Verification and Benchmarking of Porflo: An Equivalent Porous Continuum Code for Repository Scale Analysis

**L. L. Eyler
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November 1984

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

**Pacific Northwest Laboratory
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VERIFICATION AND BENCHMARKING OF PORFLO:
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SUMMARY

The objective of this work was to perform an assessment of prediction capabilities and features of the PORFLO code in relation to its intended use in the Basalt Waste Isolation Project. This objective was to be accomplished through a code verification and benchmarking task. Results were to be documented which either support correctness of prediction capabilities or identify areas of intended application in which the code exhibits weaknesses.

A test problem set consisting of 10 problems was developed. Results of PORFLO simulations of these problems were provided for use in this work. The 10 problems were designed to test the three basic computational capabilities or categories of the code. Broken down by physical process, these are heat transfer, fluid flow, and radionuclide transport. Two verification problems were included within each of these categories. They were problems designed to test basic features of PORFLO for which analytical solutions are available for use as a known comparison basis. Hence they are referred to as "Verification" problems.

Of the remaining four problems, one repository scale problem representative of intended PORFLO use within BWIP was included in each of the three basic capabilities categories. The remaining problem was a case specifically designed to test features of decay and retardation in radionuclide transport. These four problems are referred to as "Benchmarking" problems, because results computed with an additional computer code were used as a basis for comparison.

Each of the problems tested and results comparisons are presented in Section 4.0 of this report. A summary of conclusions, based on results, follows.

Operational modes and basic features of the PORFLO code which were tested and yielded acceptable results are:

- In the heat-transfer-only mode, PORFLO predicts accurate steady-state temperatures in cylindrical coordinates with constant heat generation (Problem HT-1, Section 4.1).

- In the heat-transfer-only mode, one-dimensional energy equation solution is acceptable in constant unidirectional groundwater flow. Both horizontal and vertical coordinate directions were tested independently against analytical solutions (Problem HT-2, Section 4.2).
- In the heat-transfer-only mode, repository-scale heat conduction simulation is acceptable, based on a benchmarking comparison. Transient repository heat generation was included in this two-dimensional Cartesian geometry. Nine hydrogeologic layers were modeled with differing thermal properties in each layer (Problem HT-3, Section 4.3).
- In the fluid-flow-only mode, both transient and steady-state capabilities were acceptable in representative two-dimensional regional groundwater flow problems (Problem FF-1, Section 4.4, and Problem FF-2, Section 4.5).
- In a repository scale coupled flow and heat transfer benchmarking problem, basic features of comparable PORFLO and SWENT code models are in very good agreement. Certain discrepancies occur at early times in a simulated 50,000 yr transient. Basic physical model differences in the two codes were postulated to account for the observed deviations. One difference is in treatment of coefficient of thermal expansion of water. SWENT assumes this parameter to be constant while PORFLO incorporates water density as a property which is a nonlinear function of temperature. This difference in physical modeling is shown to be significant in the predictions of buoyancy induced flow. (Problem FF-3, Section 4.6 and Appendix B).
- In the radionuclide-transport-only mode, results were found to be acceptable in a simpler unidirectional transport problem in which constant flow occurs. Results were found to be cell Peclet number dependent, however, which has accuracy implications for larger, more coarsely noded problems (Problem MT-1, Section 4.7).
- In a two-dimensional dispersive flow in which longitudinal and transverse dispersion lengths are unequal, predicted transient radionuclide distributions were in good agreement with an analytical solution (Problem MT-2, Section 4.8).

- In the radionuclide-transport-only mode, features of mass (source) injection, radionuclide decay, and retardation were tested in a constant, unidirectional mode. In comparison to SWENT code predictions, PORFLO results are acceptably accurate, (Problem MT-3, Section 4.9).
- Radionuclide transport results in a repository scale coupled flow and heat transfer problem were inconclusive. Reasonably good agreement occurs between PORFLO and SWENT predictions for transient radionuclide concentrations during the source release period. Long after the end of release, deviation between results. PORFLO results seem more reasonable than the SWENT results for this problem (Problem MT-4 Section 4.10); however no firm conclusion can be drawn without a more detailed investigation of this problem. A limitation caused by the precision of the computer which PORFLO simulations were run on was encountered when running MT-4 with different input parameters. When this limitation is inadvertently violated, PORFLO predicts nonphysical negative concentrations (Appendix B).

