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INTERNATIONAL PROJECTS IN VALIDATING GROUND-WATER FLOW AND TRANSPORT MODELS

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ABSTRACT

The U.S. Nuclear Regulatory Commission (US NRC) is involved in international projects dealing with development of validation strategies for ground-water flow (HYDROCOIN) and transport (INTRAVAL) models. The U.S. NRC staff and their contractors, along with other international participants in the "Hydrologic Code Intercomparison Study," HYDROCOIN, simulated laboratory and field experiments to gain insights into the validation process for hydrogeologic systems. Although true validation was not achieved, this phase of the HYDROCOIN effort provided the following insights on validation of ground-water flow models: (1) validation is a site specific and purpose specific issue (i.e., validity depends on both the model, and the correct interpretation and use of site data); (2) comparison of model simulations with a single spatial and temporal set of experimental results is likely to result in model calibration rather than validation; (3) more is learned when models are rigorously tested on a variety of possible site conditions than when models are tested for simple conditions which can be easily reproduced; and (4) validation can best be judged when prior performance measures are established and specific criteria for model acceptance are fully defined.

The "International Transport Validation Study," INTRAVAL, is a direct outcome of the successes and lessons learned in the HYDROCOIN project. For example, the validation studies of HYDROCOIN illustrate the need to reexamine the data base and to perform additional experiments to isolate individual processes and phenomena of the conceptual model. Based on this need, the INTRAVAL project is utilizing data bases which are amenable to later testing. Also, scale dependency of the large temporal and spatial considerations associated with radioactive waste disposal precludes complete validation. Therefore, the INTRAVAL project will examine natural analogues to radioactive repositories, and use coupled laboratory and large-scale field studies (e.g., Las Cruces Trench study) to analyze scale dependence issues. The original test cases considered for the INTRAVAL project were for saturated flow and transport in fractured and porous media (INTRAVAL Ad Hoc 1987). Unsaturated flow problems relevant to low-level and high-level radioactive repositories have recently been defined for the INTRAVAL project.

INTRODUCTION

This paper discusses the U.S. NRC staff's and contractor's computer modeling efforts as part of two international cooperative projects for studying ground-water flow modeling strategies (HYDROCOIN) and examining the validation process for geosphere transport models (INTRAVAL) associated with performance assessment of radioactive waste disposal facilities. Both studies involve member countries of the OECD including the U.S.A. (both US NRC and US DOE are participating parties) with the Swedish Nuclear Power Inspectorate serving as the managing party. Numerous publications provide a detailed discussion of both the HYDROCOIN (see HYDROCOIN 1987) and INTRAVAL (see INTRAVAL 1988 and INTRAVAL Ad Hoc 1987) projects' objectives and programmatic structure.

Validation Issues

The validation issues identified in the ground-water flow (HYDROCOIN) (see HYDROCOIN 1987 and Andersson 1988) and transport (INTRAVAL) studies (see INTRAVAL 1988 and INTRAVAL Ad Hoc 1987) deal with testing different aspects of conceptual models and related computer codes used to simulate them.

The process of model validation can be thought of as a series of questions to be asked of the experimental database and the computer models:

1. What are the relevant processes of the experiment and how does the model consider them?

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2. What is the geometric and spatial framowork of the hydrogeologic system and do the modeling assumptions conform to them?

3. Are the simplifying assumptions inherent in the model compatible to the hydrogeologic, hydraulic, and geochemical components of the system being modeled and consistent with the model use?

4. Are the model inputs representative of the system?

5. Are the field and laboratory experiments detailed enough to provide unique sets of databases that characterize the governing processes?

6. Is the measurement scale compatible to the scale of the relevant processes?

7. Is there a coherent validation strategy that allows for additional data collection and determination of "goodness of fit" criteria for comparison of the simulation results versus the independent experimental database?

Performance Assessment of HLW and LLW

The purpose of the NRC staff's involvement in the HYDROCOIN and INTRAVAL projects is to prepare for future performance assessments of high-level and low-level radioactive waste facilities. Specifically, the NRC staff will be able to examine the validity of computer codes that may be used in licensing reviews. These codes are anticipated to be used to simulate radionuclide migration over time periods and in hydrogeologic systems relevant to waste disposal. HYDROCOIN and INTRAVAL are limited to geosphere transport models and do not include waste leaching or dose assessment models.

