Developing a 3D Flow and Transport Model of the Unsaturated Zone for Performance Assessment

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Context

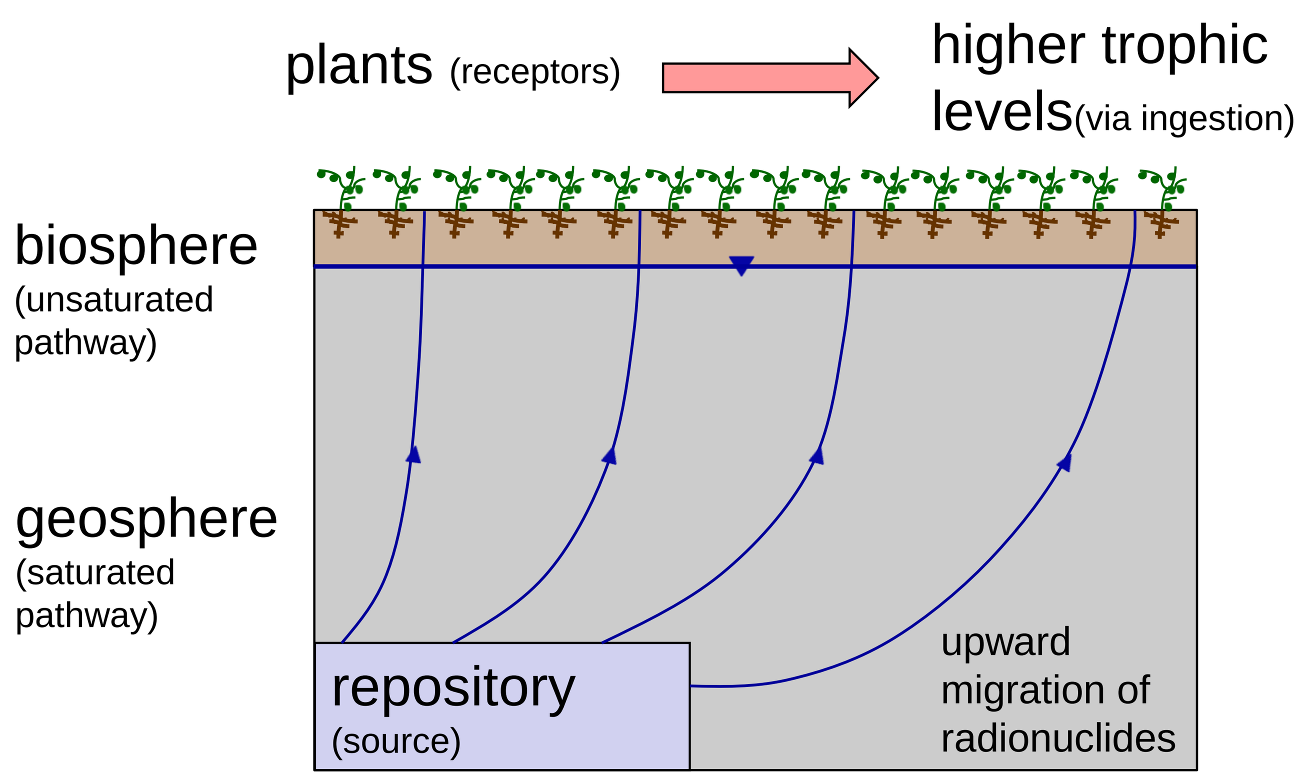


Figure 1: *Source-pathway-receptor model of radionuclide transport*

Performance assessment for nuclear waste disposal is the process of identifying the **risk** caused by geologic disposal to the ecology in general and future human populations more specifically. It involves modelling the physical and chemical processes governing radionuclide transport in groundwater, from their source in the underground repository, through the geological pathway, to a receptor within the food chain.