During the course of this work, two problems were encountered with PORFLO which have subsequently been corrected. These were a time-stepping logic problem and a multiplicative term on radionuclide decay. This latter problem directly affected results presented in Section 4.9 (Problem MT-3) of this report. Results of Problems MT-1, MT-2, and MT-4 were rechecked after the error was fixed. Results were not affected by the error because decay was not included in these problems.

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The authors would like to acknowledge the report review efforts of Budhi Sagar of Rockwell/BWIP. He is currently writing a report detailing the theoretical basis for PORFLO governing equations and solution procedure, and identified several inconsistencies in this report and in the PORFLO users manual in reference to PORFLO solution methods, options, and capabilities.

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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 analysis, it is necessary to document their computational features, capabilities, and accuracy. This process comprises verification and benchmarking. The Nuclear Regulatory Commission recently 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 procedures 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 5.6 of the PORFLO computer code (Kline, et al. 1983). 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 PORFLO code, and Pacific Northwest Laboratory (PNL) - personnel performing the results comparison and assessment conclusions. PNL had the responsibility of developing problem statements upon which PORFLO simulations were to be based. Rockwell/BWIP and BCSR personnel provided input into and review of the problem statements during their development. This was done to ensure that the problems were representative of intended PORFLO applications and that they were designed to sufficiently test pertinent features and capabilities of the code. The problem statement review also insured 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 PORFLO. 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 in performing the results comparisons.

Six verification problems and four benchmarking problems were included in this work. For verification, problems were selected which exercised the code's basic capabilities of fluid flow, heat transfer, and radionuclide transport. 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 and, although they are simple in design, parameters are chosen to be representative of intended PORFLO application. Of the four benchmarking problems, one is a decaying radionuclide transport problem and three are repository-scale problems. The TEMPEST computer code (Trent, et al. 1983) was chosen as a benchmarking code for the repository-scale problem that involved heat conduction only. The SWENT code (INTERA, 1983) was chosen for the two problems in which coupled fluid flow, heat, and radionuclide transfer occur. Both of these codes are well-documented, the former for its thermal analysis capabilities, and the latter for its groundwater flow and radionuclide transport capabilities. Both codes are also publicly available: TEMPEST from the National Energy Software Center and SWENT from the Office of Nuclear Waste Isolation (ONWI).

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 Quality Assurance (Q/A) requirements of this work. It contains, among other things, a cross-reference record of computer files and computer output listings which contain final results. These output listings are to be maintained for future reference to the results used in this work.

Section 4.0 includes the 10 problem statements upon which the simulations were based and from which comparisons of results were generated. Discussions of results are also presented as are notation of agreement or disagreement of results. Where deviations occur, a probable cause is given, if it is available. Appendix A describes the various steps that were taken in bringing up the SWENT code on the Los Alamos computer system. Special emphasis is given to the Q/A procedures that ensure traceability of the code used. Appendix B describes the chronology of two benchmark problems that revealed discrepancies between PORFLO and SWENT predictions and uncovered an undocumented limitation of the PORFLO code.

2.0 COMPUTER CODE DESCRIPTIONS

Three referenceable computer codes were used in this work. The PORFLO code (Kline, et al. 1983) was run by BCSR personnel. TEMPEST (Trent, et al. 1983) was used in one heat transfer benchmarking problem. SWENT (INTERA, 1983) was used in three benchmarking problems. The latter two codes were run as part of this work. This section contains a description of these codes.

2.1 PORFLO CODE

The PORFLO code is a two-dimensional finite-difference code applicable to an equivalent porous continuum. This computer code is capable of simulating the coupled processes of heat transfer, groundwater flow, and transport of a dissolved radionuclide in a layered hydrogeologic media. The conceptual modeling approach is based on representing the geologic system in terms of a vertical or horizontal cross section. Three-dimensional systems with axial symmetry can also be modeled with PORFLO. Analytical and Computational Research, Inc., Los Angeles, California, developed the original version of PORFLO. BCSR has since developed a double precision version to be run on the BWIP PRIME 750 computer. The version used for simulation testing in this work is Version 5.6.

The PORFLO computer code is designed to simulate time-dependent or asymptotically steady-state processes consisting of coupled groundwater flow, heat transfer, and radionuclide transport. The code is applicable to problems in two dimensions over a rectangular or axially-symmetric cylindrical domain. The mathematical model is based on the physical laws of mass, momentum, and energy conservation. A user's manual is available (Kline et al. 1983). A report detailing theoretical basis and solution procedures is in preparation.