HYDROCOIN has examined the validity of ground-water flow models primarily with respect to their impact on site characterization (see Davis, 1988 and HYDROCOIN 1987). After site characterization, the next step in a performance assessment of a radioactive waste disposal site is the prediction of performance with respect to radionuclide migration. Therefore, the INTRAVAL Project was begun to address the validity of hydrologic transport models to predict repository performance over the spatial and temporal scales of interest to radioactive waste disposal (INTRAVAL Ad Hoc 1987).

HYDROCOIN STUDY

The "Hydrologic Code Intercomparison Study," HYDROCOIN, is an international study designed to investigate various ground-water modeling strategies used to analyze the performance of nuclear waste disposal facilities (HYDROCOIN 1987). The study began in May 1984 by the Swedish Nuclear Power Inspectorate. The first workshop was held in October 1984 in Stockholm, Sweden with 19 participating groups (see HYDROCOIN 1987). Because ground-water flow modeling will be used in conjunction with site characterization and for simulation of radionuclide migration to the accessible environment through dissolution of the waste form and transport by ground water, the importance of ground-water flow modeling in performance assessment requires a thorough knowledge of the validity of ground-water models and the application of ground-water models in sensitivity and uncertainty analyses.

The HYDROCOIN study was divided into three levels to accomplish the following three basic technical objectives:

1. Benchmarking and verifying the numerical accuracy of codes by code intercomparison and by comparing code results with analytical solutions (code verification).

2. Evaluating and demonstrating the applicability of the modeling process for describing the results of experiments at both the laboratory and field scales (model validation).

3. Investigating and evaluating various methods and approaches for determining the importance of different phenomena and parameters (sensitivity analysis) and for establishing the uncertainties associated with the performance assessments obtained through this modeling process for both current and future conditions (uncertainty analysis).

Code Verification (Level 1)

Seven verification and benchmark problems were selected for the HYDROCOIN Level 1 effort (see Davis 1988 and HYDROCOIN 1987). They include:

Case 1 - two-dimensional, transient, radial flow from a borehole in a fractured permeable medium.

Case 2 - two-dimensional, steady-state flow in a rock mass intersected by fracture zones.

Case 3 - two-dimensional, saturated-unsaturated flow in a layered sequence of rocks.

Case 4 - two-dimensional, transient, thermal convection in a saturated permeable medium.

Case 5 - two-dimensional, steady-state flow and brine transport around a hypothetical salt dome.

Case 6 - three-dimensional, steady-state flow in a regional aquifer system containing bedded salt deposits.

Case 7 - two-dimensional, saturated flow through a shallow land disposal facility in argillaceous media.

The NRC staff and contractors simulated all of the Level 1 cases which are described in NUREG-1249 Vol. 1 (Davis 1988).

Model Validation (Level 2)

Five experimental data sets were selected for use in the Level 2 (validation) effort (Andersson 1985 and HYDROCOIN 1987). They include:

Case 1 - a field heat transfer experiment (Cornwall, England) involving thermal convection and conduction.

Case 2 - variable density fluid flow based on a laboratory experiment with thermal convection (Elder experiment).

Case 3 - a small ground-water flow system in fractured monzonitic gneiss (Chalk River, Ontario, Canada).

Case 4 - three-dimensional, regional, ground-water flow in low permeability rocks (Piceance Basin, Colorado, USA).

Case 5 - unsaturated zone, soil water redistribution near the surface at a field site (Central Valley, California, USA).

While none of these data sets were felt to be totally adequate for validation, it was believed that the exercise of simulating these field and laboratory experiments provided valuable information about the codes and the modeling strategies. The NRC Staff and contractors have simulated cases 1, 4 and 5 and were the pilot groups that formulated and initially modeled cases 4 and 5 (see Andersson 1988, HYDROCOIN 1987, and Nicholson 1987).

