**Verification and
Benchmarking of
MAGNUM-2D: A Finite
Element Computer Code for
Flow and Heat Transfer in
Fractured Porous Media**

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March 1985

**Prepared for
Rockwell Hanford Company
Basalt Waste Isolation Project**

**Pacific Northwest Laboratory
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SUMMARY

The objective of this work is to assess prediction capabilities and features of the MAGNUM-2D computer code in relation to its intended use in the Basalt Waste Isolation Project (BWIP). This objective is accomplished through a code verification and benchmarking task. Results are documented which support correctness of prediction capabilities in areas of intended model application.

A test problem set consisting of 10 problems is used. The problems are designed to test three basic computational capabilities or categories of the code. Broken down by physical process, these are heat transfer, fluid flow in porous media, and fluid flow in porous media with discrete fractures. Different types of problems were modeled. Several are ones for which analytical solutions are derivable. For these problems, analytical solutions are used as the basis for comparison of MAGNUM-2D results. In other test problems, geometry and flow parameters are prescribed consistent with intended applications of MAGNUM-2D in BWIP. Results of a second computer code are used as a comparison basis for these problems due to complexities which preclude analytical solutions.

Each of the test problems are presented in Section 4.0 of this report. Following is a summary of operational modes and basic features of the MAGNUM-2D code which have been tested:

- Heat Conduction in Cylindrical Geometry. Steady-state and transient heat conduction were tested in one- and two-dimensional problems. Tests included constant heat generation in a region with one uniform material (Section 4.1) and a region with four materials, each having different thermal properties (Section 4.2). For both of these cases, MAGNUM-2D results are in excellent agreement with analytical solution results.
- Heat Conduction in Cartesian Geometry. Transient and steady-state simulation capabilities were tested. In a region with one uniform material with constant heat generation, both rectangular and triangular finite elements were used. Both element configuration cases were found to

yield excellent agreement with analytical solution results (Section 4.3). A transient simulation of a waste package scale heat conduction problem modeled four materials; waste, backfill, blast affected rock, and host basalt (Section 4.4). This geometry is typical of intended code usage within BWIP. Agreement of results with a second computer code was good.

- Fluid Flows in a Porous Media. Prediction of steady-state and transient pressure field and resulting Darcian fluid flow was tested in a regional groundwater model (Section 4.5) and an areal domain model (Section 4.6). Results were in excellent agreement with corresponding analytical solutions.
- Perturbed Fluid Flow Near Waste Package Emplacement. Steady-state pressure field and resulting fluid flow in a waste package emplacement domain were predicted. Boundary conditions were perturbed to model heating effects at the waste package boundary. MAGNUM-2D results were in very good agreement with the FTRANS code which was used to generate results for comparison (Section 4.7).
- Flow in Fractures Embedded in Porous and Impermeable Media. Flow in a single discrete fracture embedded in a porous material was modeled. Steady-state pressure field results for this problem were in good agreement with the comparison basis (Section 4.8). Darcy velocities predicted in the discrete fracture are also in good agreement. For flow in a network of connected fractures in which three distinct fracture regions were modeled, pressure field results were found to be in very good agreement with results of the FTRANS code (Section 4.9) after a change to the FTRANS code was made (Appendix B). Corresponding Darcy flow velocities were also in excellent agreement.
- Flow Near A Waste Package Emplacement Intersected by Discrete Fractures. Steady-state pressure fields were well predicted and in good agreement with the comparison basis (Section 4.10). A detailed comparison of predicted Darcy flow velocities in the fractures showed excellent

agreement also. Very localized minor differences in flow velocities in fractures are attributable to differing physical models in the MAGNUM-2D and FTRANS codes.

One aspect of MAGNUM-2D capabilities was not tested in this work. This is coupled heat and fluid flow. This capability remains to be tested, both for cases of porous continua and fractured porous media.

This verification and benchmarking effort is concluded to have been successful in demonstrating that MAGNUM-2D is capable of accurate predictions of heat transfer, flow in porous continua, and flow in fractured media. This conclusion is based on the agreement of results from MAGNUM-2D predictions and the comparison basis used in each of the 10 test problems.

Additional testing needs to be conducted to specifically address fully coupled (buoyancy driven) flow and heat transfer for both transient and steady cases. MAGNUM-2D has this capability, but it was not tested in the present work. A suitable tool for use as a comparison basis was unavailable at the outset of this work. Test problems FF-4 (Section 4.7) and FF-8 (Section 4.10) would be candidate waste package emplacement test problems if heat transfer were included as a coupled process.

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1.0 INTRODUCTION

Analysis capabilities have been developed and are being used by the Rockwell Hanford Company in the Basalt Waste Isolation Project (BWIP). Computer codes which predict groundwater flow, heat transfer, and radionuclide transport are being used in this analysis. The codes, their applications, and their capabilities represent an interfaced collection of tools for waste package (very near-field), repository scale (near-field), and regional (far-field) analysis.

Although computer codes are capable of performing extensive computation, it is necessary to document their computational features, capabilities, and accuracy. This process comprises verification and benchmarking. Recently, the Nuclear Regulatory Commission issued a report which offers guidelines for qualifying computer codes that are to be used for safety and licensing analysis for repositories (Silling, 1983). Rockwell/BWIP is currently developing guidelines for verifying and benchmarking codes that are to be used in their analysis of basalt formations under consideration for high level nuclear waste storage.

This report is concerned with results of a cooperative effort directed toward verification and benchmarking Version 3.1 of the MAGNUM-2D computer code. The work was cooperative in the sense that direct interaction occurred between Rockwell/BWIP and Boeing Computer Services, Richland (BCSR), personnel closely connected with the MAGNUM-2D code and Pacific Northwest Laboratory (PNL) personnel performing the results comparison and assessment conclusions. PNL had the responsibility of developing problem statements upon which MAGNUM-2D simulations were to be based. Rockwell/BWIP and BCSR personnel provided input to and review of the problems statements during their development. This was done to ensure that the problems were representative of intended code applications and that they were designed to sufficiently test pertinent features and capabilities of the code. The interaction and problem statement review also ensured that test problems were formulated to be compatible with the codes.

Once the problem statements were completed, BCSR personnel were responsible for setting up and performing simulation analysis with MAGNUM-2D. Computer listings of output results were then provided to PNL. PNL personnel were responsible for generating analytical and benchmarking code results which were to be used in the verification and benchmarking problems and performing the results comparisons and assessment.

Ten test problems were included in this work. For verification, problems were selected which exercised the code's basic capabilities of fluid flow, heat transfer, and flow in porous media with discrete fractures. The problems selected were ones which are well recognized in the technical literature in the field of repository analysis. These are problems for which exact analytical solutions are available. Although they are not complex in design, parameters were chosen so to be representative of intended MAGNUM-2D application. Four benchmarking problems were selected which are more representative of intended code usage in BWIP analysis. The TEMPEST computer code (Trent, et al. 1983) was chosen as a benchmarking code for problems that involved heat conduction only. The FTRANS code (INTERA, 1983), was chosen for problems in which only fluid flow occurs. Both of these codes are documented, the former for its thermal analysis capabilities, and the latter for its groundwater flow capabilities in porous and fractured media.

The codes used in this work are described in Section 2.0 of this report. Section 3.0 presents the technical approach, test plan, and problem set used. It also includes a discussion of the traceability and procedures used in obtaining the simulation results of this work. A record book was kept as part of the Q/A requirements of this work. It contains, among other things, a record of computer files and computer output listings containing final results. The output listings are to be maintained for future reference of the results used in this work. Microfiche and magnetic computer tape storage are also used for more long term backup retention.

Section 4.0 includes the problem statements upon which the simulations were based and comparisons of results generated. Discussions of results are also presented. Appendix A describes the various steps that were taken in bringing the FTRANS code up on the Los Alamos National Laboratory computer system. Special emphasis is given to the Q/A procedures that ensure traceability. Appendix B details one coding change made to the FTRANS code. This change was necessary so that the code had the capability to treat variation in aperture within a fracture represented by connected line elements.

2.0 COMPUTER CODE DESCRIPTIONS

Three computer codes were utilized in this work; MAGNUM-2D, FTRANS, and TEMPEST. The former two are finite element, porous media codes and the latter is a finite-difference thermal-hydraulic code. MAGNUM-2D is one of suite of codes being developed, tested, and utilized within the Basalt Waste Isolation Project (BWIP). Simulations contained in this report with this code were set up and run by Boeing Computer Service, Richland, (BCSR) personnel familiar with the code and its use. FTRANS is available from the Office of Nuclear Waste Isolation (ONWI). Results obtained with this code and reported herein were computed as part of this work. The TEMPEST code is available from the National Energy Software Center at Argonne. It was also run as part of this work.

2.1 MAGNUM-2D

MAGNUM-2D is a computer code (numerical model) for analysis of coupled groundwater flow and coupled heat transfer in fractured or unfractured porous media. It is designed to simulate steady-state and transient processes. It is applicable to two-dimensional problems in Cartesian or axially symmetric cylindrical coordinates. The basis for the mathematical model is conservation of mass, momentum, and energy. The users manual (England, et al., 1984) presents a thorough description of the code, its capabilities and use. The governing equations in the MAGNUM-2D numerical model are included here for completeness.

The equation governing nonisothermal flow balance in a porous continuum as written in indicial notation for a Cartesian coordinate system is

$$S_s \frac{\partial h}{\partial t} = K_{ij} \frac{\partial}{\partial x_j} \left(\frac{\partial h}{\partial x_j} + \delta_{ij} \delta_{12} \right) + \gamma \frac{\partial T}{\partial t} \quad (2.1.1)$$

where

S_s = specific storage of the porous rock matrix

h = hydraulic head

t = the time coordinate
 k_{ij} = hydraulic conductivities of the rock matrix
 x_i = space coordinates (x,y)
 δ_b = density disparity
 δ_{i2} = the Kronecker delta
 γ = thermal coupling coefficient
 T = temperature of the water/rock system.

Note that K_{12} and K_{21} are assumed to be negligible and, hence, only components of flow in the principal directions are considered. Furthermore, the density disparity and thermal coupling coefficient are given by

$$\delta_b = \frac{p - p_0}{\rho^*} \quad (2.1.2)$$

and

$$\gamma = \phi\beta, \text{ respectively} \quad (2.1.3)$$

where

ρ = fluid density as a function of location and time
 ρ_0 = initial fluid density
 ρ^* = reference fluid density
 ϕ = effective porosity
 β = bulk modulus of fluid.

The equation governing nonisothermal flow balance in a fracture as written for a local one-dimensional coordinate system is

$$S_f \frac{\partial h}{\partial t} = K_f \frac{\partial}{\partial L} \left(\frac{\partial h}{\partial L} + \delta'_b \right) + \gamma \frac{\partial T}{\partial t} \quad (2.1.4)$$

where

S_f = specific storage in the fracture

K_f = hydraulic conductivity of (filled or unfilled) fracture

L = local space coordinate

δ_b^i = component of the density disparity along L .

Under the assumption that the fluid and rock mass are in thermal equilibrium, the governing thermal energy balance equation written for Cartesian coordinates using indicial notation is

$$S_t \frac{\partial T}{\partial t} + \rho c_f q_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i} (D_{ti} \frac{\partial T}{\partial x_i}) + Q \quad (2.1.5)$$

where

S_t = heat capacity of the fluid/rock system

c_f = specific heat of the fluid

q_i = component of the Darcy velocity vector

D_{ti} = effective thermal diffusivity

Q = volumetric rate of heat generation.

Moreover,

$$S_t = \phi \rho c_f + (1-\phi) \rho_s c_s \quad (2.1.6)$$

where

ρ_s = bulk density of the rock

c_s = specific heat of the rock,

and

$$\frac{D_{tx}}{\rho c_f} = \frac{\phi D_f}{\rho c_f} + \frac{(1-\phi) D_{sx}}{\rho c_f} + (\alpha_l U^2 + \alpha_r V^2) / \bar{q} \quad (2.1.7)$$

and

$$\frac{D_{ty}}{\rho C_f} = \frac{\phi D_f}{\rho C_f} + \frac{(1-\phi) D_s}{\rho C_f} + (\alpha_\tau U^2 + \alpha_l V^2) / \bar{q} \quad (2.1.8)$$

where

- D_f = thermal conductivity of the fluid
- D_s = thermal conductivity of the rock
- α_l = longitudinal dispersivity
- α_τ = transverse dispersivity
- U = horizontal component of Darcy velocity
- V = vertical component of Darcy velocity
- $\bar{q} = (U^2 + V^2)^{1/2}$, the groundwater speed.