For completeness, the governing equations are also given here. The governing groundwater flow balance equation written in indicial notation for Cartesian coordinates is

$$S_s \frac{\partial h}{\partial t} = \frac{\partial}{\partial x_i} \left(k_{ij} \frac{\partial h}{\partial x_j} + \delta_b \delta_{ij} \right) + \gamma \frac{\partial T}{\partial t} + m_r \quad (2.1.1)$$

where

S_s = specific storage of the porous rock matrix

h = hydraulic head at a reference density

t = the time coordinate

K_{ij} = hydraulic conductivity

x_i = space coordinate

δ_b = density disparity

δ_{ij} = the Kronecker delta

γ = thermal coupling coefficient

T = temperature

m_r = volumetric source term.

Furthermore, the thermal coupling coefficient is given by

$$\gamma = \phi \beta \quad (2.1.2)$$

where

ϕ = effective porosity

β = bulk modulus of fluid $\left(- \frac{1}{\rho_f} \frac{\partial \rho_f}{\partial T} \right)$.

The governing thermal energy balance equation also written for a Cartesian coordinate system in indicial notation is

$$S_t \frac{\partial T}{\partial t} + \rho_f c_f \frac{\partial}{\partial x_i} (q_i T) = \frac{\partial}{\partial x_i} \left(D_t \frac{\partial T}{\partial x_i} \right) + Q \quad (2.1.3)$$

where

- S_t = heat capacity of the fluid-rock system
- ρ_f = fluid density
- c_f = specific heat of fluid
- q_i = component of the Darcy velocity vector
- D_t = effective thermal conductivity coefficient
- Q = volumetric heat generation rate.

Moreover,

$$S_t = \phi \rho_f c_f + (1 - \phi) \rho_s c_s \quad (2.1.4)$$

and

$$D_t = \phi D_f + (1 - \phi) D_s \quad (2.1.5)$$

where

- ρ_s = density of rock
- c_s = specific heat of rock
- D_f = thermal conductivity of fluid
- D_s = thermal conductivity of rock.

Spatial components of D_t are further adjusted for dispersion.

The governing mass balance equation, also known as the concentration equation, is written for a single component as

$$R_d \phi \frac{\partial C}{\partial t} + \frac{\partial}{\partial x_i} (q_i C) = \frac{\partial}{\partial x_i} (D_{mi} \phi \frac{\partial C}{\partial x_i}) - \lambda R_d \phi C + \dot{m} \quad (2.1.6)$$

where

R_d = retardation factor

C = concentration of radionuclide mass

D_{mi} = hydrodynamic dispersion coefficient

λ = radioactive decay constant

$\dot{m}$ = mass source term.

The retardation factor and dispersion coefficients are computed according to the relations

$$R_d = 1 + K_d \rho_s (1 - \phi)/\phi \quad (2.1.7)$$

$$D_{mx} = D + (\alpha_L U^2 + \alpha_T V^2)/(\bar{q}\phi) \quad (2.1.8)$$

$$D_{my} = D + (\alpha_T U^2 + \alpha_L V^2)/(\bar{q}\phi) \quad (2.1.9)$$

while the decay constant is given by

$$\lambda = \frac{\ln(2)}{T_{1/2}}. \quad (2.1.10)$$

Terms in the above expressions are:

k_d = sorption or distribution coefficient

D = molecular diffusion coefficient

α_L = longitudinal dispersivity

α_T = transverse dispersivity

U = horizontal component of Darcy velocity

V = vertical component of Darcy velocity

$\bar{q} = (U^2 + V^2)^{1/2}$ is the groundwater speed

$T_{1/2}$ = half-life.

Equations 2.1.1, 2.1.3, and 2.1.6 are similar in form and, in fact, may be regarded as special cases of a general transport equation:^(a)

$$\tau \frac{\partial F}{\partial t} + \mu \frac{\partial}{\partial x_i} (q_i F) - \frac{\partial}{\partial x_i} \left(\Gamma \frac{\partial F}{\partial x_i} \right) = S_F - S_m F \quad (2.1.11)$$

where

τ, μ = generalized coefficients

F = transport variable (h , T , or C)

Γ = generalized transport coefficient

S_F = net source rate

S_m = net loss rate.

The PORFLO code is programmed to solve this general equation with the coefficients defined according to Equations 2.1.1, 2.1.3, and 2.1.6. The numerical solution is obtained using a nodal point integration (finite-volume) method.

The PORFLO code can accommodate two types of coordinate systems. A grid may be defined over a rectangular domain using Cartesian coordinates or an axially symmetric cylindrical domain using radial coordinates. Details of solution procedure, boundary conditions, operational modes, accuracy criteria, and code usage instructions are contained in the users' manual.

