

# International Workshop on Approaches for Upscaling Processes Affecting Radionuclide Transport through the Subsurface

Susan J. Altman  
Geohydrology Department  
Sandia National Laboratories  
P.O. Box 5800 MS0735  
Albuquerque, NM 87185-0735  
sjaltma@sandia.gov, (505) 844-2397

The *International Workshop on Approaches for Upscaling Processes Affecting Transport* was held in Albuquerque, New Mexico on June 18, 1999. Thirty-seven participants representing Belgium, Canada, Finland, France, Japan, Spain, Sweden, Switzerland, the United Kingdom, and the United States were present.

An internet web site summarizing the work on upscaling that has been performed by the participating countries' organizations has been constructed (<http://www.nwer.sandia.gov/wlp/upscaling/upscaling.htm>). The purpose of the web site is to create a framework for communications to foster international collaboration between different nuclear waste management programs on upscaling of processes affecting transport. In the web site are Master Tables that summarize the experiments each program has conducted to study the different processes, the scale at which the experiments were performed, and the scale at which the results of the experiments were applied. Associated with the Master Tables are lists of publications and contact names and in some cases short descriptions of the work so a user can attain more information. The information compiled in the Master Tables makes it easy to identify links between the programs, areas of overlap, and areas for which additional work is needed. These tables will allow the different nuclear waste programs and other groups studying flow and

transport to more fully benefit from each other's work. While the web site is focused towards the international nuclear waste community, it is useful to anyone doing research related to subsurface flow and transport.

Physical and chemical properties and processes acting in the geosphere are measured during site characterization of potential nuclear waste repository sites, and this information is used as input to performance assessment models. The temporal and spatial scales of these measurements are often orders of magnitude less than the scales over which performance assessment calculations are made. Upscaling is the means by which appropriate parameter values, processes and conceptual models are assigned to the larger-scale performance assessment models. The upscaling process must be sound and defensible to technical peer, regulatory, and stakeholder review.

The *International Workshop on Approaches for Upscaling Processes Affecting Transport* was focused on methods to upscale processes affecting geosphere transport for the purpose of developing performance assessment models that effectively balance efficiency with defensibility and realism. In the upscaling of transport processes we recognized that an integration of processes controlled by the physical system (*e.g.*, diffusion) and chemical-system (*e.g.*, sorption) as well as flow processes is needed. Acknowledging the importance of this integration, upscaling processes pertaining to physical transport was emphasized in the workshop.

To help focus the presentations and discussion during the workshop, certain topics were explicitly excluded from its scope. In order to concentrate on far-field flow and transport, alterations of the geosphere due to the repository were not discussed. Unsaturated-zone flow and general multiphase flow were also explicitly excluded from the topics of this workshop.

## **DISCLAIMER**

**This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.**

## **DISCLAIMER**

**Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.**

Exclusion of these topics does not imply that upscaling issues do not pertain to these topics. For example, unsaturated transport is an important issue for the Yucca Mountain Project (U.S.A.) where the repository could potentially be located above the water table and methane makes multiphase flow important at the Wellenberg site (Switzerland). However, both these topics were not discussed at the workshop for practical reasons.

No single program can fully address all aspects of the complex problem of upscaling of processes affecting transport. However, combining the efforts of different programs is mutually beneficial. Thus, the overriding objective of this workshop was to create a framework for communications to foster international collaboration between different nuclear waste management programs on upscaling of processes affecting transport. This framework was achieved at the workshop through an excellent series of presentations and discussions by representatives of many nuclear waste management programs. It is hoped that internet access to the Master Tables will continue to foster this dialogue and spirit of collaboration.

**RECEIVED**

**OCT 05 2000**

**O S T**

## **EXPLANATION OF THE MASTER TABLES**

An explanation of a Master Table is presented in Figure 1. Experiments are grouped into three categories: laboratory, field (or *in situ*) and numerical. The different repository programs are identified by the different colors of the bars in the Master Tables. Application scale is differentiated between the scale at which the experiments were conducted by using dashed lines and solid lines, respectively. This differentiation is not made for the numerical experiments.