Uncertainty and Sensitivity Analysis (Level 3)

The Level 3 effort includes the use of tools and techniques for sensitivity and uncertainty analysis in conjunction with ground-water flow models. Seven Level 3 problems and data sets (see HYDROCOIN 1987) have been defined, and these include:

Case 1 - near-surface disposal in argillaceous media (an extension of Level 1, Case 7).

Case 2 - unsaturated flow in fractured tuff.

Case 3 - regional ground-water flow for a bedded salt system (an extension of Level 1, Case 6).

Case 4 - coupled ground-water flow and brine transport (an extension of Level 1, Case 5).

Case 5 - crystalline rock case with two alternatives: (a) Chalk River (an extension of Level 2, Case 3), (b) Fjaellveden, Sweden, KBS-3 site.

Case 6 - three-dimensional ground-water flow in low permeable media (an extension of Level 2, Case 4).

Case 7 - particle tracking sensitivity study.

The NRC staff and contractors are presently completing simulation studies of cases 1, 2, 3, 6 and 7, and were the pilot groups for formulating and initially modeling cases 6 and 7 (Nicholson 1987 and HYDROCOIN 1987).

HYDROCOIN Products

Twenty-five project teams representing 11 countries have participated in HYDROCOIN through the simulation and analysis of the test cases (see HYDROCOIN 1987). The experiences of the various project teams resulted in a number of recommendations or "lessons learned" related to the validation and use of hydrogeologic models (see Cole 1987 and Nicholson 1987). In this report "lessons" is used in the more generic sense to mean the variety of quantitative and qualitative findings (e.g., numerical techniques, particle tracking algorithms, and problem formulations) that have resulted from this effort. Lessons include newly identified findings as well as confirmation of the importance of previously identified findings. Many of the lessons are drawn from direct experiences with numerical simulations of both saturated and unsaturated flow problems dealing with various geologic media (e.g., fractured crystalline rock, clay, bedded salt, tuff) for both high- and low-level waste disposal settings. They relate directly to the codes, numerical techniques, and details regarding the way the codes were applied, as well as the methods and approaches for interpreting the data sets. Other validation lessons developed directly from the interactions and discussions at the HYDROCOIN workshops and at specially convened symposia (Cole 1987, HYDROCOIN 1987 and Tsang 1986), and from the process of code and methodology intercomparison.

Work on Level 1, model verification, has been completed and published (see Davis 1988 and

Nicholson 1987). Work on Levels 2, model validation, and 3, model uncertainty and sensitivity analysis, has been completed and will be published soon.

Lessons Related to Validation

In the context of waste management it has been suggested that validation applies to both the code and conceptual model [IAEA definition (IAEA 1982)]:

> "A conceptual model and the computer code derived from it are "validated" when it is confirmed that the conceptual model and the derived computer code provide a good representation of the actual processes occurring in the real system. Validation is thus carried out by comparison of calculations with observations and experimental measurements."

Comprehensive databases sufficient for validation of complex ground-water flow models are not available at present (INTRAVAL Ad Hoc 1987 and Nicholson 1987). This was confirmed by extensive literature searches and technical inquiries that were undertaken to find data sets for Level 2. Numerical simulations using the Level 2 data bases, initially thought to be complete, revealed that the test case data were not sufficient for validation purposes. Earlier INTRACOIN project efforts indicated that for many field situations, especially at larger scales, there are too many degrees of problem freedom to allow validation in the traditional sense. As a result at least two aspects of validation must be addressed. One aspect involves selecting sufficiently complete data sets and well-defined experiments (at either the lab or field scale) to validate, in the traditional sense, our mathematical description of the physical processes involved in ground-water hydrology. A second aspect involves building confidence in the ground-water modeling process. Confidence in the way data are interpreted and codes are applied to assess performance is generated by the application of codes to understand and interpret hydrologic experiments having different levels of detail in databases. Patrick Goblet (Ecole des Mines, Fontainbleau, France) summarized at the 4th HYDROCOIN workshop some of the aspects of validation when he stated, "We need to validate the applicability of our characterization methods, ability to interpret, understand and model in low permeability deep hydrologic systems."