The MAGNUM computer code is programmed to solve these governing equations subject to initial and boundary conditions using a Galerkin finite-element method. A substantial derivation of the method is given by Baca et al., 1983.

2.2 FTRANS

FTRANS (Fractured Flow and Transport of RadionuclideS) was developed by Peter Huyakorn of GeoTrans, Inc. for INTERA Environmental Consultants, Inc. A report describing the code and its use is available (INTERA, 1983). It is a two-dimensional finite-element code for simulation of groundwater flow and transport of radionuclides in a porous medium. It contains capabilities to model fractures in the porous medium using one of several fracture models. The code version identified as QA CIN: 400--02C-02 was used in this work.

The code can simulate flow of slightly compressible fluid in a porous medium, spatial and temporal distributions of trace concentrations of radioisotopes in a porous medium, and total mass flux at the outlet. Only the flow mode was used in this work. In this model fracture idealizations

FIGURE 2.1.1. Comparison of MAGNUM-2D and FTRANS Finite-Element Configuration

available include rectangular prismatic block joint or spherical block joint. Fracture flow may be with either high- or low-permeable porous media.

Assumptions made in the code for flow mode include:

- Flow in the rock matrix and fractures obey Darcy's law.
- For fractured systems, the aperture of the fracture is assumed to be very small compared to other dimensions in the fracture plane.
- Boundary conditions are invariant with time.

Furthermore, the following limitations apply:

- The model does not simulate flow in an unconfined (water table) formation, nor can it simulate non-Darcian flow which may exist in fractures.

- The model does not simulate fully three-dimensional flow nor can it simulate quasi-three-dimensional flow in leaky aquifer-aquitard systems.

The governing equations which are solved and the numerical procedures which are used are detailed in the report describing the code (INTERA, 1983) and are not repeated here. The procedure used to put the FTRANS code up for use in this work is described in Appendix A. Included is a discussion of testing performed to assure the code was computing in accordance with test cases supplied with the code by ONWI.

2.3 TEMPEST

The TEMPEST computer code (Trent, et al, 1983) is a three-dimensional time-dependent computer program for hydrothermal analysis. It was chosen as a benchmarking code for heat conduction only problems. TEMPEST is well documented and validation results have been reported (Eyler, et al., 1983). Although very general in its hydrodynamic capabilities, the heat-conduction mode of TEMPEST was the only feature used in this work. No hydrodynamic features were included.

TEMPEST is a user oriented code which solves the energy equation implicitly using a three-step Douglas and Gunn algorithm described by Richmeyer and Morton (1967). The method is very efficient. The code was chosen for conduction benchmarking because of its capabilities, features, and referenceable documentation on validation studies. Because it does not contain a porosity formulation of the energy equation, it is only strictly applicable to porous media applications where equivalent thermal properties of the media are determinable or assumable. This is the case for its use in benchmarking simulation in this work. Details of the code's numerical procedures and algorithms are reported Trent, et al. (1983) and are not included herein.

TEMPEST, Version L, Mod 3, was used in this work. It is available from the National Energy Software Center at Argonne National Laboratory. This version of the code was resident on the LANL computer system for use in this work.

3.0 TEST PLAN APPROACH AND TEST PROBLEM SET

MAGNUM-2D is used to perform simulation of ten test problems in a problem set designed to evaluate particular capabilities of the code. The problems include features of heat transfer, fluid flow in porous media, and fluid flow in fracture porous media. Five problems are relatively simple ones, but which are representative of code applications and for which analytical solutions are derivable. Five problems are benchmarking problems (too complicated for an analytical solution) in which results of MAGNUM-2D are to be compared to other computer code results. Of these, three problems are concerned with a representative waste package scale solution domain and use parameters representative of intended code usage within BWIP. Although representative, these problems are not intended to be definitive characterization analyses.

This section describes the test plan approach upon which the present verification and benchmarking simulation results are based. The ten test problems chosen for the work are outlined along with the objectives and code features tested in each problem.

3.1 OBJECTIVE

The objective of this work is to perform analyses of representative applications and prediction feature capabilities of the MAGNUM-2D code. This was to be done by developing problem statements for representative problems which the code is capable of simulating, performing the simulations, and then comparing results to analytical solutions (verification) or other code results (benchmarking). Discussion of the acceptability of MAGNUM-2D prediction results are to be based on acceptance criteria. These criteria are necessarily problem dependent. Deviations, solution abnormalities, and difficulties encountered in performing simulations are to be documented along with the results.

3.2 TEST PLAN BASIS

The test plan basis under which this work was performed was developed in discussions between Rockwell/BWIP, BCSR and PNL personnel. Included directly were R. Baca and D. Sandoz of Rockwell/BWIP, D. Langford and N. Kline of BCSR, and L. Eyler and M. Budden of PNL. Others at PNL who have performed other hydrodynamic code validation analyses were also consulted during the work.

The plan under which this work was conducted included the following items:

- The general scope of the work was defined to include relatively simple, but representative, verification problems as well as more complex applications-related benchmarking problems.
- A specific problem set was developed and problem statements defined.
- The FTRANS computer code was chosen as a benchmarking code for waste package scale problems in which only flow occurs.
- The TEMPEST computer code was chosen as a benchmarking code for problems in which only heat transfer occurs.
- BCSR personnel performed the MAGNUM-2D simulations for each problem and provide PNL with computer output for results comparison.
- PNL personnel generated the analytical solution results and performed benchmarking code simulations.
- Acceptability criteria were to be defined and comparisons of results used to evaluate acceptability.

All of these steps involved close interaction between Rockwell/BWIP, BCSR, and PNL personnel involved in the work. This interaction was to ensure that the intent of the test problems was being followed, and that any deviations between originally developed problem statements and the solution simulations could be eliminated in advance or documented as a variance.

3.3 PROBLEM SET

Ten test problems were identified which were to test major capabilities and features of the MAGNUM-2D code. A list of references for ten suggested problems were provided by Rockwell/BWIP. Because of their familiarity with the code, they were best able to suggest problems within the code's capabilities which would test both basic and application scale features. A short description of each problem and its test design features is presented here. Detailed problem statements are included in Section 4.0 along with simulation results.

Each problem is given a designation broken down by the major capabilities of the code. They are: HT for Heat Transfer and FF for Fluid Flow. Verification problems were selected that are well documented in technical literature. Benchmarking problems were chosen to exercise MAGNUM-2D within the scope of normal BWIP use.

HT-1: Heat Transfer in a Cylindrical Geometry with Heat Generation (Section 4.1). This problem is a single region heat-conduction-only problem designed to test computation of steady-state temperature in cylindrical coordinates with uniform heat generation. An analytical solution is derivable for results comparison.

HT-1.1: Transient Multiregion Conduction Heat Transfer in One-Dimensional Cylindrical Geometry (Section 4.2). This problem is an extension of problem HT-1. It includes four concentric material regions with heat generation in the central region. The objective is to test transient heat up and computation of final steady-state temperatures in unfractured porous media. An analytical solution is available for comparison of steady-state temperature distribution, and TEMPEST code results are used for transient temperature comparison basis.

HT-4: Steady-State Conduction Heat Transfer in a Rectangular Geometry with Heat Generation (Section 4.3). This test is designed to test computational element configuration. Both rectangular and nonrectangular elements are used in predicting steady-state temperatures. An analytical solution is available for comparison.

HT-6: Heat Transfer Around a Waste Canister Emplacement (Section 4.4). This problem is designed to test computation of temperatures in the region around a waste canister emplacement. Waste canister, backfill, blast affected rock and the host basalt rock are included as heat conducting materials. The TEMPEST code is used as a benchmarking tool for this problem.

FF-1: Steady Flow in a Regional Groundwater System (Section 4.5). This is a fluid-flow-only problem designed to test steady-state hydraulic head distribution subject to a linear surface head gradient in a regional groundwater system. An analytical solution is available for this problem for results comparison.

FF-2: Transient Flow in a Rectangular Areal Domain (Section 4.6). This fluid-flow-only problem is designed to test prediction of transient hydraulic head and flow distribution. An analytical solution is available for results comparison.

FF-4: Steady Flow in a Porous Media (Section 4.7). This problem is one in which steady flow in the region around a waste canister emplacement is to be computed. Backfill, blast affected and host basalt rock are modeled as unfractured porous media with the waste canister boundary being unbreached. Driving force is assumed to be specified hydraulic heads at selected boundary locations. The FTRANS code is used as a benchmarking tool.

FF-6: Flow in Porous Material Containing a Single, Embedded Fracture (Section 4.8). This problem is designed to test computation of fluid flow in a porous medium in which a single, embedded fracture occurs. Results of the FTRANS code are used as a comparison basis.

FF-7: Flow in a Network of Fractures (Section 4.9). This problem is designed to test computation of fluid flow in a network of intersecting, discrete fractures which are embedded in an impermeable medium. Three fracture regions are included. Fractures in each region have differing characteristics. The FTRANS code is used as a benchmarking tool.

FF-8: Steady Flow in Porous Media with Discrete Fractures (Section 4.10).

This is an extension of problem FF-4 and includes discrete line fractures embedded in the porous materials. The fractures extend throughout the region and intersect the three modeled porous materials. FTRANS results are used as a comparison basis.

The above ten problems are designed to test the salient features of MAGNUM-2D in a progression of basic features, complexity, and application. The three waste package scale simulations are problems in which representative hydrogeologic and flow properties consistent with proposed applications of MAGNUM-2D are included.

3.4 PROBLEM STATEMENT ORGANIZATION

A detailed problem statement was developed for each problem in the test set. Each statement included a problem objective, models used, problem statement, analytical solution (where appropriate), assumptions, input specifications, and output specifications. These complete statements were then used as a basis for MAGNUM-2D simulations, generation of analytical results, and benchmarking with an additional computer code.

3.5 ACCEPTABILITY

The intention of this work is to provide a documented basis upon which conclusions can be drawn as to acceptability of MAGNUM-2D for simulation analysis of proposed waste canister emplacement in basalt rock formations. This is to be done through verification and benchmarking with a set of representative problems which are designed to test basic features of the code, particular capabilities, and simulation accuracy. In this report, verification is used to refer to code versus analytical solution comparison, while benchmarking will be reserved for code-to-code comparisons. In most real-world problems, analytical solutions are unavailable, making this type of verification impossible; hence, the importance of benchmarking.

The problem set proposed in this work consists of ten problems. For the five verification problems, parameters in the governing equations which

MAGNUM-2D approximates can be chosen so as to reduce the (exact) equations to a form which can be solved analytically. The resulting analytical solution is taken as the standard by which a particular feature or capability of the code can be "verified". The criterion for acceptability is then the allowable margin of difference between the code prediction and the standard.

Defining one limiting quantity for an acceptance criterion, such as percentage difference, is not possible in all cases. The approach taken in this work is to evaluate each problem individually. For each of the six verification problems, conclusion of acceptability is based on aspects of that problem and the judgement of senior numericists at PNL. Several guidelines are used. A principal result would be unacceptable if it is totally out of range by orders of magnitude, or in certain cases by a factor of two. A result would be unacceptable if it were not physically possible such as an incorrect sign. A result can be concluded to be acceptable if it agrees to within a realistic error band of the standard. For comparison to an analytical solution, this error band can reasonably be in the realm of 1 to 5 percent for principal variables depending on the complexity of the problem. With sufficiently supported explanations, even a larger error can still be termed acceptable in certain instances.

For the four benchmarking problems, a specific acceptability criterion is more difficult to prescribe. Each problem must be treated and assessed individually. The degree of approximation which is present in each problem must be evaluated. The departure of the computer results from reasonable physical behavior is one criterion which is used. Correctly predicted trends and gross features are others. These factors are used in evaluating and concluding acceptability of MAGNUM-2D's prediction in the benchmarking problems.

3.6 TRACEABILITY

One objective of this work was to provide traceability of predicted results which were computed with MAGNUM-2D and results which were obtained for comparison. BCSR personnel ran the MAGNUM-2D simulations for this work. PNL

was provided with computer output. This output, as identified by case number, is to be maintained as integral records of the work. A record log of output listings is to be maintained in a reference log book.

Several steps are taken in generating the analytical and benchmarking results. The final product is computer listings of pertinent source code and output files. These contain data used in comparisons and are to be maintained as integral records of the work.

