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Repository Technology Program Activities: FY 1988

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Repository Technology Program Activities: FY 1988

Background

Lawrence Livermore National Laboratory (LLNL) began conducting technical research under the auspices of the U. S. Department of Energy (DOE) Repository Technology Program (RTP) in FY 1982. The focus of this work is technology development in several areas to support the programs of the U.S. Office of Civilian Radioactive Waste Management (OCRWM). We are currently concentrating on the following tasks:

- Simulator development for coupled *in situ* hydrologic, thermal, and mechanical processes.
- Evaluation and development of experimental hydrologic, geochemical, and mechanical techniques.
- Simulator development and accompanying experimental activities for reactive transport.

Our hydrothermomechanical simulator development furnishes OCRWM with tools for calculating the responses of fractured, porous geologic media that have been perturbed by excavations, by heat sources or sinks, or by changing hydrologic conditions. The aim of our reactive transport effort is to develop significantly improved methods for evaluating the movement of chemical and radioactive contaminant species through rock mass fractures. These techniques will go well beyond the currently available simplified methods, which are subject to large cumulative errors as they step through time. New and improved experimental techniques are needed for measuring parameters that affect the performance of mined geologic disposal systems. The focus of our work in this area is on hydrologic measurements and geomechanical strain measurements, which we will use to develop and verify the performance of enhanced disposal systems under controlled laboratory conditions so that reliable field applications can be achieved.

In FY 1985, we specified and tested commercially available instruments used for making geotechnical and hydrologic measurements, and we designed a prototype borehole instrument for measuring displacements along fractures. We also performed scoping calculations for proposed field experiments using thermomechanical codes. Other FY 1985 activities included evaluating our modeling techniques and data requirements with respect to our program objectives and then establishing criteria for assessing the modeling results; these criteria were documented by reports in a letter format.

In FY 1986, we began the development of a semi-analytical approach for calculating coupled mechanical and hydrologic rock mass responses. This work improved our understanding of the processes encountered *in situ* in fractured rock, and it helped us to define the limitations of the numerical models then available for simulating such complex experiments. Based on this progress, we initiated (in FY 1986) the development of the mathematical foundations necessary to significantly improve our simulations of coupled mechanical and hydrologic phenomena; we continued this work in FY 1987 and FY 1988. Ultimately, the results of this work will be applied directly to flow and transport situations in which flow in fractures may be perturbed by excavations or by thermally induced stress changes.

Our experimental activities in FY 1987 included the following: developing and testing geotechnical instruments to be used in field experiments, assisting the RTP/DOE in developing technical objectives, and conducting field trials of geophysical methods to monitor grout injection into rock mass. Field work for the latter was carried out in mid-to-late FY 1987. Other FY 1987 activities included participation in the Excavation Response

Experiment (ERE) Planning Committee, the Buffer/Container Experiment Planning Committee, the Borehole Sealing and Shaft Sealing Experiment Planning Committees, and the Single Fracture Migration/Sorption Experiment under the auspices of the DOE/Atomic Energy Company of Canada, Ltd.,

(AECL) Subsidiary Agreement. Our involvement on these Underground Research Laboratory (URL) planning committees allowed us to provide better support to the OCRWM because we were able to coordinate the LLNL work with the activities of other U.S. and Canadian investigators.

Overview of Technical Progress in FY 1988

Our technical activities in FY 1988 included instrument selection and evaluation, calculational work, and simulator development. Near the end of the fiscal year, we began preparing several topical reports to document our results.

This fiscal year, we continued developing three-dimensional numerical simulators to model coupled hydrologic- and mechanical-rock mass responses and, thus, to provide representative numerical tools for understanding and calculating these *in situ* processes. We also began scoping calculations in the second half of FY 1988 to evaluate ERE design criteria, but this work was redirected late in the year when the DOE/AECL Subsidiary Agreement was set aside.

Our work in developing and evaluating experimental techniques focused on total

pressure measurement, moisture content measurement, and tracer detection instrumentation for sealing experiments and for rock-mass-response field tests. At the end of the fiscal year, we completed a review of measurement technology for instrumenting migration/sorption tests to help define the technological requirements in these areas.

By the end of FY 1988, we had completed a review of the existing codes for simulating reactive transport; we are using the results of this review to help formulate plans for future activities in this area.

The following sections describe the major RTP tasks and activities at LLNL in more detail, and they include our FY 1988 accomplishments in these areas.

Hydrothermomechanical Simulator Development Task

Ananda M. Wijesinghe

In this task, we are developing in stages a two- and three-dimensional hybrid boundary-element finite-element computer code named GENASYS (acronym for **G**eotechnical **E**ngineering **A**nalysis **S**ystem) for computing the coupled fracture fluid flow, heat flow, and deformation response of fractured rock masses that are subject to excavation. In the first stage of this work, which is currently in progress, the boundary element part of the code for deformation is being developed. In the subsequent stages, we will extend the code to include a finite-element formulation for computing fluid and heat flow along the fractures and a boundary-element formulation for computing heat flow in the rock mass. In GENASYS, the fractures in the rock mass are represented as one or more discrete two-dimensional curved surfaces in three-dimensional space or as one-dimensional curved lines in two-dimensional space. The fracture surfaces are allowed to have any arbitrary shape and orientation and are permitted to intersect one another and form a network of fractures.