Uncertainty and Sensitivity Analysis

Level 3 of HYDROCOIN was concerned with the application of sensitivity and uncertainty analysis techniques to hydrologic models in the context of radioactive waste disposal. Sensitivity analysis is used to evaluate the effect of changes in model parameters and modeling assumptions have on the simulation results or performance measure calculations to identify the most important parameters for the performance assessment. Uncertainty analysis is used to evaluate the effect limitations in site characterization and incomplete understanding of the hydrogeologic system have on the simulation results. In this regard, uncertainty analysis provides a quantitative measure of the reliability of the model. Data for characterizing and understanding a hydrogeologic system is primarily obtained through the drilling of wells and subsequent testing using the well field. A site conceptual model implicitly and explicitly contains many simplifications of the natural system based on extrapolations and interpolations of the database. Sensitivity and uncertainty analyses are important to understanding simulation limitations of a hydrogeologic system. Therefore, the application of sensitivity and uncertainty analyses in support of hydrogeologic investigations were examined in the final phase of HYDROCOIN.

The use of sensitivity and uncertainty analysis requires: (1) determination or selection of performance measure(s) (quantitative measure(s) that relates simulation results to the purpose of the investigation); (2) hydrogeologic simulations which investigate sensitivities and uncertainties of the hydrogeologic system; and (3) identification of important features or sensitivities of the hydrogeologic system through the analysis of the results of the performance measure(s) calculations.

Simulations, in support of the sensitivity analysis of HYDROCOIN, were comprised of variation of a single model parameter (single parametric variation) and simultaneous variation of all model parameters (global sensitivity). For the single parametric variation technique the analyst uses his knowledge of the hydrogeologic system to select certain parameters and modeling assumptions to vary to better understand system behavior. Analysis results can be biased by an incomplete or erroneous understanding of the system. Another class of sensitivity analysis, global sensitivity analysis, attempts to remove this bias by varying parametric values simultaneously via a statistical sampling scheme such as Latin Hypercube Sampling. No significant differences in results using the two different types of sensitivity and analysis were observed in the HYDROCOIN test cases. The primary reason for the similar results was that the simplicity of the test cases presented little of the interpretational difficulty and multiple processes encountered for field investigations. It would be expected that as site complexity increases and understanding the hydrogeologic system becomes more difficult the benefit of a global sensitivity analysis would increase.

Performance Measures for Validation

The HYDROCOIN group also recognized that the selection of an appropriate performance measure is an integral part of validation. One must select a performance measure suited to the modeling purpose. This issue in code validation is also a problem with real site analysis. The type of performance measure used to generate confidence in the model's results must be carefully selected to be a true measure of the model's adequacy for use in performance assessments. For example, in ground-water simulations of the Piceance Basin (Level 2, Case 4), the ability of the model to match the measured heads was dependent on whether an arithmetic mean, a root mean square error, or a kriged-weighted error was used in the comparison. The selection of the most appropriate performance measure must be resolved in order to decide which of the various simulations provides an adequate description of the flow field for the purpose of the modeling exercise.

The performance measure(s) used to evaluate system behavior were found to have a significant effect on the analysis results. For example, for test case 1 of Level 3 (concrete encapsulated waste disposed of near the surface (see HYDROCOIN 1987)) the properties of the concrete were found to be important to the calculation of one performance measure (volumetric flux through the concrete) and not the other (shortest travel time from the concrete to a boundary). The volumetric flux performance measure is a quantitative measure of the amount of ground water available for leaching nuclides from the concrete blocks while the travel time performance measure is a conservative measure of the containment ability of the geologic site. The use of multiple performance measures allow the total system to be divided into subsystems each with its own performance criteria (e.g., volumetric flux for the concrete). This increased reliability in the interpretation of results was clearly demonstrated in validation test case 1 of Level 2 (see HYDROCOIN 1987). For this test case (heater experiment in granite), project teams were able to fit either of two performance measures but not both with comparable accuracy. Validation was not achieved and the accuracy of the experimental procedure was called into question based on the simulation results for both performance measures. The multiple performance measures promoted the consideration of alternative conceptual models and yielded more focused measures of system performance.