Computation was done on computers at the Los Alamos National Laboratory (LANL) Computing Center Facility (CCF). CDC-7600 computers were used for the verification problems. Benchmarking simulations with FTRANS were computed on the CRAY-1 machine. Appendix A details the source of and the steps taken to put the FTRANS code up on the CRAY and ensure it was computing correctly. The version of the FTRANS code used was identified as QA CIN: 400--02C-02. The TEMPEST code, as discussed in Section 2.3, was resident on the CDC-7600 computer at LANL. TEMPEST Version L, Mod 3, which is available from the National Energy Software Center at Argonne National Laboratory, was used.

The Common File System (CFS) was used to store all programs, job streams, outputs, and run logs. On the CFS, a root directory was set up under the ident BWIP. Subdirectories for each of the ten problems are identified by problem (e.g./BWIP/HT2). All files pertinent to that problem are stored collectively under that problem's subdirectory. Also, all plot files are further kept under a next level subdirectory called PLOTS which is added to each problem's subdirectory in a logical root-tree setup. A cross-referenced list of printed output (results), input streams, and analytical coding listings for each problem is maintained in a laboratory record book and identifies banner page titles of final printed results.

Input files and output listings generated are maintained on the CFS even after being printed. Plot files containing all data plotted are also maintained. Each plot generated was labeled with a file name and storage location (root-tree sequence). The root-tree system on the CFS provides a very organized means of file storage and access. At the conclusion of this work, source codes, problem inputs and problem outputs were written to computer magnetic tape and microfiche for records retention.

4.0 TEST PROBLEM RESULTS

The test problem set used in this work is presented in summary form in Section 3.0. Results of verification and benchmarking problems are presented in this section. For verification, comparisons of results of the MAGNUM-2D code are made with analytical solutions. Benchmarking results are comparisons between results of comparable codes. For each test problem, a problem statement is given which describes the solution domain and required input parameters. A discussion of solution procedure or computer model setup and results comparison is included with the presentation of results for each problem.

4.1 STEADY-STATE CONDUCTION HEAT TRANSFER WITH HEAT GENERATION IN CYLINDRICAL COORDINATES

4.1.1 Problem Designation

This problem is designated: Heat Transfer Problem HT-1.

4.1.2 Objective

The objective of this test is to determine the correctness of predicting steady-state temperature distributions with MAGNUM-2D. The geometry is a right circular cylinder region with a vertical axis. Results are to be compared to an analytical solution. Aspects to be tested include cylindrical coordinate system, heat generation, and node spacing effects.

4.1.3 Problem Statement

A three-dimensional, axially symmetric cylindrical region contains heat generating solid material. The volumetric heat generation rate is constant. The problem is to determine the steady-state temperature distribution in the region. Exterior boundaries are at constant temperature and the material thermal conductivity is constant. The radial coordinate direction is horizontal and the axial coordinate direction is vertical. This problem is the same as used for MAGNUM-2D verification (Eyler and Budden, 1984).

4.1.4 Models Used

MAGNUM-2D is used to numerically model the heat generating region. Only the thermal energy equation in MAGNUM-2D is used. The analytical solution is obtained using computer mathematics library routines for Bessel functions. The TEMPEST code is used as a secondary check on the results.

4.1.5 Analytical Solution

The analytical solution to this problem is given by Ozisik (1980). Figure 4.1.1 presents a schematic of the problem and solution domain. In cylindrical coordinates the mathematical formulation of the steady-state problem is given as

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} + \frac{\dot{Q}}{D_t} = 0 \quad (4.1.1)$$

over the region

$$0 \leq r < R \quad \text{and} \quad 0 < z < Z.$$

The thermal conductivity is D_t and $\dot{Q}$ is the volumetric heat generation rate. Boundary conditions to the region are

$$T = T_b \quad \text{at} \quad r = R, \quad z = 0 \quad \text{and} \quad z = Z \quad (4.1.2a)$$

and

$$\frac{\partial T}{\partial r} = 0 \quad \text{at} \quad r = 0. \quad (4.1.2b)$$

For convenience, it can be assumed the $T_b = 0$ with no loss in generality.

A solution for the temperature in the region can be determined as the sum of a complementary, $\theta(r,z)$, and a particular $\theta_p(r,z)$ solution. Thus,

$$T(r,z) = \theta(r,z) + \theta_p(r,z).$$

A particular solution to Equation (4.1.1) is

$$\theta_p(r,z) = -\frac{\dot{Q}}{2D_t} \frac{z^2}{2} + Az \quad (4.1.3)$$

where the constant A is introduced to allow simplification of boundary conditions by proper choice of the value of this constant. Assuming

$$A = \frac{\dot{Q}}{2D_t} \frac{Z}{2}, \quad (4.1.4)$$

the solution for $T(r,z)$ becomes

$$T(r,z) = \theta(r,z) + \frac{\dot{Q}}{2D_t} z(Z - z). \quad (4.1.5)$$

Substituting Equation (4.1.5) into Equation (4.1.1) and the boundary conditions (Equation (4.1.2)) results in

$$\frac{\partial^2 \theta}{\partial r^2} + \frac{1}{r} \frac{\partial \theta}{\partial r} + \frac{\partial^2 \theta}{\partial z^2} = 0 \quad (4.1.6)$$

in the region

$$0 \leq r < R \text{ and } 0 < z < Z.$$

The boundary conditions become

$$\theta = \frac{\theta_0}{2D_t} z (z - Z) \text{ at } r = R, \quad (4.1.7a)$$

$$\theta = 0 \quad \text{at } z = 0. \quad (4.1.7b)$$

and

$$\theta = 0 \quad \text{at } z = Z. \quad (4.1.7c)$$

The solution to Equation (4.1.6) when substituted into Equation (4.1.5) becomes

$$T(r, z) = \frac{\theta_0}{2D_t} z (Z - z) - \frac{4 \theta_0 Z^2}{\pi^3 D_t} \sum_{m=0}^{\infty} \frac{1}{(2m+1)^3} \frac{I_0(\xi_m r)}{I_0(\xi_m R)} \sin(\xi_m z) \quad (4.1.8)$$

where

$$\xi_m = \frac{(2m+1)\pi}{Z} \quad (4.1.9)$$

and I_0 is the modified Bessel function of zero order.

4.1.6 Assumptions

The volumetric heat generation rate and material thermal conductivity are assumed to be constant.

4.1.7 Input Specifications

For this problem, the following parameters are to be used:

Region radius:	$R = 200 \text{ m}$
Region height:	$Z = 200 \text{ m}$
Boundary temperature:	$T_b = 0^\circ\text{C}$
Thermal conductivity:	$D_t = 5 \times 10^7 \text{ J/m-yr-}^\circ\text{C}$
Volumetric heat generation:	$\dot{Q} = 3.1536 \times 10^6 \text{ J/m}^3\text{-yr}$

4.1.8 Output Specifications

The steady-state temperature distribution in the region is to be computed. The vertical temperature profile is to be compared to analytical results at

$$r = 0, 0.25 R \text{ and } 0.5 R.$$

Horizontal distribution is to be compared to analytical results at

$$z = 0.25 Z, 0.5 Z, \text{ and } 0.75 Z.$$

MAGNUM-2D calculations are to be performed for two element sizes of

$$\text{Case 1, } \Delta Z_1 = \Delta R_1 = 10 \text{ m}$$

$$\text{Case 2, } \Delta Z_2 = \Delta R_2 = 20 \text{ m}$$

to examine for presence of discretization errors in this problem.

FIGURE 4.1.1. Problem HT-1, Solution Domain Schematic

4.1.9 Results and Discussions

MAGNUM-2D input was set up and run. Two cases for this problem were computed with the only difference being element sizes. Boundary conditions, material properties, and heat generation rates were as per the input specifications.

A transient solution to this problem was computed to 2000 yr. Monitored time-history temperatures indicated steady state had been reached. This procedure was used to reach steady state because MAGNUM-2D does not contain a steady-state solution mode with a heat load specified.

Figure 4.1.2 presents comparisons of MAGNUM-2D and analytical solution results for steady-state temperatures as a function of radial distance for vertical positions of 50, 100, and 150 m. TEMPEST code results are also plotted for this problem. Due to symmetry in the problem, results at 50 and 150 m are indistinguishable. Figure 4.1.3 presents vertical distributions at radial positions of 0, 50, and 100 m. Agreement between MAGNUM-2D and analytical solution results is excellent. Tabulated distributions in Table 4.1.1 further support this conclusion with the maximum error being -0.13 percent.

These results indicate that MAGNUM-2D is computing acceptably accurate in this mode. Results of the two element size simulations were all but identical. Thus, discretization errors due to element size were not significant in this problem. Anticipated symmetry about the horizontal midplane was computed exactly to within the digits output.

FIGURE 4.1.2. Problem HT-1: Radial Steady-State Temperature Distribution

FIGURE 4.1.3. Problem HT-1: Vertical Steady-State Temperature Distribution

TABLE 4.1.1. Steady-State Temperature Distributions

Radial Distribution (z=100 m)				Vertical Distribution (r=0)			
r(m)	T _{MAG} (°C)	T _{anal} (°C)	Error(%)	z(m)	T _{MAG} (°C)	T _{anal} (°C)	Error(%)
0	255.7	255.98	-0.11	0	0.00	0.00	0.00
20	254.3	254.51	-0.08	20	95.07	95.18	-0.11
40	249.7	249.98	-0.11	40	166.8	166.92	-0.07
60	241.8	242.06	-0.11	60	216.6	216.86	-0.12
80	229.9	230.17	-0.12	80	246.0	246.27	-0.11
100	213.2	213.42	-0.10	100	255.7	255.98	-0.11
120	190.4	190.60	-0.10	120	246.0	246.27	-0.11
140	159.9	160.01	-0.07	140	216.6	216.86	-0.12
160	119.7	119.85	-0.13	160	166.8	166.92	-0.07
180	67.3	67.39	-0.13	180	95.07	95.18	-0.11
200	0.00	0.00	0.00	200	0.00	0.00	0.00

4.2 TRANSIENT MULTIREGION CONDUCTION HEAT TRANSFER IN ONE-DIMENSIONAL CYLINDRICAL GEOMETRY

4.2.1 Problem Designation

This problem is designated: Heat Transfer Problem HT-1.1.

4.2.2 Objective

The objective of this problem is to test transient conduction heat transfer with heat generation. One-dimensional radial heat flow is to be computed through several composite layers of materials with heat generation occurring in the central most material. The TEMPEST code is to be used as a transient comparison basis. Simulations are to be carried to steady state for comparison to an analytical steady-state solution.

4.2.3 Problem Statement

A cylindrical waste canister containing heat generating material is placed in a horizontal position. Surrounding the canister are several layers of material with differing material properties as shown in Figure 4.2.1. The problem is to determine the radial temperature distribution in the material layers. Heat generation in the canister is constant and uniformly distributed over the canister volume. The following conditions are to be applied. At time $t < 0$, all materials are at an equilibrium initial temperature of 50°C . At time $t = 0$, the canister is emplaced and heat-up begins. At a distance of 10 m, the host rock is assumed to remain at a constant temperature of 50°C .

4.2.4 Models Used

The MAGNUM-2D code is to be used to predict transient and steady-state radial temperature distribution. Results of TEMPEST are to be used as a comparison basis during the transient, and an analytical solution is to be used for the comparison basis at final steady-state conditions.

4.2.5 Assumptions

- Material properties are constant.
- The time scale for waste canister emplacement is small relative to the transient heat up time and thus heat generation is assumed as a step change at arbitrary time $t = 0$.

Heat generation in the waste canister is constant for $t > 0$.

- The host rock at a distance of 10 m is assumed to be an infinite heat sink and a constant temperature boundary condition may be used.
- No contact resistance occurs at material boundaries.

4.2.6 Analytical Solution

Developing the steady solution to the present problem is straight forward. In region 1 (waste material with heat generation), the following differential equation applies:

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{dT}{dr} \right) + \frac{\dot{Q}}{D_s} = 0. \quad (4.2.1)$$

The general solution to Equation (4.2.1) is

$$T(r) = - \frac{\dot{Q} r^2}{4D_{s,1}} + A_1 \ln(r) + B_1 \quad (4.2.2)$$

where $D_{s,1}$ is the molecular thermal conductivity of the material in region 1.

In regions 2 to 4, no heat generation is present and the equation to be solved is:

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{dT}{dr} \right) = 0 \quad (4.2.3)$$

The general solution is

$$T_n(r) = A_n \ln(r) + B_n \quad (4.2.4)$$

where n refers to region number 2, 3, or 4.