2.2 SWENT CODE

The SWENT computer code (INTERA, 1983) is a three-dimensional finite-difference computer code for simulation of fluid, energy, solute, and radionuclide transport. It is a multidimensional transient code capable of modeling radionuclides in straight or branch chains in a heterogeneous geologic medium. Fluid flow, energy, and inert component are coupled through properties of viscosity and density. Porosity is treated as a function of pressure.

The code has numerous application capabilities. The user may optionally specify the spatial numerical approximation and also solution scheme (direct or iterative). Numerical differencing approximations available include centered in space (CIS), centered in time (CIT), backward in space (BIS), and backward in time (BIT). Individual transport processes or coupled processes are available including a steady-state flow with transient radionuclide transport option. Boundary condition options are also available. Most of these options are also available in PORFLD.

The SWENT code is documented and validation simulation results have been reported (INTERA, 1983). By solving a pressure equation rather than a hydraulic head equation to determine fluid flow, SWENT takes a fundamentally different approach than PORFLO. The two are generally comparable in terms of the assumptions made in each code. Because the code is documented, the details of the governing equations, the numerical approximations, and the solution techniques used in SWENT are not included herein.

SWENT was chosen as a benchmarking tool because its documentation indicated that capabilities and features were similar to those available in PORFLD. Certain differences between the two codes do exist; therefore, in the benchmark problems performed in this work, attempts were made to make test problems suitable for both PORFLO and SWENT simulation. Important differences between the codes and their impact on particular problems are included in discussions in Appendix B of this report. The version of SWENT used was QA CIN 400--OIC-D2 distributed by ONWI.

2.3 TEMPEST CODE

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 the repository scale heat conduction-only problem. TEMPEST is well-documented and validation results have been reported (Eyler, et al., 1983). Although very general in its hydrodynamic capabilities, the heat-conduction-only mode of TEMPEST was the only capability used in this work.

TEMPEST is a user oriented code which solves the energy equation using an implicit 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 and no flow occurs. 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. Validation results are reported by Eyler, et al. (1983). The version of the TEMPEST code used is Version L, Mod 2. It is publicly available from the National Energy Software Center.

3.0 TEST PLAN APPROACH AND TEST PROBLEM SET

PORFLO is used to simulate ten test problems in a problem set designed to evaluate particular capabilities of the code. The problems include features of heat transfer, fluid flow, coupled heat and fluid flow, and radionuclide transport. Six problems are relatively simple ones, but they are representative of code applications for which analytical solutions are derivable. Four problems are benchmarking problems (too complicated for an analytical solution) in which results of PORFLO are to be compared to other computer code results. Of these, three problems are concerned with a representative repository-scale solution domain and use representative parameters of a layered basalt hydrogeology. Although representative, these problems are not intended to be site 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 capabilities of the PORFLO 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 PORFLO prediction results is to be based on defined 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, N. Kline of BCSR, and L. Eyler and M. Budden of PNL. Others at PNL who have experience in hydrodynamic code validation analyses were also consulted during the work.

The plan under which this work was to be 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 SWENT computer code was chosen as a benchmarking code for repository scale problems in which flow, heat, and radionuclide transport occur simultaneously.
- BCSR personnel were to perform the PORFLO simulations for each problem and provide PNL with computer output for results comparison.
- PNL personnel were to generate the analytical solution results and perform 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 PORFLO code. A list of references for ten suggested

problems were provided by Rockwell/BWIP. Because of their familiarity with the PORFLO code, they were best able to suggest problems within the code's capabilities which would test both basic and intended application features.

The problems included three heat-transfer-only problems, two fluid-flow-only problems, one coupled fluid flow and heat transfer problem on a repository scale, three problems with radionuclide-transport-only, and one radionuclide transport problem in a coupled heat and fluid flow on a repository scale. 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, FF for Fluid Flow, and MT for radionuclide Mass Transfer. Verification problems were selected that were well documented and accepted in technical literature. Benchmarking problems were chosen to exercise PORFLO 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 heat-conduction-only problem designed to test steady-state energy equation solution in cylindrical coordinates with uniform heat generation. An analytical solution is derivable for results comparison.

HT-2: Heat Transfer in Unidirectional Flow (Section 4.2). This problem is a heat-transfer-only problem in a constant unidirectional groundwater flow in a porous medium. It is designed to test the horizontal and vertical transient energy equation solution subject to a step-change boundary condition. An analytical solution is derivable for results comparison.