The capability to compute problems in three spatial dimensions rather than in two dimensions is critical for accurately predicting the hydrothermomechanical response of a fractured rock mass subject to excavation. This is because it is necessary to be able to faithfully represent the geometry of the excavation; the geometry, orientation and connectivity of the fractures; the inhomogeneity and material anisotropy of the unfractured rock; the three-dimensionality and anisotropy of the *in-situ* stress; and the nonuniform spatial distributions of the solution variables. In typical problems, the orientations and spatial distributions of these quantities relative to one another are such that the problems cannot be simplified to two spatial dimensions without seriously compromising the accuracy of the solution.

Currently, there are no other computer codes capable of computing coupled three-dimensional hydrothermomechanical problems in fractured rock masses with discrete representation of the fracture surfaces. Furthermore, codes that

employ volume-discretization-based solution methods generate very large computational models for three-dimensional problems; these models are beyond the capabilities of even the largest supercomputers. The GENASYS code is specifically designed to efficiently compute large problems in unbounded three-dimensional domains in which the far-field response is primarily linear and in which the nonlinearities are concentrated along fracture surfaces and in highly localized regions in the interior of the problem domain (e.g., near-field damage zones).

In GENASYS, the size of the computational problem is kept at a manageable level by adopting a hybrid boundary-element finite-element approach that requires the gridding of only the external boundaries, the internal material interfaces, the fracture surfaces, and the interior regions of localized nonlinearity. This method also accurately accounts for far-field boundary conditions at infinity, thus eliminating the need in volume-discretized solution methods to extend the computational grid to an arbitrarily chosen external boundary location. Because the boundary integral equations used in the code employ singular solutions of the linearized governing equations as Green's functions, sharp variations in the solution are easily accommodated, stress discontinuities that occur at interior element boundaries in most volume-discretization methods are avoided, and highly accurate solutions can be obtained for relatively coarse boundary discretizations. Highly adaptive solution algorithms such as variable-order, variable-refinement adaptive quadrature schemes, and adaptive nonlinear equation solution methods are being implemented to exploit the power and efficiency of this hybrid computational approach.

As an integral part of the GENASYS code development effort, we will also develop a comprehensive pre-processor/post-processor graphics capability to quickly and easily generate the computational grid and material property input data, and to display and analyze the output results in two and three spatial dimensions.

Another important aspect of the development of this code is the formulation of improved theoretical models to describe the constitutive behavior of fracture deformation, fracture fluid flow conductivity, stress-induced damage, and the relationship of fracture statistics to discontinuum behavior. To validate the developed constitutive models against experimental data, we will actively participate

in laboratory and field experimental programs, such as the Canadian Underground Research Laboratory (URL) Excavation Response Experiment (ERE), that are designed to provide the required data for code validation. We will also exercise and validate the GENASYS code through participation in computational workshops at which the performances of different codes are compared.

GENASYS Code Development and Verification

In FY 1988, A. M. Wijesinghe continued the development (began in late FY 1987) of Version 1.0 of the GENASYS code, and he applied it to compute the deformation response of the rock mass at the Canadian URL to sequential excavation of Instrument Room 209. During this application of the code to an actual field problem, we found that the Barton-Bandis joint deformation model was not sufficiently general in its treatment of fracture deformation for application to multidimensional coupled-shear and normal-fracture deformations. Therefore, we initiated the development of an improved constitutive model for fracture deformation.

The GENASYS Version 1.0 code is designed to compute the three-dimensional mechanical deformation of a rock mass containing discretely represented fractures. Although the code was programmed for both unfractured and fractured domains, because of time restrictions imposed by the impending Room 209 ERE calculations, it was verified and made operational only for the deformation of unfractured three-dimensional domains. To prepare for computing these large problems, we installed the code on LLNL's CRAY-1 computers (part of the Octopus operating system). During this process, we found that some code modifications were needed to make the code compatible with the Cray Fortran (CFT) compiler and the Octopus file system.

With this capability in hand, numerical simulation of the Canadian URL Room 209 Excavation Response Experiment was begun in FY 1988. In this experiment, which is a trial run for the main ERE, the response of the rock mass to the excavation of a tunnel was measured. The tunnel was excavated in a sequence of nineteen excavation steps, and the rock mass response was measured by an array of instruments that

included borehole extensometers and stressmeters. The excavation sequence consisted of a pilot hole excavated in the first ten steps which was then enlarged to the final tunnel diameter in nine additional slash steps (see Fig. 1). The deformed cross-sections at the end of excavating the pilot hole are shown in Fig. 2. They illustrate the lack of symmetry in the three-dimensional pattern of deformation of the rock mass; this is primarily a result of the anisotropy and the lack of symmetry of the *in-situ* stress relative to the tunnel geometry.

Figure 3a shows the computed changes in the magnitudes of the principal stresses, that would be measured by the stressmeter N1 located as shown in Fig. 1. The displacements of the anchors of the extensometer EXT-08, shown in Fig. 1, relative to the displacement at the deepest anchor, are given in Fig. 3b. These instruments were installed after the initial tunnel excavation (step 0); therefore, the stresses and deformations measured by these instruments are the changes in these quantities from the initial state of stress and deformation created by the excavation of the initial access tunnel.

The principal stresses and relative displacements of the extensometer anchors change rapidly during the first few excavation steps of both the pilot hole and the additional slash steps, and they reach asymptotic values that correspond to a uniform hole of infinite length as the three-dimensional stress disturbance at the excavation face moves away from the points of measurement. These results were presented by A. M. Wijesinghe at the Eighth URL ERE Planning Committee meeting held on March 23-24, 1988 in Lac Du Bonnet, Canada.