The following boundary conditions apply:

$$r = 0 \quad \frac{dT_1}{dr} = 0$$

$$r = R_1 \quad -D_{s,1} \frac{dT_1}{dr} = -D_{s,2} \frac{dT_2}{dr}$$

$$r = R_1 \quad T_1 = T_2$$

$$r = R_2 \quad -D_{s,2} \frac{dT_2}{dr} = -D_{s,3} \frac{dT_3}{dr}$$

$$r = R_2 \quad T_2 = T_3$$

$$r = R_3 \quad -D_{s,3} \frac{dT_3}{dr} = -D_{s,4} \frac{dT_4}{dr}$$

$$r = R_3 \quad T_3 = T_4$$

$$r = R_4 \quad T_4 = T_b$$

Applying these boundary conditions to the general solutions (Equations 4.2.2 and 4.2.4), the temperature distribution can be determined in each region as

$$0 \leq r \leq R_1: T_1(r) = T_b + \frac{\dot{Q}R_1^2}{2} \left(\frac{1}{2D_{s,1}} \left(1 - \frac{r^2}{R_1^2} \right) + \frac{1}{D_{s,2}} \ln \left(\frac{R_2}{R_1} \right) + \frac{1}{D_{s,3}} \ln \left(\frac{R_3}{R_2} \right) + \frac{1}{D_{s,4}} \ln \left(\frac{R_4}{R_3} \right) \right) \quad (4.2.5a)$$

$$R_1 \leq r \leq R_2: T_2(r) = T_b + \frac{\dot{Q}R_1^2}{2} \left(\frac{1}{D_{s,2}} \ln \left(\frac{R_2}{r} \right) + \frac{1}{D_{s,3}} \ln \left(\frac{R_3}{R_2} \right) + \frac{1}{D_{s,4}} \ln \left(\frac{R_4}{R_3} \right) \right) \quad (4.2.5b)$$

$$R_2 \leq r \leq R_3: T_3(r) = T_b + \frac{\dot{Q}R_1^2}{2} \left(\frac{1}{D_{s,3}} \ln \left(\frac{R_3}{r} \right) + \frac{1}{D_{s,4}} \ln \left(\frac{R_4}{R_3} \right) \right) \quad (4.2.5c)$$

$$R_3 \leq r \leq R_4: T_4(r) = T_b + \frac{\dot{Q}R_1^2}{2} \left(\frac{1}{D_{s,4}} \ln \left(\frac{R_4}{r} \right) \right) \quad (4.2.5d)$$

4.2.7 Input Specifications

Geometry of the problem is shown in Figure 4.2.1. Dimensions of the material regions are:

$$\begin{aligned} R_1 &= 1 \text{ m} \\ R_2 &= 2 \text{ m} \\ R_3 &= 2.5 \text{ m} \\ R_4 &= 10 \text{ m} \end{aligned}$$

Material properties for each region are given in Table 4.2.1.

Heat generation in region 1 is uniform and constant. No contact resistance occurs at the boundary between material regions. Temperature at the outer boundary, R_4 , is 50°C and constant. Initial temperatures are 50°C.

4.2.8 Output Specifications

Radial temperature distributions are to be compared at transient times of 1, 2, and 5 yrs. The final steady-state distribution is to be compared to the analytical solution.

TABLE 4.2.1. Region Dependent Material Properties

Region	Heat Generation $Q(\text{J/m}^3\text{-sec})$	Density $\rho_s(\text{kg/m}^3)$	Specific Heat $C_s(\text{J/kg-}^\circ\text{C})$	Thermal Conductivity $D_s(\text{J/m-sec-}^\circ\text{C})$
1	200	2000	1500	2.0
2	0	1800	930	1.4
3	0	2780	850	1.5
4	0	2780	930	1.8

FIGURE 4.2.1. Problem HT-1.1: Solution Domain Schematic

4.2.9 Results and Discussion

MAGNUM-2D simulation of this problem utilized 30 elements and 153 nodes. The elements were aligned with the radial coordinate direction simulating a one-dimensional problem. Spacing between nodes was unequal. Boundaries and interface positions between material types were matched. The code was run in the transient, nonisothermal mode. Fixed time steps of 0.01, 0.02, 0.05, and 0.1 yr were taken over the intervals 0-.1, 0.1-0.5, 0.5-1.0, and 1.0 to 5.0 yr, respectively.

The TEMPEST code was run with 50 computational cells in the radial coordinate direction. Cell width was variable. Boundaries and material interface locations were matched. The code was run in the heat transfer-only-mode with automatic time stepping. Time steps were limited to 50 times the explicitly stable value during the implicit solution.

Figure 4.1.2 presents comparisons of transient temperatures at four locations: $R = 0.25, 1.25, 2.10,$ and 2.75 m. These are points in each of the four material regions. TEMPEST results are time-history data computed in this work. MAGNUM-2D results are at discrete times and of data obtained from computer output. Comparison of these discrete time points is also made in Table 4.2.1. Agreement is very good with percentage differences during the transient (relative to TEMPEST results) being less than 1.3 percent.

Figure 4.1.3 presents comparisons of steady-state temperature distribution in the radial direction. MAGNUM-2D and TEMPEST results are at time of 5 yr. By this time, steady conditions had been reached. Analytical steady-state results are from Equation 4.2.5. Agreement between MAGNUM-2D, TEMPEST and the analytical solution is very good. Maximum difference of MAGNUM-2D (relative to the analytical temperature) at the four locations presented in Table 4.2.2 is 0.72 percent.

MAGNUM-2D is concluded to be computing correctly in this geometry. Both transient and steady-state results are found to be in excellent agreement with the comparison basis used.

FIGURE 4.2.2. Problem HT-1.1: Transient Temperatures

FIGURE 4.2.3. Problem HT-1.1: Radial Temperature Distribution

TABLE 4.2.2. Transient Temperature Comparison

Location R(m)	Time (yrs)	T _{MAG} (°C)	T _{TEM} (°C)	Error (%)	T _{anal} (°C)	Error (%)
0.25	0.1	126.7	128.31	1.25	-	-
	0.5	176.8	177.61	-0.45	-	-
	1.0	195.5	196.28	-0.40	-	-
	2.0	209.4	209.92	-0.25	-	-
	5.0	214.5	214.67	-0.08	214.84	-0.16
1.25	0.1	93.98	94.89	-0.96	-	-
	0.5	138.6	138.88	-0.20	-	-
	1.0	156.7	156.93	-0.15	-	-
	2.0	170.2	170.20	0.00	-	-
	5.0	175.2	174.82	0.22	175.64	-0.25
2.10	0.1	67.36	67.89	-0.78	-	-
	0.5	103.7	103.93	-0.22	-	-
	1.0	120.7	120.94	-0.20	-	-
	2.0	133.6	133.60	0.00	-	-
	5.0	138.4	138.00	0.29	138.64	-0.17
2.75	0.1	58.71	58.63	0.14	-	-
	0.5	89.39	88.74	0.73	-	-
	1.0	105.6	104.81	0.75	-	-
	2.0	118.0	116.88	0.96	-	-
	5.0	122.6	121.09	1.24	121.72	-0.72

4.3 STEADY-STATE CONDUCTION HEAT TRANSFER IN A RECTANGULAR GEOMETRY WITH HEAT GENERATION

4.3.1 Problem Designation

This problem is designated: Heat Transfer Problem HT-4.

4.3.2 Objective

The objective of this problem is to test two-dimensional heat conduction simulation capability of MAGNUM-2D. Uniform heat generation is to be considered in a rectangular domain. Both rectangular and nonrectangular computational elements are to be used.

4.3.3 Problem Statement

The problem is to determine the steady-state temperature distribution in a two-dimensional slice through a waste-package scale rectangular domain. Uniform heat generation occurs in the region. The region measures 20 m by 10 m and is bounded by a fixed, uniform temperature. Material in the region is porous and contains water in the pores. Material properties of the rock and water are to be assumed constant. Only conduction heat transfer is to be considered, e.g. no flow occurs. Figure 4.3.1 presents a schematic of the problem. The initial temperature is 50°C and boundaries are to be held constant at this value.

4.3.4 Models Used

The MAGNUM-2D computer code is to be used. Analytical solution is to be generated using computer mathematics library routines.

4.3.5 Assumptions

Assumptions made in this problem include:

- Heat transfer is by molecular conduction only.
- Heat generation rate is uniform over the region and constant.
- Material properties are constant.
- Water is present in the porous medium but no flow occurs.

4.3.6 Analytical Solution

The thermal energy equation solved by MAGNUM-2D in Cartesian tensor notation is

$$S_t \frac{\partial T}{\partial t} + \rho_f c_f q_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i} (D_t \frac{\partial T}{\partial x_i}) + \dot{Q} \quad (4.3.1)$$

where the heat capacity of the water-rock system is given by

$$S_t = \phi \rho_f c_f + (1-\phi) \rho_s c_s \quad (4.3.2)$$

and D_t is the molecular thermal conductivity defined as

$$D_t = \phi D_f + (1-\phi) D_s. \quad (4.3.3)$$

The volumetric heat generation rate is $\dot{Q}$ and ϕ is the porosity. For this problem, the Darcy velocity, q_i , is zero. In Cartesian coordinates, Equation 4.3.1 can be reduced to

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = - \frac{\dot{Q}}{D_t} \quad (4.3.4)$$

for steady-state, no-flow, constant property conditions. Solution to Equation 4.3.4 is given by Carslaw and Jaeger (1959, p. 170) as

$$T = \frac{\dot{Q} (a^2 - x^2)}{2 D_t} - \frac{2 \dot{Q} a^2}{D_t} \sum_{n=0}^{\infty} \frac{(-1)^n \cos \left(\frac{\xi_n x}{a} \right) \cosh \left(\frac{\xi_n y}{a} \right)}{\xi_n^3 \cosh \left(\frac{\xi_n b}{a} \right)} \quad (4.3.5)$$

where

$$\xi_n = \frac{(2n + 1)\pi}{2}$$

4.3.7 Input Specifications

Solution domain and material properties for this problem are:

Domain length	$L = 2a = 20 \text{ m}$
Domain width	$W = 2b = 10 \text{ m}$
Porosity	$\phi = 0.2$
Water thermal conductivity	$D_f = 2.1 \times 10^7 \text{ J/m-yr-}^\circ\text{C}$
Rock Thermal conductivity	$D_s = 5.6 \times 10^7 \text{ J/m-yr-}^\circ\text{C}$
Heat generation rate	$\dot{Q} = 3 \times 10^8 \text{ J/m}^3\text{-yr}$

4.3.8 Output Specifications

Predicted steady-state temperature distributions are to be compared to the analytical solution in both the horizontal and vertical centerplanes. Two MAGNUM-2D cases are to be computed, one with rectangular computational elements and one with nonrectangular computational elements.

FIGURE 4.3.1. Problem HT-4: Solution Domain Schematic

4.3.9 Results and Discussion

Two cases of this problem were simulated with MAGNUM-2D. One used 72 elements and 253 nodes. For this case, the elements were rectangular. The other used 144 elements and 325 nodes. The elements were triangular in this case. The triangular elements were formed by dividing each rectangular element in the former case. Figure 4.3.2 presents a comparison of the element configuration for the two problems. As can be observed, the "triangulation" was done in a rather helter-skelter manner, thus creating a complex element configuration.

The code was run in the nonisothermal mode for both cases with specified temperatures boundary conditions and uniform heat generation rate. Fixed time steps of 0.1 and 0.2 yr were used over the intervals 0 to 1, and 1 to 5 yr, respectively. At $t=5$ yr, steady conditions had been reached. This was determined by monitoring transient temperatures as was done in Problem HT-1.1 (Section 4.2).

Water properties are coded directly in MAGNUM-2D. Thus, although reference thermal conductivity for water in the porous medium was included in the problem statement because it is needed to determine the equivalent value for the analytical solution, it was not input to MAGNUM-2D. Neither was it output for comparison. Thus, there was no way to determine if the MAGNUM-2D and the analytical solution were utilizing exactly the same equivalent thermal conductivity of the porous medium as defined by Equation 4.3.3.