INTRAVAL STUDY

The "International Transport Validation Study," INTRAVAL, which formally began in Stockholm, Sweden in October 1987, is a direct outcome of the successes and lessons learned in the HYDROCOIN project. For example, the validation studies of HYDROCOIN illustrate the need to reexamine the database and assumptions used to develop the model input and to perform additional experiments to isolate individual processes and phenomena of the conceptual model.

Based on this need, the INTRAVAL project is utilizing data bases which are amenable to later testing. Also, scale dependency of the large temporal and spatial considerations associated with radioactive waste disposal precludes true validation. Therefore, the INTRAVAL project will examine natural analogues to radioactive repositories and use coupled laboratory and large-scale field studies (e.g., Las Cruces Trench study) to analyze scale dependence issues.

The original test cases considered for the INTRAVAL project were for saturated flow and transport in fractured and porous media (INTRAVAL Ad Hoc 1987). Unsaturated flow problems which are relevant to low-level and high-level radioactive repositories have since been defined for the INTRAVAL project. The US NRC staff and contractors have prepared test case descriptions for both the experimental studies and the associated modeling activities for both porous and fractured unsaturated media.

The purpose of INTRAVAL is to increase the understanding of how various processes and hydrogeological structures of importance for the transport of radionuclides from a repository to the accessible environment can be properly described by mathematical models, and how models developed for this purpose can adequately simulate radionuclide transport during short as well as very long time periods (INTRAVAL 1988). Additional benefits from the INTRAVAL project involvement are active interchange between experimentalists and modelers on state-of-the-art experiments for validating geosphere flow and transport models for radioactive waste disposal. Discussions on improvements to these experiments and suggested new experiments also will be pursued.

INTRAVAL Cases

The study cases adopted and assigned "Pilot Group Leaders" by the Co-ordinating Group in April 1988 for Part I and Part II were:

Part I

Case 1a Radionuclide migration in intact rock and clay samples by diffusion and advection based on laboratory experiments performed at Harwell, U.K.
Pilot Group Leader: David Lever, Harwell.

Case 1b Uranium migration in crystalline bore cores based on laboratory experiments performed at EIR, Switzerland.
Pilot Group Leader: Jorg Hadermann, EIR.

Case 2 Radionuclide migration in single natural fissures in granite based on

laboratory experiments performed at KTH, Sweden.
Pilot Group Leader: Tryggve Eriksen, KTH.

Case 3 Tracer tests in a deep basalt flow top performed at the Hanford reservation, Washington, USA.
Pilot Group Leader: Charles Cole, PNL.

Part II

Case 4 Flow and tracer experiments in crystalline rock based on the Stripa 3-D experiment performed within the international Stripa project.
Pilot Group Leader: Ivars Neretnieks, KTH.

Case 5 Tracer experiments in a fracture zone at the Finnsjon research area, Sweden.
Pilot Group Leader: Peter Andersson, Swedish Geological Co.

Case 6 Withdrawn.

Case 7 Natural Analogue studies at the Pocos de Caldas site, Minas Gerais, Brazil.
Pilot Group Leader: Neil Chapman, BGS.

Case 8 Natural Analogue studies at the Koongarra site in the Alligator Rivers area of the Northern Territory, Australia.
Pilot Group Leader: Peter Duerden, ANSTO.

Case 9 Radionuclide migration in a block of crystalline rock based on laboratory experiments performed at AECL. Whiteshell, Canada, in cooperation with the U.S. DOE.
Pilot Group Leader: To be appointed by Norman Eisenberg, USDOE.

Case 10 Unsaturated flow and transport in porous media at the Las Cruces Trench Experiment with emphasis on assessing spatial variability.
Pilot Group Leader: Thomas J. Nicholson, USNRC

Case 11 Unsaturated flow and transport in fractured tuff at the Apache Leap Tuff Site with emphasis on assessing matrix-fractured flow systems.
Pilot Group Leader: Thomas J. Nicholson, USNRC.