Figure 1. The nineteen excavation steps needed to construct Instrument Room 209 at the URL. The pilot hole was excavated in the first ten steps, then enlarged in nine additional steps. The approximate location of one extensometer (EXT-08) and one stressmeter (N1) are shown.

Figure 2. Cross-section geometry and calculated deformed cross sections after the Room 209 pilot hole was completely excavated through step 10. (a) Left face, $y = -21.7$ m, (b) initial excavation face, $y = 0$ m, (c) right face, $y = 24.9$ m. Displacements shown are magnified 500 times.

Figure 3. (a) Calculated principal values of stress change at stressmeter N1. (b) Calculated change in displacement between anchors of extensometer EXT-08 relative to the deepest anchor 1.

These calculations assume linearly elastic rock deformation and primarily account for the three-dimensional geometry of the excavation and the strongly nonisotropic *in-situ* stress state that preclude two-dimensional idealizations. To model this excavation sequence with GENASYS Version 1.0, we discretized the surface of the tunnel using 50 to 100 curved eight-noded quadratic isoparametric boundary elements and 150 to 300 boundary nodes. The computational time for a run ranged from 30 to 60 minutes on a CRAY-1 computer, with the input/output operations accounting for a significant fraction of this time owing to out-of-core solution of the

matrix equations. The \$8000 computational cost for calculating the entire sequence of nineteen excavation steps using the GENASYS boundary element code was more cost effective by a factor of 20 to 30 than the three-dimensional finite-element computations reported by others at the URL ERE Planning Committee meetings. To perform these computations conveniently, we added to the GENASYS code the capabilities to directly input instrument location data and to compute output results in a form that can be directly compared with the measurements made at these locations.

Constitutive Model for Fracture Deformation

In the URL Room 209 excavation, the stresses acting on a steeply-dipping water-filled fracture that would be intersected by the tunnel were measured after each excavation step. Fluid flow pressure tests were also performed to measure the change in the hydraulic conductivity of the fracture before and after excavation of the tunnel. The computations described previously yielded the displacements and stresses induced in the rock mass by excavation of Room 209 with the rock assumed to be unfractured and homogeneous. The normal traction and the two shear traction components acting on the fracture can be computed from these numerical results if we also assume that the deformation of the fracture does not alter the stress state in the

vicinity of the fracture so that the computed traction is *impressed unaltered* on the fracture. This assumption will be tested later using the fully coupled version of GENASYS that accounts for the effect of fracture deformation on the stress state. Subject to this condition, we will be able to use a constitutive model for fracture deformation to compute the changes in fracture aperture due to the changes in the tractions acting on the fracture. These aperture values can then be used with an appropriate flow law to compute the hydraulic conductivity of the fracture for comparison with the experimental data.

To predict the aperture changes from the stress changes predicted by the uncoupled GENASYS stress calculations, Wijesinghe wrote

a stand-alone post-processing computer program, based on the Barton-Bandis constitutive model for fracture deformation. The Barton-Bandis model describes one-dimensional joint deformation under conditions when either the normal traction or the shear traction is held fixed. It, therefore, provides an incomplete description of the joint deformation that would occur under the simultaneous multidimensional normal and shear traction changes predicted by the GENASYS code. Also, the Barton-Bandis model cannot be systematically modified to account for complex stress variations in which different traction components follow complicated loading, unloading, and cyclic stress paths. Calculations, based on the Barton-Bandis model, which assume uncoupled normal and one-dimensional shear modes of deformation, yielded substantially different fracture displacements when compared with a modified Barton-Bandis type model that approximately accounted for the coupling between these modes.

From these studies, it became clear that an improved model for fracture deformation was needed to account for the following:

- Multidimensional fracture deformation in the normal and two shear directions.
- The coupling between the normal and shear modes of deformation.
- Complex loading, unloading, and cyclic stress paths encountered in real excavation problems.

To fill this need for a more accurate description of fracture deformation, Wijesinghe developed a new elasto-plastic constitutive model for joint deformation that employs the Barton-Bandis constitutive parameters as a subset of the required input data. We coded this constitutive model in the stand-alone joint deformation model computer program and tested it for specific combinations of traction and displacement specified input-load paths. For example, Fig. 4 shows the variation of

Figure 4. Response of the elasto-plastic joint deformation model for a cyclic direct shear test at constant normal traction equal to -7.05 MPa.

shear-stress versus shear-displacement in a cyclic direct-shear test at constant normal traction. The model successfully exhibits the characteristic peak in shear stress, the post-peak softening of the joint, and the different load-deformation paths followed by the joint when loading and unloading in shear. The model also reproduces the dilatant normal displacement upon shearing, the hysteresis in the shear stress response upon repeated cyclic shearing of the joint, and the asymptotic approach of the shear-stress/shear-displacement cycle to a fixed limit cycle as the roughness asperities are degraded. We intend to further enhance this model so that it can mimic

the phenomenon of reverse yield in the normal-stress/normal-deformation response when the joint is unloaded. We will then be able to compare the results from the model with any experimental data available in the literature. When testing is complete, this elasto-plastic constitutive model will be incorporated in the GENASYS code.

We presented the above results to RTP/DOE managers at a project review meeting held on September 26-27, 1988. We will also document the results of this work on constitutive modeling of joint deformation in a formal LLNL report and in journal articles.