The analytical solution, Equation 4.3.5, was coded and run. Results comparisons are made in Figure 4.3.3 for the horizontal temperature distribution at the midplane ($y = 0$ m) and halfway to the boundary ($y = 2.5$ m). Similar comparisons of vertical temperature distribution at two locations is made in Figure 4.3.4. Agreement of the MAGNUM-2D and analytical results is very good. Graphically, the case 1 and case 2 results for MAGNUM-2D are indistinguishable. Comparison of output data also showed the code to be predicting symmetrically about the $x = 0$ and $y = 0$ planes as it should for this problem. A limited tabulation of midplane results is presented in Table 4.3.1. As apparent in the table, agreement of the code results with analytical results is excellent. The maximum deviation (for both cases) is

FIGURE 4.3.2. Problem HT-4: Comparison of MAGNUM-2D Element Configuration for Case 1 and Case 2

FIGURE 4.3.3. Problem HT-4: Comparison of Horizontal Temperature Distributions

FIGURE 4.3.4. Problem HT-4: Comparison of Vertical Temperature Distributions

TABLE 4.3.1. Steady-State Temperature Distribution, Case 1

x(m)	Horizontal Distribution at y=0			y(m)	Vertical Distribution at x=0		
	T _{MAG} (°C)	T _{anal} (°C)	Error (%)		T _{MAG} (°C)	T _{anal} (°C)	Error (%)
0.00	120.3	119.98	0.26	0.00	120.3	119.98	0.26
0.83	120.1	119.74	0.30	0.83	118.4	118.08	0.27
1.67	119.4	119.02	0.32	1.67	112.7	112.36	0.30
2.50	118.1	117.76	0.29	2.50	103.0	102.78	0.21
3.33	116.2	115.80	0.35	3.33	89.45	89.28	0.18
4.17	113.6	113.25	0.31	4.17	71.80	71.70	0.14
5.00	110.0	109.68	0.29	5.00	50.00	50.00	0
5.83	105.2	104.96	0.23				
6.67	98.98	98.75	0.23				
7.50	90.89	90.68	0.23				
8.33	80.40	80.26	0.17				
9.17	67.00	66.92	0.12				
10.00	50.00	50.00	0				

less than 0.4 percent. The only difference found between case 1 and case 2 temperatures was a change of one digit in the second decimal point. Thus only case 1 results are tabulated.

MAGNUM-2D is concluded to be calculating acceptably accurate in this configuration for both rectangular and triangular elements.

4.4 HEAT TRANSFER AROUND A WASTE CANISTER EMPLACEMENT

4.4.1 Problem Designation

This problem is designated: Heat Transfer Problem HT-6.

4.4.2 Objective

The objective of this problem is to test steady-state heat conduction capabilities of MAGNUM-2D around a waste canister for an in-tunnel emplacement configuration. The geometry is an approximated model of intended code application and includes waste canister, backfill, blast affected (disturbed rock), and host (basalt) rock material zones. This is a benchmarking problem in that results of another computer code are to be used for comparison basis.

4.4.3 Problem Statement

The steady-state temperature distribution around a waste canister for an in-tunnel emplacement configuration is to be determined. The cylindrical waste canister is surrounded by a concentric region of back-fill material. Surrounding the backfill is a blast affected region of basalt rock. Material properties for this region are assumed to be disturbed and different than the surrounding host basalt rock.

The modeled region is to include two vertical boundaries, one through the centerline of the waste canister and one through a symmetry plane located equidistant between two adjacent emplacement tunnels. Upper and lower boundaries of the modeled region are to be horizontal and at a fixed temperature. Figure 4.4.1 presents the basic geometry of the modeled region. The problematic emplacement is presented schematically in the lower half of the figure. The four material regions are identified. In the upper half of the figure, the Cartesian approximation to be used for the numerical model is presented. The Cartesian approximation is to be used for reasons discussed in Section 4.4.4. Heat generation is assumed to be constant and uniform in the waste canister zone.

4.4.4 Models Used

The MAGNUM-2D code is to be used in the heat-transfer-only mode to compute transient and steady-state temperatures in and around the waste canister. The approximated Cartesian geometry shown in the upper half of Figure 4.4.1 is to be used in the simulation. This model geometry is prescribed because a suitable benchmarking tool that satisfies the objective of this and subsequently related problems (see Section 4.7, Fluid Flow Problem FF-4) was not available. Computational results of the TEMPEST code is to be used as a benchmarking comparison basis in the approximated Cartesian geometry model.

4.4.5 Assumptions

Assumptions made for the present problem are:

- Heat generation is uniform and constant in the modeled waste canister volume.
- Thermal conductivity is constant in each material and isotropic.
- Vertical boundaries are to be zero flux.
- Horizontal boundaries are to be fixed temperature.
- No thermal resistance occurs at material boundaries.

4.4.6 Input Specifications

The geometry and pertinent dimensions of the "Cartesian approximation" model of the waste canister simulation domain are shown in Figure 4.4.2. This model maintains volumes nearly equivalent to the cylindrical region for each of the materials.

Material properties for each region are given in Table 4.4.1. Both vertical boundaries are to be zero flux boundaries. Upper and lower horizontal boundaries are to be maintained at constant temperature of 50°C. Initial temperatures are to be 50°C. Heat generation rate for the waste canister is 100 J/m³-sec.

TABLE 4.4.1. Solid Material Properties by Region

Region	Thermal Conductivity D_s (J-sec/m-°C)	Density ρ_s (kg/m ³)	Specific Heat c_s (J/kg-°C)	Porosity ϕ
1	3.00	2500	1500	0.01
2	1.40	1800	930	0.30
3	1.78	2780	930	0.00022
4	1.78	2780	930	0.0001

Properties of water present in the pore volume are to be assumed constant at a reference temperature of 50°C. These are:

Density	$\rho_f = 990 \text{ kg/m}^3$
Specific heat	$c_p = 4188 \text{ J/kg-°C}$
Thermal conductivity	$D_f = 0.61 \text{ J-sec/m-°C}$

4.4.7 Output Specifications

Transient temperature distributions at times of 5 and 10 yr are to be compared along the horizontal plane and the vertical plane through the canister centerline. Steady-state temperatures are also to be computed and compared.

FIGURE 4.4.1. Problem HT-6: Simulation Region Schematic

The MAGNUM-2D and the TEMPEST code were used to model this problem. The MAGNUM-2D model contained 394 elements and 1233 nodes. Element configuration was mixed; both rectangular and nonrectangular elements were used. The TEMPEST model used 1458 computational cells, variably spaced. Grid structure for the two models over equivalent regions reflected about the centerplane are presented in Figure 4.4.3. In the MAGNUM-2D simulation, time steps of 1, 2.5 and 5.0 yr were used over intervals of 0-5, 5-15, and 15-30 yr, respectively. TEMPEST was used in an automatic time-stepping mode with the limitation that the time step be restricted to a maximum of 1000 times the explicit stable value during implicit solution over the time step.

Steady-state isotherms predicted by the two codes are presented in Figure 4.5.4. Agreement is very satisfactory. Both code's results indicate expected symmetry about the horizontal centerplane. Transient temperatures at four locations are presented in Figure 4.4.5. During the transient heat up, MAGNUM-2D underpredicts temperatures compared to TEMPEST results. The underprediction is not excessive. For example, at 5 yr, the underprediction is typically less than 0.3°C , at location (0.2, 0.2). This is about 1.5 percent at this point in time. One point to note is that the TEMPEST results indicate a smooth curve as material heats up. The MAGNUM-2D results at location (0.2, 0.2), for example, show a distinct deviation from a smooth curve. This is evidenced by temperatures plotted at 1, 2, 3, and 4 yr. Noting that MAGNUM-2D results were computed using a one year time step over this interval, TEMPEST results were also computed again but using a 1 yr time step out to 5 yr. These later results are also included in Figure 4.5.5. These latter TEMPEST results show considerable deviation from the anticipated smooth curve. This tends to indicate (it is well known for the TEMPEST solution procedure (Eyler, et al. 1983)) that implicit solution procedures may become inaccurate at extremely large time steps relative to an explicit stable value.

Figures 4.4.6 and 4.4.7 present horizontal and vertical temperature distributions, respectively, at times of 5 and 10 yr. With the exception of those very near the center of the modeled waste canister, agreement of the results is excellent. The cause of the nominal disagreement at the center point is unknown.

These results indicate that MAGNUM-2D is capable of computing accurately in this geometry. Results tend to indicate though that MAGNUM-2D and TEMPEST may produce inaccurate results at very large time steps. This has been observed in this and other TEMPEST simulations, but data are unavailable to determine the relation between accuracy and time step for the MAGNUM-2D solution.

FIGURE 4.4.3. Problem HT-6: MAGNUM-2D and TEMPEST Computational Domain Comparison (Partial)

FIGURE 4.4.4. Problem HT-6: Comparison of Steady-State Isotherms

FIGURE 4.4.5. Problem HT-6: Transient Temperatures

FIGURE 4.4.6. Problem HT-6: Horizontal Temperature Distribution at Times of 5 and 10 yr

FIGURE 4.4.7. Problem HT-6: Vertical Temperature Distribution at Times of 5 and 10 yr

4.5 STEADY FLOW IN A REGIONAL GROUNDWATER SYSTEM

4.5.1 Problem Designation

This problem is designated: Fluid Flow Problem FF-1.

4.5.2 Objective

The objective of this problem is to test computation of steady-state fluid flow in a regional groundwater system modeled with the MAGNUM-2D code. Results are to be compared to an analytical solution.

4.5.3 Models Used

The MAGNUM-2D code is to be used in the steady-state, fluid-flow-only mode. The analytical solution is to be generated using computer mathematics library routines.

4.5.4 Problem Statement

A uniformly sloped water table exists over a region in which groundwater flow is to be computed. Figure 4.5.1 presents a schematic of the region. The region is bounded on the bottom by an impermeable layer. Each lateral boundary is a major groundwater divide and can thus be treated as impermeable. The material in the region of interest is isotropic and homogeneous. Under steady, isothermal conditions, an analytical solution for hydraulic head distribution and, hence, flow, in this region can be determined.

4.5.5 Analytical Solution

The groundwater flow equation for steady, isothermal, isotropic, and homogeneous conditions, can be reduced to

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = 0. \quad (4.5.1)$$

Boundary conditions for this problem (see Figure 4.5.1) are specified as

$$\frac{\partial h}{\partial x}(0,y) = \frac{\partial h}{\partial x}(L,y) = \frac{\partial h}{\partial y}(x,0) = 0 \quad (4.5.2)$$

along the bottom and lateral boundaries, and

$$h(x,H) = f(x) \quad (4.5.3)$$

along the top surface of the solution domain. For an assumed linear water table, the functional form can be expressed as

$$f(x) = H + x \tan \alpha \quad (4.5.4)$$

where H = elevation of the water table above the datum, and

α = angle of slope of the water table.

The analytical solution for the hydraulic head distribution has been obtained and is given by Domenico (1980)^(a) as

$$h = \left(H + \frac{L \tan \alpha}{2} \right) - \frac{4 \tan \alpha}{L} \sum_{m=0}^{\infty} \frac{\cos(\xi_m x) \cosh(\xi_m y)}{\xi_m^2 \cosh(\xi_m H)} \quad (4.5.5)$$

where

$$\xi_m = \frac{(2m+1) \pi}{L}.$$

(a) There is an error in the cosh term in the numerator of the solution given by Domenico (Equation (6.7), p. 259, 1980). It has been corrected in Equation (4.5.5) given here.

Differentiating Equation 4.5.5 with respect to x and y , respectively, and multiplying by the hydraulic conductivity, K , results in an analytical expression for horizontal and vertical Darcy velocities. The result is

$$U = - \frac{4K \tan \alpha}{L} \sum_{m=0}^{\infty} \frac{\sin(\xi_m x) \cosh(\xi_m y)}{\xi_m \cosh(\xi_m H)} \quad (4.5.6)$$

and

$$V = \frac{4 K \tan \alpha}{L} \sum_{m=0}^{\infty} \frac{\cos(\xi_m x) \sinh(\xi_m y)}{\xi_m \cosh(\xi_m H)}. \quad (4.5.7)$$

4.5.6 Assumptions

The principal assumptions in this problem are:

- The sloped water table can be approximated as a specified linear head distribution at the solution domain boundary.
- The groundwater flow is steady and isothermal.
- Material in the region is isotropic and homogeneous.
- The bottom of the region is bounded by an impermeable material.
- The lateral boundaries are theoretically impermeable such as might be exhibited by major groundwater divides.

4.5.7 Input Specifications

The parameters required for simulation of this problem are space dimensions, water table angle, and hydraulic conductivity. These are to be:

Region Depth	$H = 500 \text{ m}$
Region Width	$L = 1000 \text{ m}$
Water Table Angle	$\alpha = 1.7184 \text{ degrees}$
Hydraulic Conductivity	$K = 1 \text{ m/yr}$

This water table angle corresponds to a lateral hydraulic gradient of 0.03 m/m.