The goal of this project is to develop a three dimensional model of the **biosphere ,** the part of the pathway which lies above the water table. It focuses on modelling soil heterogeneity in the **unsaturated zone**

Within the **DIAMOND** framework, this project falls squarely into the Environment, Migration and Risk Work Package (WP1), but has links to Project Cluster 2.3.3 and Project 1.3.2.1

Model Results

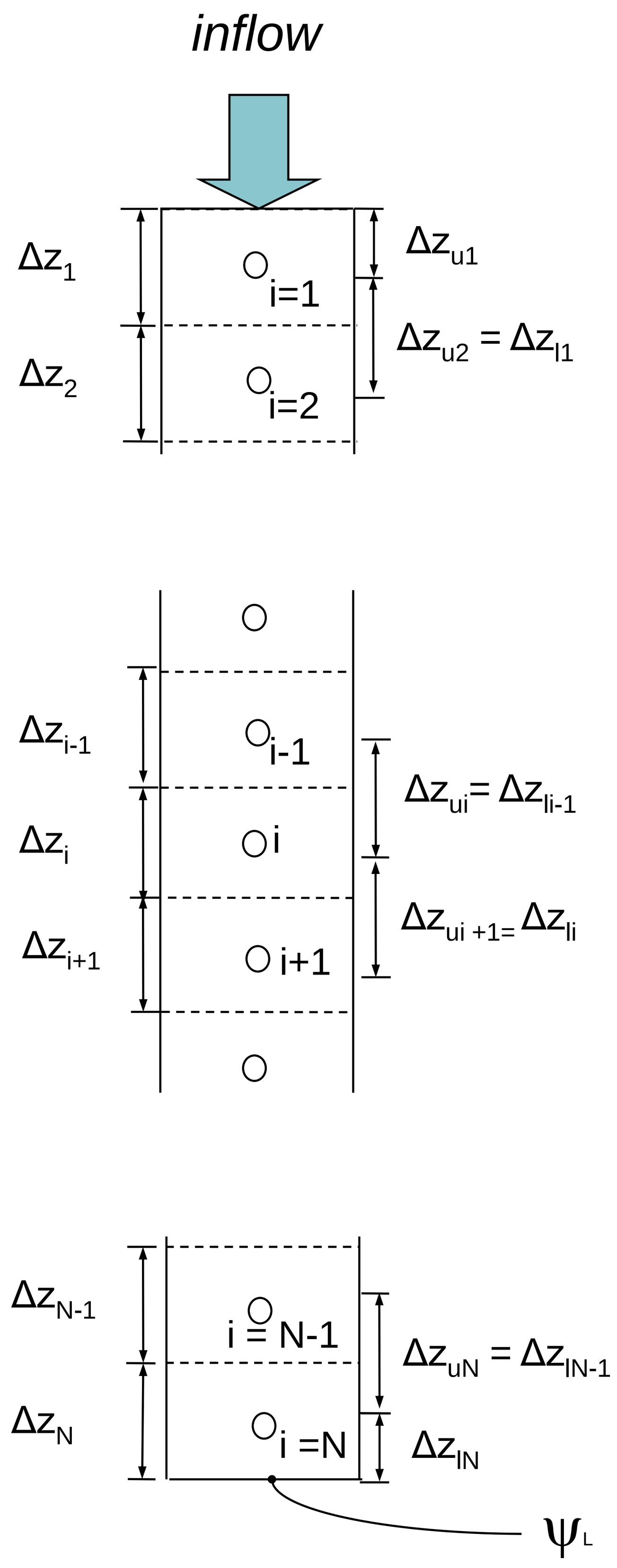


Figure 2: *1D finite difference model*

A 1D finite difference model has been developed (figure 1) was built in the MATLAB environment. Two solution method were used: the **Method of Lines** (**MoL**), and a non-iterative, **simple implicit method** (**SIM)** for this problem. The results were verified using EPA CHEMFLO and show excellent agreement (figures 3 and 4).

In general, SIM was faster than the MoL code but the level of agreement depended on the users choice the number of time and space steps, especially as the spatial grid became denser. However, there is a need to able to control the accuracy by an internal error tolerance to avoid relying on benchmark codes, while retaining the time-saving advantages of the implicit method. An implicit method which iteratively converges using a specified error tolerance is a suitable next step. A **root extraction model** will also be added, and the code will be extended to include various types of boundary conditions.