Pre-Processor/Post-Processor Software Development

The most important factor that currently hinders the use of the GENASYS code in practical applications is the lack of general input data generation, output results processing, and graphical display capabilities. For example, when the URL Room-209 calculations were being performed, it consumed one man-month to prepare by hand one set of three-dimensional computational grids for the nineteen excavation steps. Manual grid generation is error prone and is not practical for the more complicated three-dimensional problems that GENASYS is designed to handle. Examining the voluminous tabular data produced by the code, and scanning and plotting the results, are also very laborious and time-consuming tasks. In FY 1988, we studied this problem, and proposed the development of a comprehensive pre-processing/post-processing software package that can be used for all versions of GENASYS.

We received approval from RTP/DOE to initiate the development of this pre-processing/post-processing software package in mid-FY 1988. We evaluated the following

alternatives available for developing this capability:

- Develop the code from scratch at LLNL.
- Acquire and modify an existing LLNL or public domain code.
- Purchase a commercial stand-alone software package with a user-programmable software interface, and develop an application interface to GENASYS at LLNL.

After surveying the available codes and their hardware, operating system, and licensing requirements, we selected the last option as having the best chance for success in the shortest time. Our survey indicated that the most suitable commercial packages were PATRAN, AUTOCAD/AUTOSOLID, and SUPERTAB. In vendor demonstrations, PATRAN proved to be the most suitable alternative, so we decided to license PATRAN and develop an application interface for GENASYS. Also, because PATRAN runs only on workstations and mainframes, we have decided to acquire two SUN workstations for running PATRAN and GENASYS interactively. We will implement this plan when we receive funds from RTP/DOE for the software, hardware, and graphics programming staff.

Canadian URL ERE Scoping Calculations

In the second quarter of FY 1988, the Repository Technology Program at LLNL was assigned the task of performing scoping calculations in support of the design of the main Excavation Response Experiment at the URL in collaboration with the Atomic Energy Company of Canada, Ltd., (AECL). In this experiment, the mechanical and hydrologic response of the granitic rock mass to sequential excavation of one or more tunnels will be measured. The rock at the URL is sparsely fractured, but one or more fractures will be targeted for study with instruments installed specifically to measure the response of those fractures. Other instruments will measure the overall response of the rock mass.

The general experimental concepts and geometries to be examined in our scoping computations were developed under a DOE/AECL Subsidiary Agreement. The scoping calculations were simplified calculations undertaken in support of experiment design to help determine the best experiment configuration and to optimize the locations of the measuring instruments. More complicated detailed calculations were also planned as part of the predictive and back-analysis computations, but they were to be performed at a later date.

Two experimental configurations for the ERE were identified by the URL ERE Planning Committee during the Eighth URL ERE Meeting held in March 1988. In the first test configuration, a sequentially excavated horizontal drift intersected a single vertical fracture located normal to the direction of the drift. In the second configuration, the vertical fracture was assumed to be located on one side of the drift and was oriented parallel to the direction of excavation of the drift. In both cases, the minimum *in-situ* principal stress was assumed to act normal to the plane of the fracture and to lie in the horizontal plane.

We decided to perform the scoping calculations as simply as possible without compromising the essential three-dimensional aspects of the problem. To this end, we decided to perform full three-dimensional computations while employing a linearly elastic isotropic material model for the intact rock and thin low-modulus elastic or elasto-plastic layers to represent the fractures. We needed a three-

dimensional computer code with sophisticated data preparation and results-analysis capabilities because of the large number of computer runs that would be required for grid and parameter sensitivity studies. LLNL's finite element structural analysis code NIKE3D, the associated pre-processor INGRID, and the post-processor TAURUS partially met our requirements, but NIKE3D did not have the capability to handle initial stress, shear-traction boundary condition, and material-excitation capabilities. We arranged for the NIKE3D, INGRID, and TAURUS codes to be expanded to include these features, but we did not have the funds available to have comprehensive changes incorporated in the codes. The developers of these codes at LLNL, however, agreed to implement these features as temporary simple modifications to the existing codes.

While the codes were being modified, E. J. Kansa (in collaboration with other RTP/LLNL staff) began to prepare input data for the scoping calculations for the two test configurations using the preliminary data we received from AECL. Using the pre-processing code INGRID, we generated three-dimensional computational grids for both test configurations. At the end of June 1988, the code developers at LLNL provided us with modified versions of the NIKE3D, INGRID, and TAURUS codes that could account for initial stresses, shear traction boundary conditions, and material excavation in their calculations.

In June 1988, our work on performing the actual URL ERE scoping calculations was halted at the request of RTP/DOE because a new collaborative agreement needed to be negotiated between DOE and AECL. We were instructed to limit our work to verifying and documenting the modifications made to the codes. Also, a portion of the funds originally allocated to the scoping calculation task was diverted to performing calculations in support of RTP instrument development at LLNL.

To verify the modifications made to the NIKE3D code and to evaluate its sensitivity to computational parameters such as the degree of grid refinement and the location of the external grid boundary, Kansa set up and computed solutions to the problem (see Fig. 5) of a spherical hollow cavity deformed by a uniform

uniaxial far-field stress. The analytical solution for this three-dimensional test case was derived by A. M. Wijesinghe because the complete solution for the displacements and stresses could not be found in the literature. Figure 6a shows a typical grid used for computing this problem with the NIKE3D code (Fig. 6b is an expanded view of the grid near the cavity surface). This numerical model uses 5146 nodes and 3734 eight-noded brick finite elements to model one-eighth of the solution domain. To model the full problem at this level of discretization, approximately eight times as many nodes and elements would be needed. This small problem required about 62% of the CRAY-1 computer's two-megaword memory and needed about 19 CPU minutes to compute. Typical numerical and analytical results for the displacements along the x , y , and z axes, and the stress distributions along the x axis are given in Figs. 7 and 8, respectively. These results showed that the displacements are accurate to within 2% everywhere within the solution domain. The accuracy of the computed stresses was poor near the cavity wall but improved rapidly with distance away from it. For example, the stresses were as much as 50% in error at the cavity wall itself, but improved to within 10 and 5% at distances of one and two cavity radii,

Figure 5. Test problem for the NIKE3D structural analysis code—a spherical cavity deforming under a uniform uniaxial far-field stress S .

respectively. These results indicate that, if the grid can be refined further in the immediate neighborhood of the cavity, the accuracy of the stresses computed using NIKE3D can be improved to acceptable levels.