4.5.8 Output Specifications

MAGNUM-2D computed output for this problem is to be compared to analytical results for the following locations:

- horizontal distribution at $y = 250$ m
- vertical distribution at $x = 50$ m, 500 m, and 950 m.

These latter positions will yield data for expected symmetry comparisons.

FIGURE 4.5.1. Groundwater Region Schematic

4.5.9 Results and Discussion

The MAGNUM-2D code was run using steady-state and flow-only options. There were 84 rectangular elements and 291 nodes in the problem. Hydraulic head at nodes along the top surface were specified corresponding to a gradient of 0.03 m/m using zero as a reference value. The analytical solution, Equation 4.5.5, was coded and run.

Horizontal distribution of steady-state hydraulic head at the midplane ($y/H = 0.5$) is presented in Figure 4.5.2. Vertical distribution of hydraulic head is presented in Figure 4.5.3. Horizontal positions of $x/L = 0.05, 0.50,$ and 0.95 are included. Agreement of MAGNUM-2D and analytical solution results is excellent. Table 4.5.1 lists certain of these data. Maximum deviation of code results is less than 0.1 percent of the analytical solution. This is excellent agreement in light of the fact that the hydraulic head boundary conditions specified on the top boundary of the MAGNUM-2D model were 0.07 percent less than that which corresponding to a gradient of 0.03 m/m. This minor deviation occurred as a result of computing the top boundary condition value of $\alpha = 1.7184$. For the analytical solution, it was assumed that $\tan\alpha$ was identically 0.03 m/m.

Figures 4.5.4 and 4.5.5 present comparison of horizontal and vertical distributions of Darcy velocities, respectively. The velocities presented are those computed at element centers; thus the positions of the distributions are different than those presented for hydraulic head. Agreement of MAGNUM-2D and analytical results is very good. The code predicts the similitude between horizontal velocities at $x/L = 0.025$ and 0.975 exactly within the accuracy of the four digits output.

Based on these hydraulic head and Darcy velocity results, MAGNUM-2D is concluded to be predicting accurately in this mode for this problem.

FIGURE 4.5.2. Problem FF-1: Horizontal Distribution of Hydraulic Head at $y/H = 0.5$

FIGURE 4.5.3. Problem FF-1: Vertical Distribution of Hydraulic Head at $x/L = 0.05, 0.50, \text{ and } 0.95$

FIGURE 4.5.4. Problem FF-1: Horizontal Distribution of Vertical Darcy Velocity

FIGURE 4.5.5. Predicted Vertical Distribution of Horizontal Darcy Velocity

TABLE 4.5.1. Steady-State Hydraulic Head Distribution

Horizontal at $y/H = 0.5$				Vertical at $x/L = 0.05$			
$x(m)$	$h_{MAG}(m)$	$h_{anal}(m)$	Error (%)	$y(m)$	$h_{MAG}(m)$	$h_{anal}(m)$	Error (%)
0	8.436	8.442	-0.07	0	10.19	10.192	-0.02
50	8.533	8.538	-0.06	90	9.985	9.992	-0.07
275	10.94	10.944	-0.04	180	9.359	9.365	-0.06
500	14.99	15.000	-0.07	250	8.533	8.538	-0.06
725	19.04	19.056	-0.08	320	7.337	7.341	-0.05
950	21.45	21.462	-0.06	410	5.052	5.050	0.04
1000	21.55	21.559	-0.04	500	1.499 ^(a)	1.500 ^(a)	-0.07

(a) Boundary condition

4.6 TRANSIENT TWO-DIMENSIONAL FLOW

4.6.1 Problem Designation

This problem is designated: Fluid Flow Problem FF-2.

4.6.2 Objective

The objective of this problem is to test computation of transient groundwater flow in a two-dimensional region with MAGNUM-2D which occurs because of an initial hydraulic head distribution which is not in equilibrium.

4.6.3 Problem Statement

The problem is to determine transient groundwater flow in a two-dimensional region. The hydraulic head in the region is an initial potential mound with a sinusoidal distribution,

$$h = h_{\max} \sin \left(\frac{\pi x}{X} \right) \sin \left(\frac{\pi y}{Y} \right). \quad (4.6.1)$$

With no sources or sinks in the region, the hydraulic head in the region will asymptotically decrease with time as groundwater is forced out of the region. Boundaries of the region are maintained at constant head. Figure 4.6.1 presents a schematic of the problem. Solution of a similar problem for which $X = Y$ is given by King, et al. (1981).

4.6.4 Models Used

The MAGNUM-2D code is used in a fluid-flow-only mode. Results are compared to an analytical solution developed and solved for the problem.

4.6.5 Analytical Solution

The governing groundwater flow balance equation for the case of constant hydraulic conductivities and isothermal flow, written in Cartesian coordinates, becomes

$$\frac{S_s}{K} \frac{\partial h}{\partial t} = \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}. \quad (4.6.2)$$

An analytical solution to this equation can be obtained subject to initial conditions of Equation 4.6.1 for $0 < x < X$, $0 < y < Y$ and for boundary conditions of

$$\begin{aligned} h(0, y, t) = h(X, y, t) = h_b &= 0 \\ h(x, 0, t) = h(x, Y, t) = h_b &= 0 \end{aligned} \quad (4.6.3)$$

for all t . Without any loss in generality it is convenient to define h_b , the constant boundary head, to be zero. The solution to Equation 4.6.2 is

$$h(x, y, t) = h_{\max} \left[\exp \left(-\frac{\pi^2 K t}{S_s} \left(\frac{1}{x^2} + \frac{1}{y^2} \right) \right) \sin \left(\frac{\pi x}{X} \right) \sin \left(\frac{\pi y}{Y} \right) \right]. \quad (4.6.4)$$

This solution can be readily verified by substitution into Equations (4.6.2) to (4.6.4).

Transient horizontal and vertical Darcy velocities are obtainable by differentiating Equation 4.6.4 with respect to x and y , respectively, and multiplying the result by hydraulic conductivity. The result is

$$U = \frac{K h_{\max} \pi}{X} \left[\exp \left(-\frac{\pi^2 K t}{S_s} \left(\frac{1}{x^2} + \frac{1}{y^2} \right) \right) \cos \left(\frac{\pi x}{X} \right) \sin \left(\frac{\pi y}{Y} \right) \right] \quad (4.6.5)$$

and

$$v = \frac{K h_{\max} \pi}{Y} \left[\exp \left(- \frac{\pi^2 K t}{S_s} \left(\frac{1}{X^2} + \frac{1}{Y^2} \right) \right) \sin \left(\frac{\pi X}{X} \right) \cos \left(\frac{\pi Y}{Y} \right) \right] \quad (4.6.6)$$

for horizontal and vertical components, respectively.

4.6.6 Assumptions

Assumptions made in this problem include:

- The flow domain is finite and all boundaries are maintained at constant head, $h_b = 0$.
- The flow domain is isotropic and the hydraulic conductivity is constant.
- There are no sources or sinks.
- The flow domain is isothermal.

4.6.7 Input Specifications

Parameters required for solution are specified as follows:

Domain length	$X = 2,000 \text{ m}$
Domain width	$Y = 1,000 \text{ m}$
Hydraulic conductivity	$K = 3.0 \times 10^{-3} \text{ m/yr}$
Specific storage	$S_s = 2.3 \times 10^{-4} \text{ m}^{-1}$
Maximum head	$h_{\max} = 100 \text{ m}$

4.6.8 Output Specifications

The transient hydraulic head distribution is to be computed to a time of 10,000 yr and results presented in increments of 2000 yr. Computed distributions in the x- and y- coordinate directions are to be compared to analytical solutions at selected locations to ensure symmetry about the $\frac{x}{X} = \frac{1}{2}$ and the $\frac{y}{Y} = \frac{1}{2}$ planes.

FIGURE 4.6.1. Problem FF-2: Sinusoidal "Potential Mound" Problem Schematic

4.6.9 Results and Discussions

The simulation region was modeled with MAGNUM-2D using 128 elements and 433 nodes. The elements were rectangular and uniform in size measuring 125 m by 125 m. The code was run in the transient, isothermal, flow-only mode. Time steps of 25, 50, 100, 200, and 400 yr were taken over intervals from 0-100, 100, -300, 300-1000, 1000-2000, and 2000-10,000 yr, respectively. Results were printed at 25 yr and 1000 yr and subsequently at each 2000 yr interval to a total simulation time of 10,000 yr. No time-history data were included in the MAGNUM-2D output, thus comparisons can only be made at these discrete times. Initial conditions were generated in a format required by MAGNUM-2D by a preprocessor specifically coded to generate appropriate values from Equation 4.5.1. Hydraulic head at boundary nodes were maintained constant at $h_b = 0$ m throughout the simulation.

Figure 4.6.2 compares the transient predicted hydraulic head. Agreement with the analytical results is very good over the whole transient. Table 4.6.1 presents a tabulated comparison. The maximum relative deviation between the

data and MAGNUM-2D predictions is less than 1.5 percent. This maximum occurs at the end of the simulation. Over the period from 1,000 to 10,000 yr, the absolute difference has only increased less than three-fold, whereas the relative difference has increased over eight-fold. This characteristic is a consequence of the asymptotic decay to zero and is not of particular significance.

Thus, it is concluded that MAGNUM-2D is predicting acceptably accurate in this transient problem.

TABLE 4.6.1. Transient Hydraulic Head

Location	Time (yr)	h_{MAG}	h_{anal}	Diff (m)	Error (%)
x = 1000 m y = 500 m (curve 1)	0	100.00	100.00	0	0
	1,000	85.26	85.136	0.124	0.15
	2,000	72.64	72.481	0.159	0.22
	4,000	52.81	52.536	0.274	0.52
	6,000	38.40	38.079	0.321	0.84
	8,000	27.92	27.600	0.320	1.16
	10,000	20.30	20.005	0.295	1.25
x = 1000 m y = 250 m (curve 2)	0	70.71	70.711	0	0
	1,000	60.29	60.200	0.090	0.15
	2,000	51.37	51.252	0.118	0.23
	4,000	37.35	37.149	0.201	0.54
	6,000	27.15	26.923	0.227	0.85
	8,000	19.74	19.516	0.224	1.15
	10,000	14.35	14.146	0.204	1.44
x = 500 m y = 250 m (curve 3)	0	50.00	50.000	0	0
	1,000	42.63	42.568	0.062	0.14
	2,000	36.32	36.241	0.079	0.22
	4,000	26.41	26.268	0.142	0.51
	6,000	19.20	19.039	0.161	0.89
	8,000	13.96	13.800	0.160	1.16
	10,000	10.15	10.003	0.147	1.12

FIGURE 4.6.2. Problem FF-2: Transient Hydraulic Head

4.7 STEADY FLOW IN A POROUS MEDIA

4.7.1 Problem Designation

This problem is designated: Fluid Flow Problem FF-4.

4.7.2 Objective

The objective of this test problem is to test computation of steady-state flow in a porous medium. Three porous materials are present in a geometry typical of anticipated MAGNUM-2D analysis usage within BWIP.

4.7.3 Problem Statement

The region to be modeled is shown in Figure 4.7.1. The region spans a total height of 41.1 meters and a width of 5 meters. The vertical boundaries at $x = -5$ m and $x = 0$ m are symmetry planes. The horizontal boundaries at $y = -5$ m and $y = 36.6$ m are fixed hydraulic head planes. The center of the 0.37-m diameter waste canister is taken as the origin. The outer diameter of the waste canister is the simulation region boundary.

Concentrically surrounding the waste canister is a 0.15-m thick layer of porous backfill material. Surrounding that is a 0.33-m thick region of blast-affected porous material.

Hydraulic heads at the upper and lower boundaries are fixed at 2.5 and 5.0 m, respectively. Around the outer diameter of the waste canisters, hydraulic heads are specified at several locations to model a perturbation to the pressure field such as may occur due to heating in the waste canister.

4.7.4 Models Used

The MAGNUM-2D and FTRANS codes are to be used.

4.7.5 Assumptions

Assumptions made for the present problem are:

- Flow is isothermal.
- Vertical boundaries are symmetry planes; horizontal boundaries of fixed hydraulic head.

- No fracture flow paths are present in the porous media or at material boundaries.

4.7.6 Input Specifications

The center of the waste canister is taken as the origin. The solution domain is to be from 5 meters below the origin to 36.6 meters above the origin. Vertical symmetry planes are at $x = -5$ m and $x = 0.0$ m. The waste canister surface defines the boundary to the backfill region.

Properties of the porous materials are listed in Table 4.7.1.

