of metals in plants), to compare them with the results included in the first contribution, and thus to identify explanatory mechanisms.

Â Â Â Â Â Â All the contributions will have in their structure mathematical formalism, and consequently it will be possible to check their general applicability in other contaminated areas, and in this way to improve the formalism. From a basic science point of view, the contributions are of interest for experts in the area of metals biogeochemistry (both for those working on the big picture “models for whole ecosystems, and for those focusing on the interactions between key groups of organisms “ plants, micro organisms, and the abiotic reservoirs of metals in sol).