HT-3: Repository Scale Transient Heat Conduction (Section 4.3). This problem is a transient heat-conduction-only problem in a repository scale solution domain. Repository volumes are modeled along with nine hydrogeologic layers. Realistic repository heat generation rates, as a function of time, are to be specified according to an assumed waste material heat loading. The PORFLO results are to be benchmarked against TEMPEST.

FF-1: Steady Flow in a Regional Groundwater System (Section 4.4). 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 results comparison.

FF-2: Transient Flow in a Rectangular Areal Domain (Section 4.5). 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-3: Repository Scale Coupled Flow and Heat Transfer (Section 4.6). This problem is designed to test features of coupled fluid flow and heat transfer in a repository scale solution domain over a simulated time span of 50,000 yr. Two separate heat-generating repositories are modeled with transient-decreasing heat generation rates. Nine composite material layers are modeled and representative hydrogeologic properties are used. Results of a SWENT code simulation are to be used for a benchmarking comparison.

MT-1: Radionuclide Transport in a Unidirectional Flow Field (Section 4.7). This problem is similar to problem HT-2 except that a mass transport-only mode is used. Two solution domains are used: 1,000 m and 10,000 m long. Results of an analytical solution are used for comparison.

MT-2: Two-Dimensional Radionuclide Transport from a Modeled Line Source (Section 4.8). This problem simulates radionuclide transport in a two-dimensional vertical plane in which unequal longitudinal and transverse dispersion exists. Results are compared to an analytical solution.

MT-3: Radionuclide Transport with Decay and Retardation (Section 4.9). This problem simulates a decaying radionuclide transport with retardation in a constant, unidirectional, groundwater flow. Results are compared to an equivalent SWENT code simulation.

MT-4: Radionuclide Transport on a Repository Scale with Coupled Fluid Flow and Heat Transfer (Section 4.10). This problem is the same as FF-3 with the added feature of a transient release of a radionuclide in the repositories over a

span in time from 1050 to 9200 yr. Results are compared to an equivalent SWENT code simulation.

The above ten problems are designed to test the salient features of PORFLO in a logical progression of basic features, complexity, and application. Fluid flow, heat, and mass transport are included in the simpler but representative problems. The three repository scale simulations are problems in which representative hydrogeologic and flow properties consistent with proposed applications 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 PORFLO simulations, generation of analytical results, and benchmarking with an additional computer code.

Originally, for each problem, parameters representative of PORFLO application were specified. It was found, however, that for some problems it was necessary to redefine certain parameters. This was necessary for several reasons. In certain cases, analytical solution results could not be obtained directly with the use of computer mathematics library routines, because specified parameters in the problems resulted in function arguments being out of range. In these cases, the problem statement parameters were modified to accommodate the analytical solution and still be representative for PORFLO simulation. The analytical solutions could probably have been evaluated with the use of an asymptotic expression, but that approach would not have been a significant enhancement to the objectives of this work. It would have also been more difficult to ensure that the analytical solutions were being correctly determined. Thus changing parameters was a logical option which did not detract from this work's objectives but did allow timely completion.

For the benchmarking cases, it was also necessary to modify certain input specifications. This was done for reasons of model simulation compatibility

between the PORFLO and SWENT codes in problems FF-3 and MT-4. The two codes have similar, but not identical, capabilities, which is one reason SWENT was chosen as a benchmarking code. There are two features to the SWENT code, however, which precluded performing simulation of Problem MT-4 as originally specified. One is that SWENT was found not have the capability to treat longitudinal and transverse dispersion lengths from input [α_L and α_T], respectively] that are unequal in different rock layers. While it was determined that, internally, the code is programmed to handle differing values in different rock types, there is no mechanism described in the code's input manual to prescribe them. It was not within the objectives of the present work to perform any code modifications. Thus, it was decided, in consultation with Rockwell/BWIP personnel, that the problem statement would be modified to specify only one value of α_L and one value of α_T throughout all rock types in the layered media.

The other significant modification had to do also with problems FF-3 and MT-4. PORFLO used a specific storage concept in its modeled pressure equation. SWENT, on the other hand, uses water compressibility and rock compressibility. Because the specific storage is defined in terms of these two parameters, equivalent modeling can be accomplished. However, as with α_L and α_T , only one value of rock compressibility may be input to SWENT. Thus, again, the problem statements were modified to assume only one value of specific storage for all rock types.

The effect of these two problem modifications on the benchmarking problems FF-3 and MT-4 was minimal with respect to the objectives of this work. While they essentially simplified the problems, they did not detract from the goals of the benchmarking effort.