There is one Master Table for each process thought to be important to transport (dispersion, diffusion, chemical retardation, colloid transport, flow through heterogeneous fractured media, and flow through heterogeneous porous media). Chemical retardation is divided into three

different Tables: one summarizes experiments providing information for using the  $K_d$  mass modeling approach (Chemical Retardation,  $K_d$ ), another summarizes experiments providing information for using the  $K_a$  surface area modeling approach (Chemical Retardation,  $K_a$ ), and the third summarizes the experiments used for alternative modeling approaches for chemical retardation (Chemical Retardation, other). Processes that are only being studied by a few programs are grouped into another Master Table labeled “other processes” (osmosis, thermal diffusion, electrokinetic diffusion, precipitation, radioactive decay, and coupled phenomena). The Master Table for “flow through heterogeneous porous media” is shown in Figure 2.

The web-site users can view the Master Tables for the different processes by linking back and forth from the List of Processes. This list also provides brief definitions of the different processes that affect transport. Definitions of the different experiments are linked to the experiment names listed on each table (List of Laboratory Experiments, List of Field Experiments). Each numerical experiment has a unique link to descriptions of the modeling exercises provided by the different programs. In order to gain more information about the different programs, links are provided between the legend and short descriptions of the programs written by each representative.

## **CONCLUSION AND RECOMMENDATIONS FROM THE WORKSHOP**

The following summary points from the Upscaling Workshop are made:

- Upscaling methods are rock-type specific. This was clearly demonstrated by comparing conclusions made by programs working on clay media versus fractured crystalline rocks.

- The relative importance or function of a process depends on the given medium, which in turn affects the characteristic length scale of the process. An example is diffusion: diffusion could act as a primary transport process in clay (length scale on the order of 100s of meters) whereas in fractured crystalline rocks diffusion could act as retardation process (length scale on the order of decimeters of meters). This function needs to be recognized for each system.
- In order to define and defend upscaling methods, a variety of studies are needed at different spatial and temporal scales: lab, field, and numerical. A variety of scales within the laboratory and field setting are also recommended.
- The key to understanding the upscaling of a process is to understand the basic physical and chemical mechanisms controlling the processes. One needs to understand if there are interfering processes in the system and if the system is in equilibrium. For example, one needs to understand the relative importance of hydraulic conductivity heterogeneity versus diffusion in order to be able to interpret tracer test breakthrough curves.
- One needs to know if they can measure a representative elementary volume (REV).
- The physics of a system can change with time, especially with the introduction of a repository. While the scope of this workshop did not address this issue, it cannot be ignored when determining how to upscale a process.
- There is still much to learn about flow and transport processes and there is a desire for more data to study these processes. Areas deserving further study include:
  - Understanding discrepancies between transmissivity measurements made under convergent flow conditions versus natural flow conditions.

- Understanding discrepancies between lab and field measurements of sorption.
- Understanding diffusive properties of low-porosity materials.
- Understanding exactly what is being measured in field tests.

Based on these conclusions, the following recommendations are made:

- Experiments need to be defined for the purpose of understanding the basic physics of a system including understanding the relative importance of interfering processes.
- It is critical to characterize the characteristic length scale of a process at both the experimental and application scale when designing laboratory, field and/or numerical experiments and when determining how to upscale. If the characteristic length scale of the experiment is not relevant to the application scale, then the results of the experiment could be of little use.
- The approaches discussed in this workshop need to be communicated to groups working on near-field issues. Although this workshop has been constrained to issues related to far-field transport, much of what has been discussed is relevant to processes important in the near field. It is up to each participant in the workshop to communicate this information within their project.
- Physical transport processes must be well integrated with processes affecting chemical retardation. There is a need to develop experiments that can integrate these processes.



*More detailed reporting of the workshop has been published as:*

*Altman, S. J., International Workshop on Approaches for Upscaling Processes Affecting Radionuclide Transport through the Subsurface. SAND2000-0208, Sandia Natl. Lab., Albuquerque, NM, 2000.*

## **ACKNOWLEDGMENTS**

Patti Comisky, Peter Davies, Tina Goodrich, Kathy Hart, Allen Lappin, Shermi Liang, Sean McKenna, Lucy Meigs, Paul Reeves, and Vince Tidwell contributed to organization of the workshop. Cheryl Allen, Bill Arnold, Julio Astudillo, Tina Goodrich, Yuji Ijiri, Mark Jensen, Martin Mazurek, Simon Norris, Gerald Ouzounian, Martin Put, Klaus Schelkes, Jan-Olof Selroos, and Timo Vieno contributed to the web site development. I also thank Mark Matthews, Department of Energy/Carlsbad Area Office for his support. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000