Figure 6. (a) Typical three-dimensional linear brick finite-element computational grid for the spherical-cavity test problem. (b) Magnified view of the grid near the cavity surface.

Figure 7. Displacements (a) u_x , (b) u_y , and (c) u_z along the x , y , and z coordinate axes, respectively, in the spherical-cavity test problem computed using the unmodified NIKE3D code.

Figure 8. Stresses (a) S_{xx} , (b) S_{yy} , and (c) S_{zz} along the x-coordinate axis in the spherical-cavity test problem computed using the unmodified NIKE3D code.

This test problem was simulated in four different ways, as indicated in Fig. 9a-d, to separately exercise the unmodified code, and the initial stress, shear-boundary traction, and material excavation options of the modified code. The initial stress and shear traction boundary condition code options produced correct results that were as accurate as those produced by the unmodified code, but the excavation option results were very inaccurate. This is probably due to an error in implementing this code modification or is due to numerical

instabilities produced by the method of simulating excavation by reducing the elastic modulus in the excavated region to a value far below that of the unexcavated rock.

These results are documented in detail in the LLNL report: *Verification of the NIKE3D Structural Analysis Code by Comparison Against the Analytic Solution for a Spherical Cavity Under a Far-Field Uniaxial Stress*, by E. J. Kansa (January 1989). This report was submitted to RTP/DOE for review and will be formally released upon approval.

Figure 9. Spherical-cavity test problems computed for verifying (a) the unmodified NIKE3D code, (b) the shear boundary traction option, (c) the initial stress option, and (d) the excavation option.

In summary, the initial stress and shear traction options that were installed work correctly as intended. The excavation option does not function correctly and needs further work (and funds) for correction. The NIKE3D code, in principle, is capable of producing quantitatively accurate results in rapidly varying stress fields on sufficiently refined grids. However, because of the low-order interpolation and quadrature

schemes employed in the code, the level of grid refinement needed to compute complex problems may require more computer storage and memory than currently available on LLNL's CRAY-1 computers. Therefore, codes such as GENASYS that employ higher order algorithms to reduce the computer resource requirement will be necessary to efficiently compute these large problems.

Canadian URL ERE Planning Committee Activities

J. L. Yow, Jr. and A. M. Wijesinghe served on the URL Excavation Response Experiment Planning Committee until July 1988, when this activity was halted because the DOE/AECL collaborative agreement had been terminated. In support of the Room 209 ERE, we submitted two reports in letter form to the URL ERE Committee. In the first report, J. Ueng reviewed the Room 209 ERE analysis reports submitted by the AECL and University of Alberta modeling groups. In the second report, Yow and Wijesinghe presented and discussed a set of criteria for evaluating the

Room 209 analyses submitted by the modeling groups. This report was prepared in response to an action item assigned to LLNL at a URL ERE Committee meeting, and it formed the basis for discussions at the modelers workshop held subsequently. We participated in this modelers workshop on June 12, 1988 in Minneapolis, Minnesota. Since that meeting, in response to the instructions from RTP/DOE, we have suspended computational work geared specifically to analysis of the URL ERE until the DOE/AECL agreement is renegotiated.

Experimental Technology Task

Richard K. Thorpe

Earth Pressure Instrumentation

Two types of earth pressure measurement devices were evaluated for possible use in the Buffer/Container Experiments at the Canadian Underground Research Laboratory (URL). Both were of the rigid diaphragm design, but had different mechanisms for detecting deflection of the diaphragm (i.e., bonded resistance strain gauge vs vibrating wire). Similar units have been deployed in previous high temperature (90°C or higher) applications. Based on the results of the buffer mass experiments at Stripa, Sweden (Pusch et al., 1984), hydraulic membrane gauges were not considered for high temperature tests at the URL.

The strain gauge cell was developed by M. Molecke of Sandia National Laboratory, Albuquerque, and was fielded for the Waste Isolation Pilot Project (WIPP) (Tyler, 1984). Three prototype gauges were fabricated and delivered to LLNL by S. Breeze of Sandia, who also provided details on gauge construction and calibration techniques. Figure 10 is a photograph of one of the disassembled units.

In conjunction with the Engineering Measurements Section at LLNL, we tested the thermal stability and hydrostatic pressure calibration of the Sandia gauges (designated as 1, 2, and 3). Cells 1 and 2 were tested in an autoclave to determine their calibrations at temperatures of 28, 100, 150, and 65°C (listed in the order the tests were run); the results of these tests are shown in Fig. 11. The calibration sensitivities, in $\mu\text{V}/\text{V}/\text{psig}$, increased only slightly over this temperature range.

Cell 3 was monitored at atmospheric pressure in an oven held constant at nominally 150°C. Periodic readings over a one-month period indicated the monotonically increasing output (drift) shown in Fig. 12. Clearly, this output is unacceptable for any experimental situation. We then conducted a second long-term thermal drift test on cell 1, which had been subjected to short-term calibrations. Holding this cell at 95°C and at atmospheric pressure, we observed a small amount of drift; however, it was in the opposite sense of what was obtained from the test at 150°C.