Case 12 Unsaturated flow and transport in fractured welded tuff at the G-Tunnel, Nevada Test Site, Nevada with emphasis on varying moisture content and temperature gradients
Pilot Group Leader: Dwight Hoxie, US Geological Survey

NRC Activities in INTRAVAL

NRC staff involvement in this project is extremely beneficial to the waste management program for two reasons. First, a number of issues relevant to assessing the adequacy of a license application will be addressed, such as: the validity of hydrogeologic models, hydrogeologic characterization of a field site, extrapolation of laboratory measurements to field experiments, and extrapolation of short-term test (e.g., days to months) data to long-term (e.g., thousands of years) performance assessments. Second, the staff analysis performed to evaluate a hydrogeologic data base will be similar, regardless of whether the purpose is to judge the adequacy of (1) an INTRAVAL database to support a hydrogeologic hypothesis, or (2) a licensee's database in support of his application. Therefore, involvement in INTRAVAL will afford staff "hands-on" experience with some of the analysis work which will be required during license reviews. A further benefit of INTRAVAL involvement is the interaction with experts from around the world with the NRC staff analysing the same waste management issues.

Specifically, NRC staff evaluations will entail: (1) analysis of the collected data to construct a conceptual model(s); (2) simulation of the experiment, based on the constructed conceptual model(s), with an available NRC computer program; (3) evaluation of the simulation results to validate the conceptual model(s) and/or suggest further testing/characterization needed to prove and/or disprove the various conceptual model(s); and (4) revision and reevaluation of these conceptual model(s) and the need for additional data. These analyses will be reported through the INTRAVAL Project workshops and reports. The NRC staff will be further assisted by the review and recommendations provided by INTRAVAL participants on the NRC staff analyses.

The INTRAVAL project structure is based on a participating organization having one or more project team(s) performing the technical work. Presently there are nine INTRAVAL test cases with more being proposed. Although it would benefit the NRC to follow the work performed by all participants as it relates to generic issues (i.e., time and spatial scale issues, extrapolation of laboratory data), the most important INTRAVAL test cases which the NRC staff and contractors will simulate first are:

Case 10 Las Cruces Trench Study (New Mexico State University/PNL/MIT)
- Infiltration and solute transport under variably-saturated conditions for heterogeneous porous media in the near surface;

Case 11 Apache Leap Tuff Study (University of Arizona)
- Fluid flow and solute transport experiments in unsaturated fractured tuff at both the laboratory and field scales;

Case 12 Borehole Experiment in G-Tunnel, Nevada Test Site (USGS)
- Fluid flow and solute transport at elevated temperatures and various moisture contents in the vicinity of boreholes in fractured tuff;

Case B Alligator Rivers Analogue (Australia Nuclear Science & Technology Organization)
- Solute transport in a reducing and oxidizing environment over extremely long time scales (thousands of years) relevant for waste management performance assessments.

Additional cases will be simulated as time and resources permit.

CONCLUSIONS

The most significant conclusions taken from the HYDROCOIN study were:

(1) validation is a site specific issue (i.e., validity depends on both the model and the correct interpretation and use of site data);

(2) comparison of model simulations with a single spatial and temporal set of experimental results is likely to result in model calibration rather than validation;

(3) a variety of conceptual models should be examined when evaluating hydrogeologic site conditions to determine if simplifying assumptions are valid;

(4) with respect to validation, more is learned when models are rigorously tested on a variety of possible site conditions than when models are tested for simple conditions which can be easily reproduced;

(5) validation can best be judged when prior performance measures are established and specific criteria for model acceptance are fully defined.

The NRC staff and contractors will be involved in the INTRAVAL study to fully address model validation. Future efforts will involve both field and laboratory experimentalists and modelers. These efforts will require experiments specifically designed to address model validation issues in the context performance assessment. These experiments must be formulated and developed by both laboratory and field experimentalists to provide the comprehensive database for validation. Efforts must provide a better understanding of the limitations that incomplete system characterization poses in terms of hydrogeologic system interpretation and conceptual model development. The validation process will involve iteration between experimentation and simulation wherein the database is reexamined and additional data is collected. Additionally, we must be able to demonstrate what effect incomplete characterization has on model validation and performance assessment uncertainty.

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