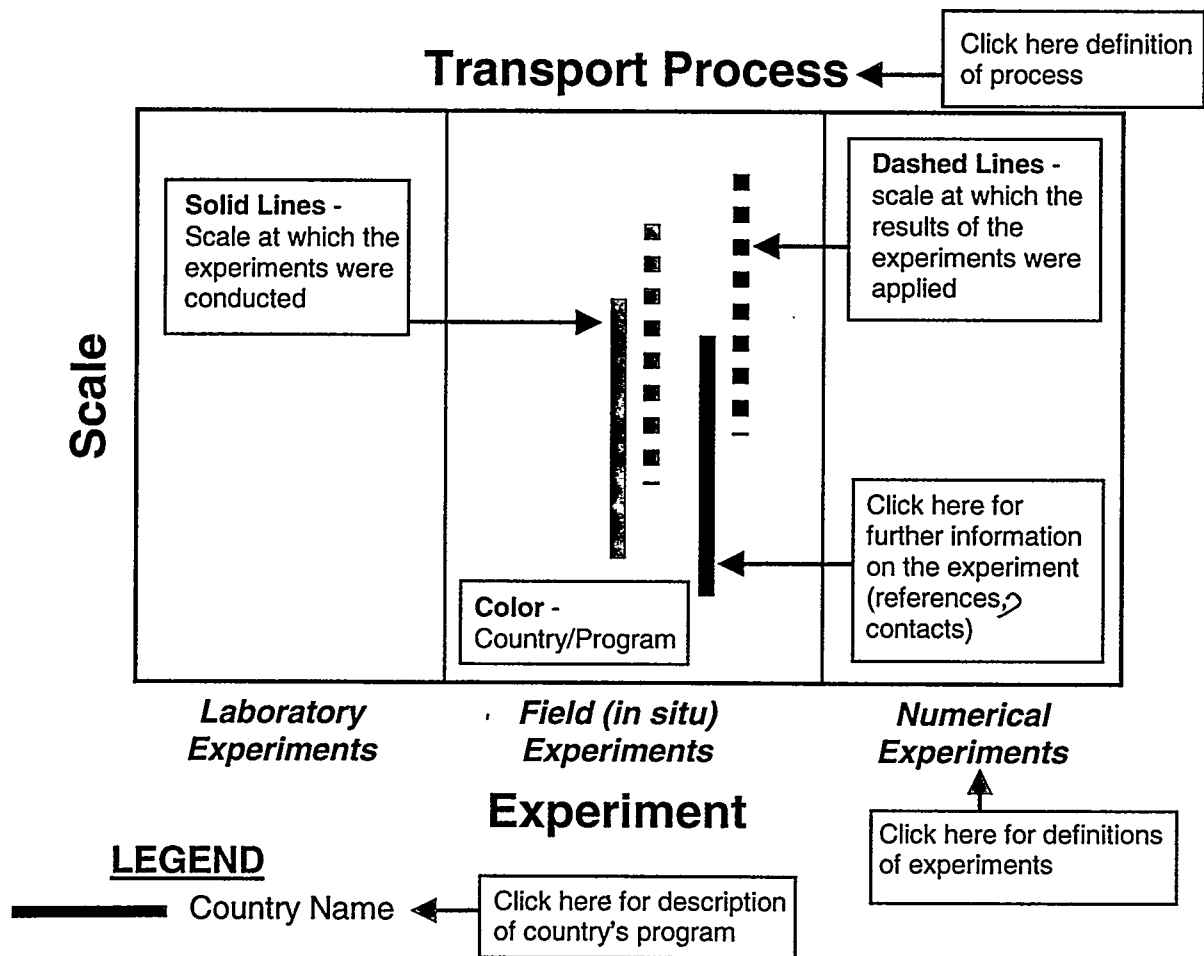


Figure 1: Explanation of the master tables.