TABLE 4.7.1. Porous Material Properties

<u>Material</u>	<u>Material Number</u>	<u>Hydraulic Conductivity (m/sec)</u>	<u>Specific Storage (m^{-1})</u>
Basalt	1	1×10^{-13}	4.6×10^{-7}
Blast affected	2	1×10^{-12}	2.0×10^{-3}
Backfill	3	1×10^{-10}	2.0×10^{-3}

Hydraulic head at the lower boundary is to be fixed at 5.0 m and hydraulic head at the upper boundary is to be fixed at 2.5 m boundary. At the waste canister boundary at locations shown in Figure 4.8.1, hydraulic heads are:

$$h_1 = 4.700 \text{ m}, h_2 = 4.696 \text{ m}, \text{ and } h_3 = 4.962 \text{ m}.$$

4.7.7 Output Specifications

Steady-state hydraulic head distributions and Darcy flow velocities in the porous materials are to be compared at selected locations.

FIGURE 4.7.1. Problem FF-4: Problem Schematic

4.7.8 Results and Discussions

The MAGNUM-2D code was set up using 174 elements and 591 nodes for this problem. Figure 4.7.2 presents a schematic of the element configuration and material numbers over a portion of the vertical dimensions spanning the waste canister region. The FTRANS model was set up using virtually identical element geometry. However, because FTRANS uses 4 nodes per element (one at each corner) and MAGNUM-2D uses 8 (one at each corner and one at the middle of each side), the FTRANS model had exactly 4 elements located within each MAGNUM-2D element for a total of 696 elements. Thus, the two models were as identical as could be for this problem.

Figure 4.7.3 presents MAGNUM-2D predicted hydraulic head contours over the vertical region $-5.0 < y < 5.0$ m. The perturbation effect of specified hydraulic heads at the waste canister boundary is evident. (FTRANS results are not included in the figure because a contour plotting capability for nonrectangular elements was not readily available in this work.)

Figure 4.7.4 presents a comparison of predicted hydraulic head. The plot is of a vertical distribution at $x = 0.0$ and -5.0 m (right and left edge vertical planes, respectively). Agreement of the results is excellent. At right boundary ($x = -0.0$), both codes predict the same deviation from a linear head distribution which results because of the perturbation of the waste canister boundary. The local variation from $-3.0 \leq y \leq 3.0$ m is expanded in Figure 4.7.5. Also included in this figure is data predicted at the boundary between materials 1 and 2. This is a circumferential distribution at a radial distance of 0.665 m around the origin. Excellent agreement is evident with the maximum deviation of head data being less than 1 percent along the right vertical boundary plane. Further agreement is evidenced in the horizontal hydraulic head distributions at $y = -1.2, 0.0$, and $+1.2$ m shown in Figure 4.7.6. In this figure, the MAGNUM-2D results exhibit more smoothness in the distributions. Only the curve at $y = 0.0$ m crosses material types. The apparent discontinuous slope of the FTRANS results at $x = \pm 1.2$ m corresponds to the location where the models switch from rectangular to nonrectangular element shapes.

Table 4.7.2 presents a comparison of predicted vertical Darcy velocities at three discrete position in the domain. One is near the lower left hand corner, one is near the upper left hand corner, and one is adjacent to the waste canister boundary. Values presented are within the same element location but the codes do not predict Darcy velocities at the same physical location. Thus values tabulated are at slightly different physical locations.

In the absence of the waste canister boundary perturbation the vertical Darcy velocity in the host basalt would be

$$V = -K_1 \frac{dh}{dy} = 1.893 \times 10^{-7} \text{ m/yr.}$$

This velocity results from the impressed vertical hydraulic gradient of $h_{top} = 2.5 \text{ m}$ and $h_b = 5.0 \text{ m}$. The tabulated data at the two points on the left boundary span this value because of the perturbation of the waste canister boundary. Results of the two codes are in very good agreement even though locations of the comparison are only approximate.

MAGNUM-2D is predicting acceptable results based on the comparisons made here using the FTRANS code as a comparison basis. For comparable models, predicted hydraulic head data agrees to within 1 percent. Darcy velocity predictions at one selected location near the waste canister boundary agree to within 3 percent. Other positions compared were in better agreement. Physical position of the predicted velocity differs slightly in each model, however, which may partially explain these differences.

TABLE 4.7.2. Comparison of Predicted Steady-State Darcy Velocities

Approximate Position (x,y)	Vertical Darcy Velocity		Error (%)
	V_{MAG} (m/yr)	V_{FTRANS} (m/yr)	
(-5.0, -5.0)	1.6625×10^{-7}	1.6686×10^{-7}	-0.37
(-5.0, 36.6)	1.9523×10^{-7}	1.9490×10^{-7}	0.17
(-0.185, 0.0)	-2.6191×10^{-3}	-2.5503×10^{-3}	2.63

FIGURE 4.7.2. Problem FF-4: MAGNUM-2D Element Configuration and Material Number

FIGURE 4.7.3. Problem FF-4: MAGNUM-2D Predicted Hydraulic Head Contours

FIGURE 4.7.4. Problem FF-4: Comparison of Vertical Hydraulic Head Distribution

FIGURE 4.7.5. Problem FF-4: Comparison of Vertical Hydraulic Head Distribution Near Waste Canister Level

FIGURE 4.7.6. Problem FF-4: Comparison of Horizontal Hydraulic Head Distribution

4.8 FLOW IN A SINGLE FRACTURE

4.8.1 Problem Designation

This problem is designated: Fluid Flow Problem FF-6.

4.8.2 Objective

The objective of this problem is to test computation of steady-state flow in a porous media with a single embedded fracture.

4.8.3 Problem Statement

A schematic of the problem to be solved is shown in Figure 4.8.1. The region consists of a porous media with a highly permeable fracture centrally located at the base of the domain. A uniform horizontal hydraulic gradient of -10^{-3} m/m is imposed by specifying hydraulic head values at the left and right boundaries. This problem is similar to the one presented by Baca, et al. (1984).

4.8.4 Models Used

The MAGNUM-2D and FTRANS codes are to be used.

4.8.5 Assumptions

Assumptions made for this problem include:

- The highly permeable fracture is discrete and embedded in a homogeneous porous medium.
- Boundary conditions are constant.
- The flow is isothermal.

4.8.6 Input Specifications

Parameters for this problem are:

Domain width	$W = 1000$ m
Domain height	$H = 200$ m
Fracture length	$L_f = 100$ m
Boundary head	$h_{left} = 6$ m
Boundary head	$h_{right} = 5$ m
Porous media hydraulic conductivity	$K_{PM} = 10^{-13}$ m/s

Fracture hydraulic conductivity

$$K_f = 10^{-9} \text{ m/s}$$

Fracture aperture

$$A_f = 1 \text{ m}$$

4.8.7 Output Specifications

Steady-state hydraulic head distributions computed by MAGNUM-2D and FTRANS are to be compared. Darcy velocities computed by the codes are to be compared also.

FIGURE 4.8.1. Problem FF-6: Single Fracture Embedded in a Porous Medium

4.8.8 Results and Discussion

The MAGNUM-2D model of this problem was set up using 178 rectangular elements. Eight line elements modeled the discrete fracture along the central portion of the bottom boundary. The hydraulic gradient was imposed by specifying left and right boundaries at fixed head values of 6.0 and 5.0 m, respectively. The code was run in the steady-state, flow-only mode.

The FTRANS model was set up similarly but with 200 elements. Five line elements modeled the fracture. The code was run in a transient mode and results monitored until no variation in primary variables occurred, thus indicating steady state.

Figure 4.8.2 presents the predicted hydraulic head. Results are plotted along the lower boundary ($y = 0.0$ m), through the fracture, and along the upper boundary. Agreement between the two codes is excellent. The upper boundary is sufficiently removed from the fracture so as not to be noticeably affected by its presence. Thus a linear hydraulic gradient is predicted by both codes along the upper boundary. The region from $300 < x < 700$ is expanded in Figure 4.8.3 to show the perturbing effect of the fracture more clearly. Along the whole lower boundary, agreement of predicted hydraulic head is excellent.

In the fracture itself, the hydraulic gradient is nearly constant due to the significantly reduced flow resistance. Figure 4.8.4 presents a comparison of predicted Darcy velocities in the discrete fracture. Although node placements differ, agreement is good. At the center of the fracture, for example, the two codes predict velocities to within 1 percent. In the porous media, along the top boundary, agreement between predicted Darcy velocities were found to be within 0.2 percent.

One aspect of the Darcy velocities predicted by MAGNUM-2D should be noted. The code predicts Darcy velocities in each line element at four Gauss points located within the line element where a line element is defined by three nodes (see Figure 2.1.1). The code computes Darcy velocity at these Gauss points by linearizing the head distribution. If the mid-side node is not centered a weighted averaging is used. Thus, velocity is predicted as constant in the fracture (line element) at each of the four Gauss points. The single

velocity values in Figure 4.8.4 in each line element are thus the value at each of the four Gauss points. FTRANS, on the other hand, predicts flows in each line element as a consequence of the hydraulic head at each end (node point) of the line element and a leakage source (sink) from adjacent porous rock. Thus, only one Darcy velocity is predicted for each fracture (line element). As Figure 4.8.4 indicates, results from these two different methods are very consistent.

Based on the predicted hydraulic heads, MAGNUM-2D is concluded to be predicting accurately for this problem and operating mode. Darcy velocities in both the fracture and porous medium are also in good agreement.

FIGURE 4.8.2. Problem FF-6: Predicted Hydraulic Head Over the Region $0 < x < 1000$ m

FIGURE 4.8.3. Problem FF-6: Predicted Hydraulic Head Over the Fracture Affected Region

FIGURE 4.8.4. Problem FF-6: Predicted Darcy Velocities in the Discrete Fracture

4.9 FLOW IN A NETWORK OF FRACTURES

4.9.1 Problem Designation

This problem is designated: Fluid Flow Problem FF-7.

4.9.2 Objective

The objective of this problem is to test computation of steady-state hydraulic head and flow in a network of connected fractures. The fractures are embedded in an impermeable medium.

4.9.3 Problem Statement

A schematic of the solution domain to be modeled is presented in Figure 4.9.1. The domain consists of an impermeable medium cross-hatched with a network of highly permeable fractures. The fractures intersect at 90° angles. A uniform hydraulic gradient of -1.25 m/m is imposed by specifying hydraulic head values at the left and right boundary nodes. Additionally, hydraulic head is to be specified at one interior lower boundary node to model a local perturbation as shown in the figure.

Three regions are to be included in the solution domain. The fracture aperture and hydraulic conductivity differ in each region. With this exception, this problem is similar to that presented by Baca, et al. (1984).

4.9.4 Models Used

The MAGNUM-2D and FTRANS codes are to be used to model the system of intersecting fractures.

4.9.5 Assumptions

Assumptions made for this problem include:

- Fractures are discrete and imbedded in an impermeable medium.
- Boundary conditions are fixed and constant.
- The flow is isothermal.

4.9.6 Input Specifications

Parameters for this problem are:

Domain length	$L = 8 \text{ m}$
Domain width	$W = 2 \text{ m}$
Boundary head	$h_{\text{left}} = 15 \text{ m}$
Boundary head	$h_{\text{right}} = 5 \text{ m}$
Central node head	$h_{\text{cent}} = 14 \text{ m}$
Fracture intersection angle	$\alpha = 90^\circ$

Fluid properties are to be constant and at a reference temperature of 25°C .

Fracture properties, by region are:

Region	Aperature	Hydraulic Conductivity
	(μm)	(m/sec)
1	5	8×10^{-3}
2	10	4×10^{-3}
3	20	2×10^{-3}

Regions are defined in Figure 4.9.1.

4.9.7 Output Specifications

Steady-state hydraulic head distributions computed with the MAGNUM-2D and FTRANS code are to be compared at selected locations.

FIGURE 4.9.1. Problem FF-7: Network of Fractures Solution Domain Schematic

4.9.8 Results and Discussion

The MAGNUM-2D code was setup and run using line elements to model the network of discrete fractures. A total of 64 line elements and 107 nodes were used. Boundary conditions of fixed hydraulic head were specified at the left and right ends of the network and at the lower central node. The code was run in the steady-state flow-only mode.

The FTRANS model of this problem was set up using rectangular elements, and defining discrete line fractures across diagonal nodes. The hydraulic conductivity of the host material was set to 10^{-20} m/sec and thus impermeable relative to fracture conductivities which are of the order of 10^{-3} m/sec. A total of 64 elements were used and the code was run in a transient mode. Fifty time steps were computed and the results were monitored to determine that steady-state conditions had been reached. No discernable variation in results occurred beyond 10 time steps.