3.5 ACCEPTABILITY

The intention of this work is to provide a documented basis upon which conclusions can be drawn as to acceptability of PORFLO for simulation analysis of proposed waste repositories 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, the term verification is used to refer to code versus analytical solution comparison, while benchmarking is used in reference to code-to-code comparisons. In most real-world problems, analytical solutions are unavailable, making this type of verification impossible; hence, benchmarking is of significant value.

The problem set proposed in this work consists of ten problems. Six of these are simple, yet representative, and intended to test particular code features or main capabilities. For PORFLO, major capabilities can be delineated as fluid flow, heat transport, and mass (radionuclide) transport as they apply in an equivalent porous continuum. Among other features, PORFLO includes source terms, decay, retardation, variable material and hydrogeologic properties, and coordinate system.

For the six verification problems, parameters in the governing equations which PORFLO 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". (Having a mathematical expression for an analytical solution, of course, is one thing; generating numbers to which code predictions are to be compared is oftentimes a problem in itself.) 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 as 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 and the degree of noding resolution. With sufficient explanation, 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 PORFLO'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 PORFLO and results which were obtained for comparison. BCSR personnel ran PORFLO simulations for this work with Version 5.6 on the BWIP PRIME 750 computer. 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 SWENT were computed on the CRAY-1S machine. Appendix A details the source of and the steps taken to put the SWENT code up on the CRAY and ensure it was computing correctly. The version of the SWENT code used was 400--01C-02. The TEMPEST code, as discussed in Section 2.3, was resident on the CDC-7600 computer at LANL. TEMPEST Version L, Mod 2, which is publicly 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 and date of final printed results.

At the completion of the project, input, output, and code source listings were transmitted to Rockwell/BWIP. Paper, microfiche, and computer magnetic tape copies were sent for future use and for record keeping requirements.

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.

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 PORFLO 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 PORFLO. 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.

4.1.4 Models Used

PORFLO is used to numerically model the heat generating region. Only the thermal energy equation in PORFLO is used. The analytical solution was 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

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

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

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

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

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

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

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

The boundary conditions become

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

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

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

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

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

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

PORFLO calculations are to be performed for two node spacings 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.

4.1.9 Simulation Results and Discussion

The PORFLO code was used to simulate the stated problem. A 22 by 22 noding was set up in cylindrical coordinates using constant distance between nodes with $\Delta R_1 = 10 \text{ m}$ and $\Delta Z_1 = 10 \text{ m}$. This node spacing was taken as the reference case 1 listed in output specifications.

The analytical solution, (Equation 4.1.8), was computed using computer mathematics routines for the modified Bessel function, I_0 . Results were obtained on a CDC-7600 computer. Hand calculation checking of the coded analytical solution confirmed its correctness.

Results of PORFLO and the analytical solution are compared in Figures 4.1.2 and 4.1.3 for the predicted horizontal distribution at $z = 100$ m, and the vertical distribution at $r = 0$, respectively. Agreement of PORFLO results with the analytical solution and the TEMPEST results is excellent. Maximum centerline temperatures listed in Table 4.1.1 agree within 1 percent. The coarser noding case 2 results are also in very good agreement. Other results comparisons in the output specifications were made. Results were found to be symmetric about the $z = 100$ m plane and, like those shown in Figures 4.1.2 and 4.1.3, were in good agreement.

Based on these results, the PORFLO code is computing correctly and accurately in this geometry.

TABLE 4.1.1. Steady-State (Maximum) Centerline Temperatures

	<u>Analytical</u>	<u>PORFLO⁽¹⁾ (22 by 22)</u>	<u>PORFLO⁽¹⁾ (12 by 12)</u>	<u>TEMPEST (20 by 20)</u>
T =	255.95°C	256°C	255°C	256.09°C

(1) PORFLO output in D10.2 format results in only three digits

FIGURE 4.1.1. Problem HT-1: Solution Domain Schematic

HEAT TRANSFER PROBLEM HT1

PLOT FILE=/BWIP/HT1/PLOTS TPLTTVSAZ100 - - PROBLEM HT1: T VS R AT Z=100 METERS.

FIGURE 4.1.2. Problem HT-1: Radial Temperature Distribution Comparison at Vertical Midplane (Z = 100 m)

FIGURE 4.1.3. Problem HT-1: Vertical Temperature Distribution Comparison at Centerline ($R = 0$ m)

4.2 TRANSIENT-ADVECTED THERMAL ENERGY IN UNIDIRECTIONAL FLOW

4.2.1 Problem Designation

This problem is designated: Heat Transfer Problem HT-2.