# Flow Through Heterogeneous Porous Media

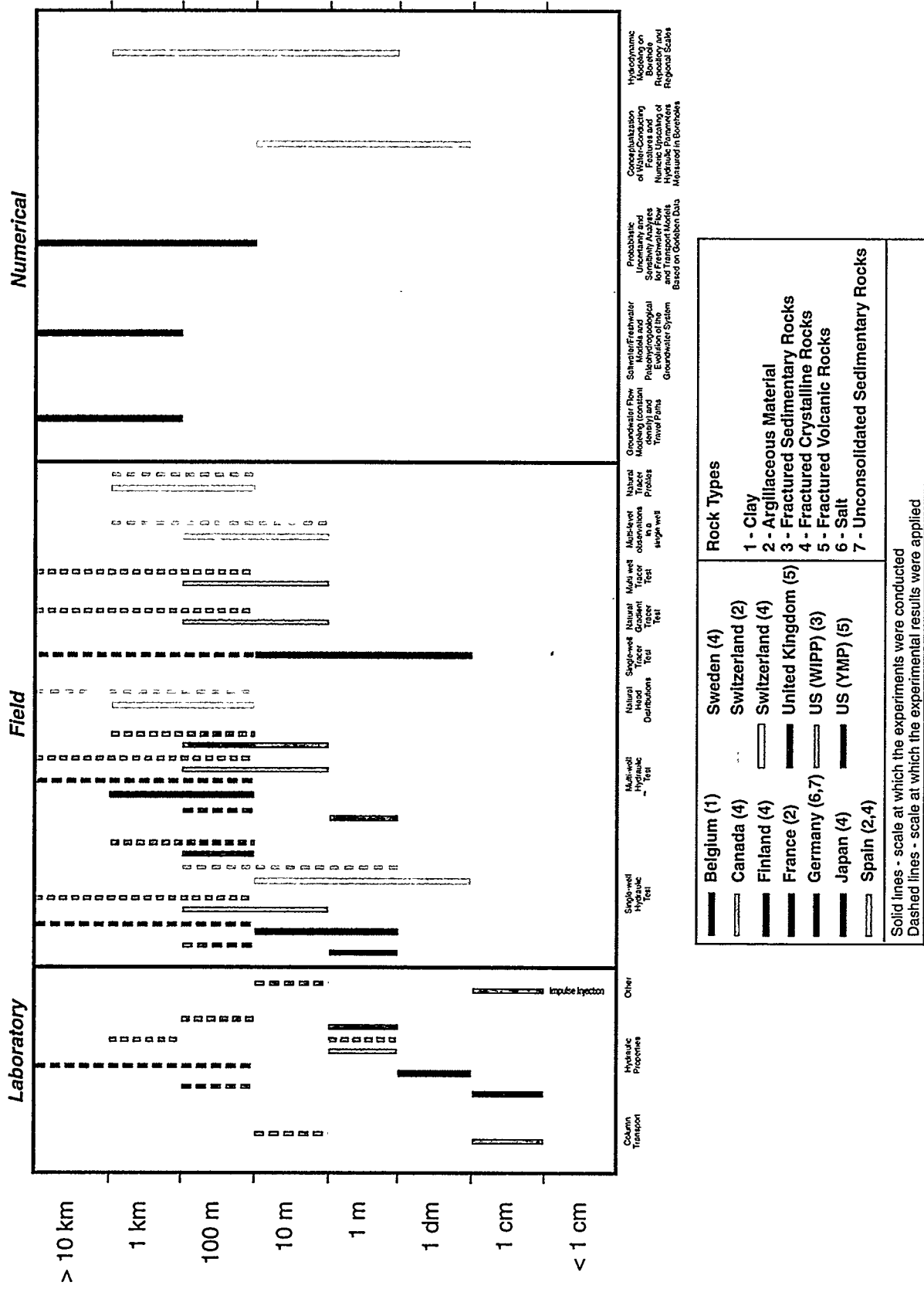


Figure 2: Master Table for Flow through Heterogeneous Porous Media. This is one of many Master Tables for a process that affects transport on the web page (<http://www.nwerner.sandia.gov/wlp/upscale/upscale.htm>). Summarized in the Tables are the experiments each program has conducted, the scale at which the experiments were performed, and the scale at which the results of the experiments were applied. The web page provides links from the Master Table to lists of publications and contact names for each experiment, definitions of the different experiments, and short descriptions of the programs written by each representative.