Figure 10. Disassembled Sandia earth-pressure cell.

Figure 11. Hydrostatic pressure calibration sensitivities for Sandia cells 1 and 2 at selected temperatures.

In an attempt to reduce the drift, we replaced the circular strain-gauge package in cell 3 with a rosette of four linear (Karma) gauges whose backing material was more resistant to high temperature creep. This cell was retested under atmospheric pressure at a temperature of 150°C; the results of this test are shown in Fig. 13. Over a period of 63 days, the cell drifted only 4 psig (0.028 MPa), compared with over 400 psig (2.76 MPa) for the original strain gauge system. These results demonstrate that with proper choice and installation of strain gauges, the Sandia cells may be suitable for high temperature applications at the URL.

The vibrating wire diaphragm cell was fabricated by Geonor, USA, and is shown in Fig. 14. This cell was considerably larger than the Sandia gauges, and it would have required modification for use in the URL Buffer/Container Experiment. Also, having been designed for measuring contact earth pressures at a structural

interface, it would not have been suitable for free-field pressures. Nonetheless, since it is the only such "off-the-shelf" gauge designed for 95°C and up to 12 MPa total stress, it afforded an opportunity for us to evaluate the calibration and thermal stability of the vibrating wire design.

Figure 15 is a schematic of the calibration setup for the Geonor cell. Because of the limited size of our pressure vessel, the back edge of the cell required machining (see Fig. 14). The cell case remained rigid enough, however, for its performance to remain unaffected. The pressure calibration determined in our laboratory precisely matched the data supplied by Geonor, as indicated by Fig. 16. Although the calibration curve is nonlinear, we found it to be completely reproducible, with essentially no hysteresis. Temperature calibrations for the gauge were still in progress at the close of FY 1988.

Figure 12. Drift (apparent pressure) vs time for "as received" transducer.

Figure 13. Drift (apparent pressure) vs time for regauged transducer. Note the difference in scale from Fig. 12.

Figure 14. Geonor vibrating-wire earth-pressure cell.

Figure 15. System used to pressure calibrate Geonor vibrating-wire transducer.

Figure 16. (a) Pressure calibration data supplied by Geonor for the 12 MPa earth-pressure cell. (b) Results of the LLNL pressure calibration at room temperature.

Moisture Measurement Instrumentation

Our work in this subtask focused on microwave-resonator measurements of the moisture content of a bentonite/sand mixture known as the Reference Buffer Material (RBM). We first completed the preliminary testing of a brass microwave resonator in direct contact with the medium. The tests were performed by pressing the resonator against the flat face of a cylindrical specimen. Three RBM samples with saturation levels of 1.6, 49.0, and 90.8% were prepared for measuring frequency sensitivity as a function of water content. The test data are presented in Fig. 17, and the correlation between resonant frequency and saturation is shown in Fig. 18. The resonant frequencies for the three saturations were 642, 587, and 520 MHz, respectively. The variation, although not exactly linear, demonstrates that this method is at least feasible (i.e., that the output sensitivity is suitable for detecting small changes in moisture content).

Several different resonators were designed and tested as prototypes for use in the URL experiments. Resonators similar to the one tested in the above study were used to monitor small changes in the moisture content of air. Such devices allow for the medium (air) to enter the cavity and, thereby, produce large changes in the resonant frequency. Also, they typically are

Figure 17. Preliminary measurements on the surface of RBM.

Figure 18. Preliminary results from microwave resonator tests on RBM.

flared at one end to optimize the shape of the external microwave field. However, neither of these features could be accommodated in a prototype soil moisture sensor. First, the microwave generator coil at the closed end of the cavity would be shorted if liquid water were to come in contact with it. Second, a flared end would make it very difficult to achieve a uniform density in the surrounding medium under either an emplacement (i.e., boring a hole and inserting the probe) or embedment (i.e., compacting material around the probe) installation.

Therefore, the final design incorporated a straight, cylindrical barrel, and a ceramic disk placed over the sensing end of the resonator to hermetically seal the cavity. A schematic of the unit is shown in Fig. 19. We found that it performed as well as the flare-ended resonators, except that some sensitivity was lost because of the end seal.

Three specimens of buffer material at different densities and saturation levels were prepared for calibrating the prototype microwave moisture sensors. As before, we performed the tests in direct contact with the RBM. Both

the top and bottom faces of each specimen were tested to detect possible density variations, and identical results were obtained in each case; the results are given in Fig. 20. For a saturation range of 44 to 77%, the resonant frequency of the sensor varied from 899 to 895 MHz, respectively. These data indicate that the sensitivity is reduced by the ceramic end seal; however, the range is still well within the resolution of the recording instrumentation.

We also completed thermal stability and low-pressure leakage tests for the prototype sensors. Our results indicate that the signal remains stable and that there is no apparent leakage when the sensor is submerged in water heated to 100°C. We observed spurious signals near the boiling point, however, which were probably caused by vaporization bubbles impinging on the ceramic end piece. This not only demonstrates the sensitivity of the sensor but underscores the importance of the contact conditions. When emplaced or embedded *in situ*, any separation between the sensor and medium could lead to nonuniform moisture distribution and misleading measurements.

Figure 19. Resonant-cavity microwave moisture sensor.

Figure 20. Results of prototype microwave resonator tests.