Upon initial comparison of results from FTRANS and MAGNUM-2D for this problem, significant differences in head distribution and Darcy velocity in the

fractures was found. To isolate the cause, both codes were used to simulate sequentially simplified problems. First, the perturbed head value at the center of the lower boundary was removed as a boundary condition. Then, fracture aperture was set to a single value over the whole network. For both these cases, an analytical solution for the head distribution can be determined. MAGNUM-2D results were in agreement with the analytical solution whereas FTRANS results were not.

Discussions with FTRANS code developer^(a) supported the observations of these results. It was determined that FTRANS was coded to utilize only a single fracture aperture. Subsequent to these discussions a coding change was made to the version of FTRANS used in this work as detailed in Appendix B. After making the coding change, FTRANS results for the simplified network problem were in complete agreement with the analytical results and MAGNUM-2D results. Results for the case of the network with three aperture regions and no perturbation at the lower boundary are included in Table 4.9.1. Agreement is excellent.

Results for the problem as stated in Section 4.9.6 are presented in Figures 4.9.2 and 4.9.3. The hydraulic head as a function of horizontal position in the uppermost and lowermost fracture are presented. Results identified as Case 1 are for the problem as stated; those of Case 2 are for the lower, centered head value removed as a boundary condition. MAGNUM-2D and FTRANS results are in excellent agreement for both cases.

These results indicate that MAGNUM-2D is correctly predicting flow in this geometry with a network of intersecting fractures.

(a) Peter Hyakorn, GEOTRANS, Inc., personal communications.

TABLE 4.9.1. Comparison of Fracture Network Hydraulic Head (Case 2)

<u>x(m)</u>	<u>Analytical</u>		<u>FTRANS</u>		<u>MAGNUM-2D</u>	
	<u>h(m)</u>	<u>V(m/yr)</u>	<u>h(m)</u>	<u>V(m/yr)</u>	<u>h(m)</u>	<u>V(m/yr)</u>
0.0	15.000	2.229x10 ⁵	15.00	2.227x10 ⁵	15.00	2.229x10 ⁵
1.0	13.750		13.75		13.75	
2.0	12.500		12.50		12.50	
3.0	11.250	1.115x10 ⁵	11.25	1.115x10 ⁵	11.25	1.115x10 ⁵
4.0	10.000		10.00		10.00	
5.0	8.750		8.75		8.75	
6.0	7.500	5.575x10 ⁵	7.50	5.576x10 ⁵	7.50	5.575x10 ⁵
7.0	6.250		6.25		6.25	
8.0	5.000		5.00		5.00	

Note:

1. Results in lowermost fracture
2. Head (h) is at node location (x). Velocity (V) is between node locations.
3. MAGNUM-2D velocity is that predicted for all four Gauss points in the (fracture) line element.

FIGURE 4.9.2. Problem FF-7: Hydraulic Head Distribution in the Uppermost Fracture

FIGURE 4.9.3. Problem FF-7: Hydraulic Head Distribution in the Lowermost Fracture

4.10 STEADY FLOW IN A FRACTURED POROUS MEDIA

4.10.1 Problem Designation

This problem is designated: Fluid Flow Problem FF-8.

4.10.2 Objective

The objective of this problem is to test computation of steady-state flow in a porous medium. Three porous materials are present along with several discrete fractures.

4.10.3 Problem Statement

The region to be modeled is shown in Figure 4.10.1. It geometrically is identical to the region modeled in problem FF-4 (Section 4.6), but with discrete fractures added. The region spans a total height of 41.1 meters and a width of 5 meters. The vertical boundaries at $x = -5$ m and $x = 0$ m are symmetry planes. The horizontal boundaries at $y = -5$ m and $y = 36.6$ m are fixed hydraulic head planes. The center of the 0.37-m diameter waste container is taken as the origin. The outer diameter of the waste container is the boundary of the simulation domain.

Concentrically surrounding the waste container is a 0.15-m thick layer of porous backfill material. Surrounding that is a 0.35-m thick region of blast-affected porous material. With fixed hydraulic heads at the upper and lower boundaries, steady-state flow distribution is to be computed.

Discrete fractures extend vertically through the solution domain as shown in the figure. Two of the lines are discontinuous and extend partially through the blast-affected zone as depicted by the detail inset. The x-y coordinate positions of the fractures near the waste canister are shown in parentheses.

4.10.4 Models Used

The MAGNUM-2D and FTRANS codes are to be used.

4.10.5 Assumptions

Assumptions made for the present problem are:

- Flow is isothermal.

- Vertical boundaries are symmetry planes; horizontal boundaries of fixed hydraulic head.
- Fractures are discrete, and embedded in a porous medium.

4.10.6 Input Specifications

The center of the waste container is taken as the origin. The solution domain is to be from 5 meters below the origin to 36.6 meters above the origin. Vertical symmetry planes are at $x = -5$ m and $x = 0.0$ m. The waste canister surface defines the boundary to the backfill region.

Properties of the porous materials and discrete fracture are listed in Table 4.10.1.

TABLE 4.10.1. Porous Material Properties

<u>Material</u>	<u>Material Number</u>	<u>Hydraulic Conductivity (m/yr)</u>	<u>Specific Storage (m^{-1})</u>	<u>Aperature (m)</u>
Basalt	1	3.15×10^{-6}	4.6×10^{-7}	-
Blast affected	2	3.15×10^0	2.0×10^{-3}	-
Backfill	3	3.15×10^{-3}	2.0×10^{-3}	-
Fractures		3.15×10^{-2}	0.0	2.0×10^{-3}

Hydraulic head at the lower boundary is to be fixed at 5.0 m and hydraulic head at the upper boundary is to be fixed at 2.5 m.

4.10.7 Output Specifications

Steady-state hydraulic head distributions and Darcy flow velocities in the porous materials and line fractures are to be compared.

4.10.8 Results and Discussion

The MAGNUM-2D code was run in the steady-state mode for this problem. A total of 286 elements (including fracture line elements) and 591 nodes were included in the model. Geometry, boundary conditions, and material properties

were as prescribed by the problem specifications. Figure 4.10.2 presents the finite element configuration for this problem. This is the element structure used in the FTRANS model and includes 696 elements and 765 nodes.

Additionally, 244 line elements were included to model the fractures. This element structure is equivalent to the MAGNUM-2D model in that four FTRANS elements are required to match one MAGNUM-2D element (see Figure 2.1.1).

Figure 4.10.3 presents a comparison of predicted hydraulic head. Plotted are distributions as a function of horizontal position at vertical positions of $y = -1.2$ m and $y = +1.2$ m. Agreement between the two codes is excellent. A good comparison of the tabulated data showed head values that differed by one digit in the third decimal place. Maximum relative error of data compared was less than 0.1 percent. Similarly, excellent agreement is evident in the vertical distribution of head shown in Figure 4.10.4. Results are plotted over the vertical distance domain for $x = 0.0$ and -5.0 m, the right and left vertical boundary planes, respectively. At the $x = -5.0$ m plane, results are within less than 0.1 percent over the whole range plotted.

Further comparison of the predicted head and flow in the fractures is presented in Figure 4.10.5. In this figure, hydraulic head and predicted Darcy velocity are compared in the lower region in each of the modeled discrete fractures. (See Figure 2.1.1 for a description of relative location of FTRANS and MAGNUM-2D node point, element boundaries, and predicted velocities.) Results of the FTRANS code are those enclosed in parentheses. In all cases, the agreement between FTRANS and MAGNUM-2D is excellent.

Figure 4.10.7 presents a comparison of hydraulic head and flow velocities in fractures 1 and 2 near their termination in material 2, the blast affected rock. Hydraulic head values are in good agreement, as are Darcy velocities. The only significant deviation in results is in the fractures in the line elements at their termination. MAGNUM-2D, using a four-point Gauss procedure, is predicting constant velocity over the whole length of a single line element. FTRANS, in using two-line elements for each equivalent MAGNUM line element, predicts differing velocities. This results directly from the modeling approach used in each code. The velocity MAGNUM-2D predicts is

essentially the average of the two FTRANS velocities, indicating that it computing correct flow rate in the fracture, on the average.

Several observations based on the process of producing these simulation results should be noted. The corrections that were put into MAGNUM-2D to create and fix Version 3.1 (used in this work) significantly improved prediction of Darcy velocity distribution at the four Gauss points in a line element. In summary, the corrections had to do with using a weighted averaging of head values when a mid-side node was not centered. Additionally, the FTRANS code results (those presented herein) were greatly improved for this problem when the correction described in Appendix B was enabled. For prior results, certain characteristics of the solution results were difficult to explain on a physical basis. Also, it was found that when the value of K_2 (hydraulic conductivity in material 2) was set to 3.15×10^{-5} m/yr, with no other changes to the input, FTRANS predicted results which were even more difficult to explain.

Results presented for this problem indicate, that relative to the comparison basis, MAGNUM-2D is predicting flow in this geometry and operational mode correctly.

Horizontal Distance (meters)

FIGURE 4.10.1. Problem FF-8: Solution Domain Schematic

FIGURE 4.10.2. Problem FF-8: Finite Element Structure

FIGURE 4.10.3. Problem FF-8: Horizontal Distribution of Hydraulic Head

FIGURE 4.10.4. Problem FF-8: Vertical Distribution of Hydraulic Head

FIGURE 4.10.5. Problem FF-8: Comparison of Head and Darcy Velocity Predicted in the Fractures

FIGURE 4.10.6. Problem FF-8: Comparison of Hydraulic Head and Flow Velocity in Fractures Terminating in Material 2

Figure 1.10.10. Graph showing the relationship between velocity, head and flow rate for a pump. The curves are for constant velocity, constant head and constant efficiency.

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APPENDIX A
FTRANS CODE MANIPULATIONS

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FTRANS CODE MANIPULATIONS

The version of the FTRANS code used as a benchmarking tool in this work is identified as QA CIN: 4D0--02C-02. It was obtained, upon request, from ONWI. The code was received on a magnetic computer tape. Included on the tape were the source deck (card images), six test problem input decks and the corresponding test problem output listings. These six problems are as described in the users manual for the code (INTERA, 1983).

Upon receipt of the computer tape, it was read on the PNL B-VAX-11/780. The source code and the six input decks were then transmitted via XNET to a CDC-7600 computer at Los Alamos National Laboratory (LANL) Central Computing Facility (CCF). The code was compiled and the six test problems executed. Outputs were then printed and compared to the listings provided on the original ONWI tape. All six problems were in agreement and the code was concluded to be working correctly.

Because two of the problems to be run (problems FF-4 and FF-8) required that the code be redimensioned, the FTRANS card deck file was transmitted (using the LASL CCF MAGIC file transfer utility) to a CRAY-1 computer. Prior to compilation, several changes were made to input and output formatting. This was done using a text editor and was for ease and improved convenience in interpreting output results. The code was then put into a HISTORIAN creation run format. This involved preceding each subroutine with a *DECK card.

Once the HISTORIAN creation run was complete and the code compiled, each of the six standard test problems were executed again to assure that the code was still computing correctly. Subsequently, a HISTORIAN correction run was performed to redimension appropriate arrays. After compilation, the test problems were run again. After being checked, the code was stored on the Common File System (CFS) for future use. The installed FTRANS code was used to produce results for all flow problems included in this report.

APPENDIX B

FTRANS CODING CHANGES FOR FRACTURE FLOW

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FTRANS CODING CHANGES FOR FRACTURE FLOW

In running test problem FF-7, it was determined^(a) that FTRANS is coded to treat only a single aperture width along the length of the fracture when the code is operating in the flow mode. This is not an error in the code, per se, but is a limitation not pointed out or discernable in the users manual. For cases where aperture width were constant along the total length of a fracture, no problem occurs. For cases where aperture width in a model varied along the fracture length, incorrect flow velocities would be predicted in the fracture without any direct indication to the user. This deficiency is correctable with a minor modification in the subroutine EBJNT1. The correction is as follows:

Replace

BW = 1

Line Identification

J 27 (or EBJNT1.27)

With

BW = BWLJ(IEL)

IF(BW.EQ.0.0)BW=1.

This coding change was made to run Problem FF-7 to produce results reported in Section 4.9 of this report. Testing of the correction is also discussed in that section. Problem FF-8 was also run with this corrected code.

Because the FTRANS code was obtained from ONWI for use in this work, they were informed of the above via written correspondence to Leslie Scott, a code custodian.

^(a) Confirmed by Peter S. Huyakorn, GEOTRANS, Inc., personal communication.

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