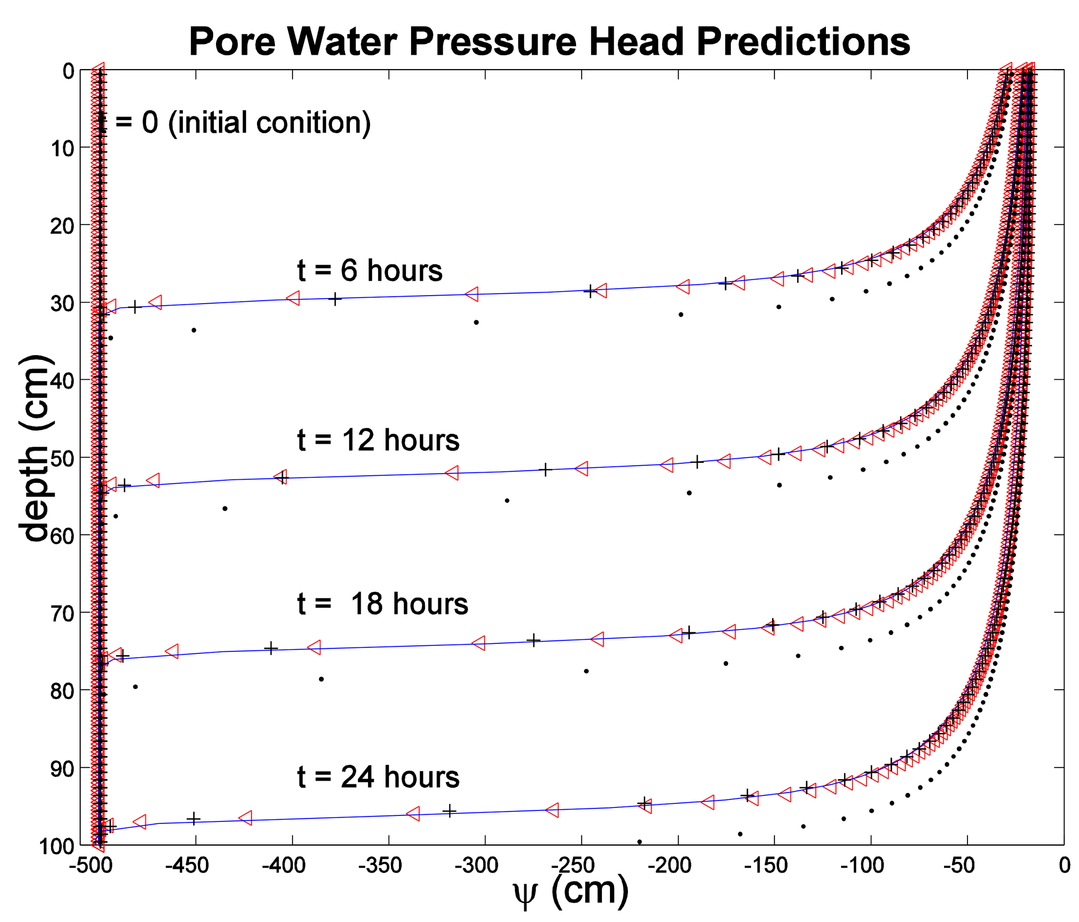
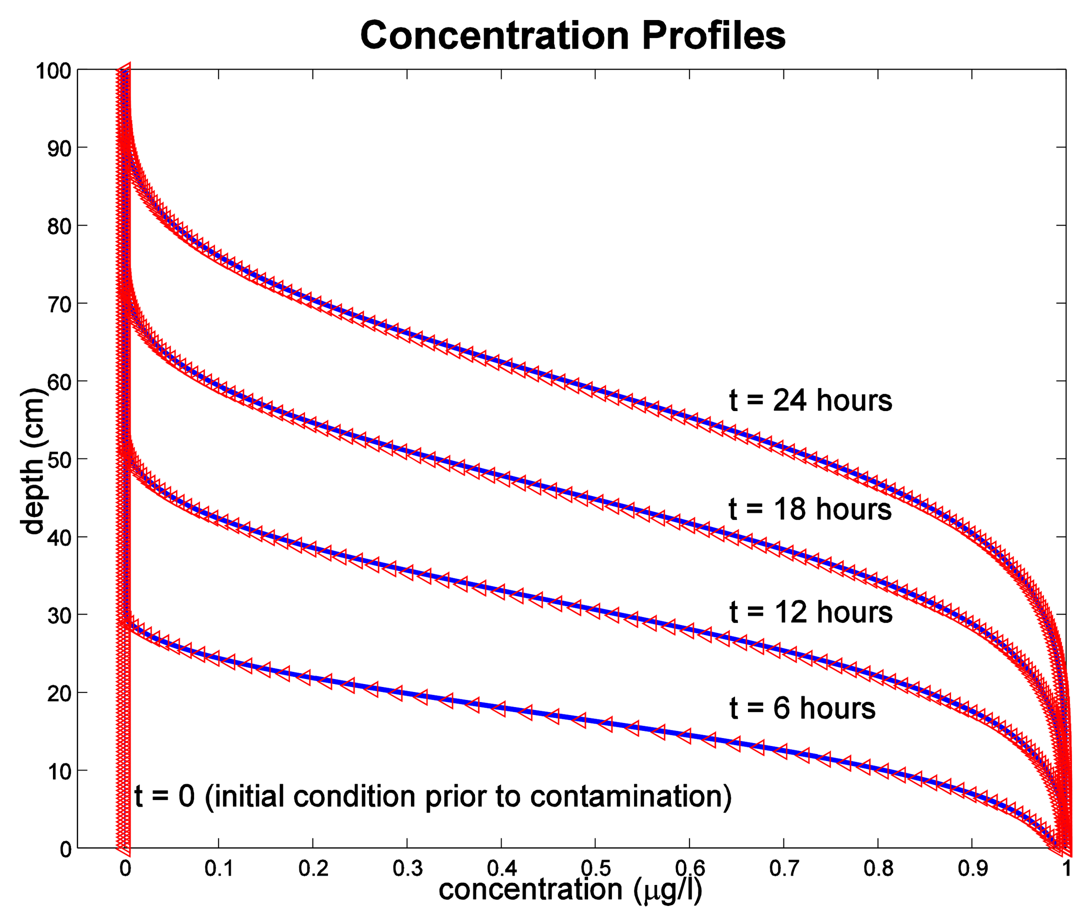