Fiber-Optic Applications

In this subtask, we conducted experiments to verify methods for detecting tracers with fiber-optic probes (optrodes). We first investigated the suitability of several different fluorescent tracers by conducting short- and long-term static-adsorption tests on loose RBM. We also conducted initial tests on three dyes to determine their thermal stability at room temperature and at 90°C. The higher temperature tests were conducted in sealed, Teflon-lined vessels for one week; the results are shown in Table 1. All of the dyes were found to be fairly stable over the short term; however, results of the long-term tests may show greater degradation. Our preliminary conclusion is that the dyes would be useful for qualitative transport measurements (i.e., breakthrough times) in the Buffer Container Experiments, as long as expected transport times were on the order of a few weeks. Further work is needed, however, to determine the sorption and dispersion characteristics of the dyes in field-emplaced RBM, so as to interpret pore fluid velocities.

As a first step toward measuring transport velocities in RBM, we constructed a linear (column) flow device (see Fig. 21). This device is a standard compaction permeameter used for

measuring the permeability of compacted soils, with modifications for tracer injection and optrode emplacement. A maximum hydraulic differential pressure of 2 MPa could be applied at the inlet. To prevent potential hydraulic fracturing of the medium, we used a pressure of 1.4 MPa so that the expected RBM swelling pressure of 2.5 MPa (Dixon and Gray, 1985) would not be exceeded. A dual reservoir system with a cross-over connection permitted injection of the tracer under steady-state flow conditions, without altering the gradient.

Preparation of the specimen and conduct of the flow tests were as follows. The compaction mold was assembled with the porous disk, baseplate, and cylindrical extension collar attached. The RBM column was then compacted according to AECL specifications, the extension collar was removed, and the top of the specimen was cut even with the end of the mold. Next, a second baseplate and porous disk were clamped onto the top of the specimen. Finally, the entire vessel was submerged in deionized water with the inlet and outlet ports open to permit the escape of air bubbles. The specimen was allowed to saturate over a period of about two months.

Table 1. Results of short-term tracer evaluation tests showing thermal stability and sorption characteristics in the buffer material. All solutions were 13-ppm dye in water, and the tests lasted 7 days.

Test	Dye remaining in solution (%)		
	Eosin	Fluorescein	Amaranth
No RBM, 90°C	91	72	88
10% RBM-dye solution, 90°C	76	100	51
10% RBM-dye solution, 20°C	67	100	49

Figure 21. Column flow system for testing optrode detection of dye tracers.

Preliminary tests indicated that steady-state flow conditions could be achieved within a few days after applying the gradient. We hypothesized that this was indicative of full saturation in the specimen; therefore, Darcy's law could be applied for interpreting the flow regime. We calculated a hydraulic conductivity of 2.36×10^{-11} m/s for the first test, as shown in Fig. 22. This was somewhat higher than the range of 10^{-12} to 10^{-13} m/s previously reported for the RBM by Dixon and Gray (1985).

After verifying the flow conditions, the system was disconnected from the pressure source, and two optrodes were emplaced. This was accomplished by drilling holes radially through the mold and into the specimen. Copper tubes containing the optrode fibers were then inserted and sealed at the mold wall by means of compression fittings. The system was repressurized, and a subsequent steady-state flow test yielded a conductivity of 2.02×10^{-11} m/s. The apparent increase in permeability in the second test indicated that some change in saturation may have occurred during optrode installation or that steady-state conditions had not been achieved. In either case, we elected to begin the tracer injection, assuming that the breakthrough time could be estimated by dividing the Darcy

velocity by the porosity of the medium. Contrary to our calculations, we found that the fluorescent dye appeared in the discharge about one week before the expected arrival time. At this point, neither of the optrodes showed any indication that dye had reached them. The experiment was stopped in order to determine if the system were at fault or if the optrodes had failed to detect the tracer. Subsequent disassembly of the system and dissection of the RBM specimen showed that the tracer had travelled primarily along the walls of the mold. Along the axis of the specimen, the dye had penetrated <1 cm, which was far short of the first optrode.

Insofar as verifying optrode performance in RBM, the experiment was inconclusive. It was, however, an interesting demonstration of the behavior of a clay-bentonite mixture during the saturation phase. Apparently, the swelling pressure generated by increased saturation was not sufficient to prevent preferential flow along the interface. The driving mechanism for this flow may have been the high capillary suction, rather than the positive pressure gradient applied externally; this, of course, casts some doubt on the ability of RBM to act as a sealing agent in repository applications, at least in the resaturation phase.

Figure 22. Flow test in compacted RBM.

Buffer/Container and Borehole/Shaft Sealing Experiment Planning Committee Activities

Tasks in support of the Buffer/Container and Borehole/Shaft Sealing Experiments include (1) providing representation on the joint DOE/AECL Planning Committees and (2) evaluating and developing instrumentation for the experiments.

At meetings held on March 1 and 2, 1988, R. K. Thorpe presented the results of the two activities assigned to LLNL. The first activity consisted of developing a laboratory experiment plan to determine differences in behavior between precompacted and compacted-in-place RBM. The second activity involved describing possible stress distributions around proposed tunnels in which the experiments will be performed at the Canadian URL.

R. K. Thorpe and B. Kjartanson (AECL coordinator for the Buffer/Container Experiment) attended a geotechnical instrumentation course together from March 28 through April 1, 1988. At this course, they had a greater opportunity to brainstorm than is usually possible at formal DOE/AECL meetings. Primarily, they discussed the role of scoping calculations. They concluded that greater emphasis should be placed on rock mechanics and hydrologic calculations. Because the rock mass at the URL is relatively unfractured, these experiments afford an opportunity to validate the continuum aspects of existing codes. They also discussed rock instrumentation, and the results of their discussion further emphasized the need for design calculations. More important, however, is the need for buffer response calculations. Predicting the fully coupled response for the experiment is not currently possible, so they proposed various types of approximate, decoupled calculations. From these talks, it was evident to them that further design decisions depend on such results, and B. Kjartanson pledged that AECL would pursue the scoping calculations with vigor.