4.2.2 Objective

The objective of this problem is to test the transient-advected thermal energy capabilities of the PORFLO code. Cartesian x- and y-coordinate flow directions are to be tested independently and predictions compared to analytical solution of a modeled, constant, unidirectional groundwater flow in a porous medium.

4.2.3 Problem Statement

Unidirectional groundwater flow is occurring in a porous media. At a given location, an array of heat generating material is put in place. The transient thermal response of constant flow groundwater and porous media is to be computed to a time of 2000 yr and subject to a step-change in temperature boundary condition.

This problem is similar to that of Coats and Smith (1964) and is one which has been solved as a validation problem for the SWIFT code (Ward et al. 1983). The analytical solution is also presented by Carslaw and Jaeger (1959). A schematic of the present problem is presented in Figure 4.2.1.

4.2.4 Models Used

The heat-transfer-only mode of the PORFLO code is to be used with porous media parameters specified to reduce the problem to one that is analytically solvable. The transient analytical solution is obtained using a computer mathematics library routine for the complementary error function which occurs in the analytical solution. Parameters are chosen so as not to exceed function argument limitations on the computer.

4.2.5 Analytical Solution

The analytical solution to this problem can be obtained subject to several assumptions. The equation to be solved is

$$\frac{\partial T}{\partial t} + v \frac{\partial T}{\partial x} = D \frac{\partial^2 T}{\partial x^2} \quad (4.2.1)$$

over the region

$$0 < x < \infty. \quad (4.2.2)$$

The thermal energy equation solved by PORFLO (Equation 2.1.3) may be reduced to that of Equation (4.2.1) by defining an interstitial velocity as

$$v = \rho_f C_f U / S_t \quad (4.2.3)$$

where the heat capacity of the fluid-rock system, S_t , is

$$S_t = \phi \rho_f C_f + (1 - \phi) \rho_s C_s. \quad (4.2.4)$$

The diffusivity contains both dispersion and conduction and is defined as

$$D = \frac{\alpha_L U \rho_f C_f + D_t}{S_t}. \quad (4.2.5)$$

For this problem the molecular thermal conductivity of the porous medium is

$$D_t = \phi D_f + (1 - \phi) D_s. \quad (4.2.6)$$

Subject to the initial conditions

$$\text{at } t = 0, T = T_0 \text{ for all } x \quad (4.2.7)$$

and boundary conditions

$$\begin{aligned} \text{at } x = 0, T &= T_1 \text{ for all } t, \text{ and} \\ \text{at } x = \infty, T &= T_0 \text{ for all } t \end{aligned} \quad (4.2.8)$$

the solution to Equation (4.2.1) is

$$T = T_0 + \left(\frac{T_1 - T_0}{2} \right) \left[\operatorname{erfc} \left(\frac{x-vt}{2\sqrt{Dt}} \right) + \exp \left(\frac{vx}{D} \right) \operatorname{erfc} \left(\frac{x+vt}{2\sqrt{Dt}} \right) \right]. \quad (4.2.9)$$

4.2.6 Assumptions

Assumptions made in the present problem include the following:

- The problem domain is semi-infinite, with the physical heat source being small relative to the domain, and it can be treated as a step change in temperature at the boundary of the solution domain.
- The analytical problem domain boundary at ($x=\infty$) is modeled at a finite distance in the PORFLO solution domain. Results are to be assumed valid until a nonnegligible temperature rise occurs at 0.9L of the solution domain.
- Material properties are constant.
- Flow and heat transport are in one direction which is consistent with the assumption that buoyancy is negligible and there is no cross flow heat transfer.

4.2.7 Input Specifications

The parameters required for PORFLO solution are:

Fluid density	$\rho_f = 1000 \text{ kg/m}^3$
Fluid specific heat	$c_f = 4185 \text{ J/kg-}^\circ\text{C}$
Fluid conductivity	$k_f = 2.05 \times 10^7 \text{ J/m-yr-}^\circ\text{C}$
Rock density	$\rho_s = 2780 \text{ kg/m}^3$
Rock specific heat	$c_s = 850 \text{ J/kg-}^\circ\text{C}$
Rock conductivity	$k_s = 5 \times 10^7 \text{ J/m-yr-}^\circ\text{C}$
Porosity	$\phi = 0.001$
Longitudinal dispersion length	$\alpha_L = 2.0 \text{ m}$
Darcy velocity	$U = 0.03 \text{ m/yr}$