Figure 3 (left): *Pore water pressure predictions. CHEMFLO (red triangles), MoL (blue line), SIM, dt=1/500 days (black dots), SIM, dt=1/5000 days (black crosses)*

Figure 4 (right|): *Concentration predictions. CHEMFLO (red triangles) and MoL (blue line)*



Upscaling

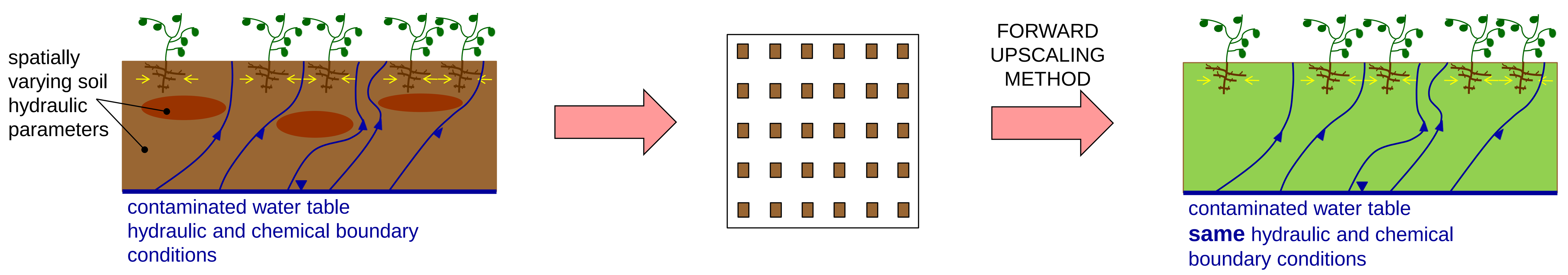


Figure 5: *Upscaling methodology*

Soil variability will be generated as a statistical distribution of hydraulic properties, or as a hypothesised but realistic soil structure. From this local structure, the **plant uptake response** of an entire field can be determined by running the detailed model.

The model can be used to simulate **field sampling programs** by discretising the hypothetical heterogeneous field. **Forward upscaling techniques** will then be used to predict the combined plant uptake response of a whole field. Comparing these predictions to the response of the model using the whole data set, we can assess both the effect of sampling patterns and the choice of forward upscaling technique on the effectiveness of prediction. By comparing 1D and 3D upscaling methods, insight into the benefits of 3D modelling over 1D or 2D models should be gained.

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