Thorpe delivered a progress report on LLNL activities and, at the request of AECL, presented an overview of instrumentation requirements for the Buffer/Container Experiment. This information, plus results of scoping calculations by Ontario Hydro and the Battelle Memorial Institute, Office of Waste Technology Development, led to the consensus that the Buffer/Container Experiment, as currently envisioned, would be very difficult to instrument and analyze; therefore, the following revisions to the test objectives and procedures were recommended: (1) limit the maximum buffer temperature to 100°C, and (2) separate the drying and resaturation phases so that the two processes can be distinguished independently. Interim reports for the Buffer/Container Experiment and Borehole/Shaft Sealing Experiments were also discussed at the meetings, and tentative writing assignments for the participants were assigned. (The necessity for publishing these reports, however, is uncertain in light of the cancellation of the DOE/AECL Subsidiary Agreement.)

Prior to the meetings, S. Alcorn of IT Corp., met with R. K. Thorpe at LLNL to discuss tracer detection methods applicable to the Buffer Container Experiment. Since Alcorn was a new participant in the project, we briefed him on our optrode development work and the status of the experiment planning effort.

In preparation for planning meetings held on June 16-17, 1988, Thorpe discussed experimental designs and measurement techniques with various participants from Office of Waste Technology Development (OWTD), IT Corp., and AECL. Specific topics included rock mechanics scoping calculations (OWTD) and tracer test concepts (IT Corp.). Alcorn visited LLNL in early June 1988 to review progress on the optrode development and discuss tracer testing in more detail.

Reactive Transport Task

Richard B. Knapp

The primary goal of this task is to develop a reactive transport simulator for modeling fracture-confined transport. During FY 1988, we reviewed the capabilities, performance, and deficiencies of existing, public domain reactive transport codes. A total of 21 codes were evaluated in the following nine categories: media type, transport mechanisms, reaction types, reaction thermodynamics, spatial dimensions, numerical solution methods, process coupling, treatment of kinematic shock fronts, and status of verification and validation. All but one of the existing codes are written for porous or equivalent porous media; only one software package incorporates fracture-confined advection with diffusive transport into the fracture-bounding matrix. This latter software package has simplifications that limit its application to practical problems.

Most codes incorporate the three major transport mechanisms (advection, dispersion, and diffusion). In addition to these processes, there is also a chemical dispersion term that should be included in the code, but the magnitude of this term is unknown, and it is not incorporated into any of the current simulators.

The greatest difference among the codes and the single most important factor affecting their applicability to practical problems is their treatment of chemical reactions. There are five classes of chemical reactions: irreversible dissolution, precipitation, ion exchange, adsorption, and radioactive decay. Any practical simulator must include irreversible dissolution and precipitation since fluids circulating around a cooling radioactive waste container will, in general, be out of equilibrium with the rock. Many current simulators do not incorporate these types of reactions. Others assume a condition of local equilibrium (LEQ) and apply the concept of sorption coefficients. LEQ is a good approximation if an initial disequilibrium condition relaxes to an equilibrium state over a distance and time period that is less than the spatial and temporal scales of interest. These scales of

interest depend on the particular problem under investigation, and they include the hundreds of meters scale for field investigations, the sub-meter scale for laboratory investigations, and the sub-crystal scale for certain other investigations. The computational step size and grid block size define the scales of interest for the computer experimentalist.

We calculated the time t_{eq} and distance l_{eq} required for an impulse of fluid (initially undersaturated with respect to quartz) to relax to equilibrium for a wide range of reactions rates and transport conditions. Typically,

$t_{eq} = 1$ yr and $l_{eq} = 10$ m for sedimentary basins,

$t_{eq} = 3$ days and $l_{eq} = 10$ mm for host rocks in magma-hydrothermal systems,

$t_{eq} = 10$ hr and $l_{eq} = 250$ μ m for regional metamorphic environments,

$t_{eq} = 1$ yr and $l_{eq} = 100$ m for injection wells,

$t_{eq} = 300$ yr and $l_{eq} = 35$ km for laboratory core flow experiments.

These values depend on the specifics of each environment and can vary over orders of magnitude.

LEQ is a good approximation if t_{eq} and l_{eq} are less than the scales of interest. This analysis, though quantitative, is only approximate because it does not include the effects of competing heterogeneous reactions. These effects result in an over-estimation of t_{eq} and l_{eq} for low-temperature silicate environments and an under-estimation of t_{eq} and l_{eq} for high-temperature environments. A manuscript ("Spatial and Temporal Scales of Local Equilibrium in Dynamic Fluid-Rock Systems," R. B. Knapp) describing this work has been accepted by *Geochimica et Cosmochimica Acta* for publication in FY 1989.

Of the remaining categories, the most important are the numerical solution techniques. The most rigorous codes are often impractical because of excessive computational times. This is especially true in radioactive disposal situations where there can be 40 chemical components and a legion of solid phases. Often the numerical

experimenter is forced to arbitrarily simplify the chemical system or to use the LEQ approach whether or not it is valid. We recommend that improvements to current techniques be applied concurrently with efforts to develop a more novel approach that would permit more efficient computing.

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