For these, computed values required for the analytical solution are

Advection velocity	$v = 0.0511 \text{ m/yr}$
Thermal dispersivity	$D = 21.134 \text{ m}^2/\text{yr}$

The solution domain for PORFLO is a one-dimensional region defined by

Length	$L = 1000 \text{ m}$
Initial temperature	$T_0 = 10^\circ\text{C}$
Boundary temperature at $x = 0$	$T_1 = 20^\circ\text{C}$
Boundary temperature at $x = L$	$T_L = 10^\circ\text{C}$

4.2.8 Output Specifications

The transient temperature is to be computed as a function of time. Results are to be compared at 500, 1000, and 2000 yr as a function of position in a 1000-m solution domain. Separate computations with PORFLO are to be done in the x (horizontal) and y (vertical) coordinate direction to ensure correct similitude in each. Because PORFLO must model the semi-infinite domain at a finite distance, computed results are only to be compared to the analytical solution to 0.9L or 900 m.

4.2.9 Simulation Results and Discussion

PORFLO was used to simulate the problem as stated above. A total of 41 nodes were used in the direction of advection. Four nodes were used in the transverse coordinate direction with zero flux boundary conditions to simulate the infinite extent of the region in cross stream direction. Results were computed with equal-spaced nodes ($\Delta x = 25$ m) over the 1000-m simulation distance. A fixed temperature boundary condition was used at a distance of 1000 m.

Results were computed using central differencing, and the code was operated in the heat-transfer-only mode. An initial time step of 5 yr was used with a time-step-growth factor of 1.1. The maximum time step to be allowed was 20 yr.

Two cases were computed with PORFLO. One used the horizontal coordinate, x , as the advection direction. The other used the upward vertical coordinate, y , as the advection direction. The transient temperature results of both cases were identical. This agreement substantiates that the basic thermal energy equation is being solved correctly in both the x and y coordinate directions.

The analytical solution for this problem was coded. Mathematics library routines were used to compute the complementary error function which occurs in the solution (Equation 4.2.7). The correctness of the coded solution was confirmed by computing the SWIFT verification case (Ward et al. 1983). Results for their parameters were reproduced and the analytical solution coding for the present problem was concluded to be correct.

Results are compared in Figure 4.2.2 for times of 500, 1000, and 2000 yr. Tabulated results are presented in Table 4.2.1 for selected points for the horizontal case. Agreement between PORFLO and the analytical solution is excellent. The PORFLO solution algorithm for heat transfer-only is acceptable based on these results in both the x - and y -coordinate direction. Within the three digits PORFLO outputs, temperatures agree with the analytical results to less than a 0.5 percent deviation.

TABLE 4.2.1. Problem HT-2: Transient Temperature Comparison

x(m)	Time 500 yr		Time 1000 yr		Time 2000 yr	
	$T_p^a(^{\circ}\text{C})$	$T_A^b(^{\circ}\text{C})$	$T_p(^{\circ}\text{C})$	$T_A(^{\circ}\text{C})$	$T_p(^{\circ}\text{C})$	$T_A(^{\circ}\text{C})$
0	20.0	20.00	20.0	20.00	20.0	20.00
50	17.8	17.74	18.6	18.54	19.1	19.10
100	15.5	15.51	17.0	17.00	18.2	18.13
150	13.6	13.59	15.5	15.51	17.2	17.12
200	12.2	12.13	14.2	14.14	16.2	16.10
250	11.2	11.14	13.0	12.98	15.2	15.12
300	10.6	10.55	12.1	12.03	14.3	14.20
350	10.3	10.24	11.4	11.33	13.4	13.37
400	10.1	10.10	10.8	10.81	12.7	12.63
500	10.0	10.01	10.3	10.27	11.5	11.50
600	10.0	10.00	10.1	10.07	10.8	10.76

(a) T_p : PORFLO temperatures; computer output to D10.2 format yields only three digits

(b) T_A : Analytical solution; reported to four digits

FIGURE 4.2.1. Problem HT-2: Solution Domain Schematic

PLOT FILE = /BWIP/HT2/PLOTS PLTHT2.500, PLTHT2.1000, AND PLTHT2.2000
 PROBLEM HT2. T VS X AT TIME = 500, 1000, AND 2000 YEARS.

FIGURE 4.2.2. Problem HT-2: Comparison of Temperature Distribution at 500, 1,000, and 2,000 yr

4.3 TRANSIENT HEAT CONDUCTION IN THE VICINITY OF A REPOSITORY

4.3.1 Problem Designation

This problem is designated: Heat Transfer Problem HT-3.

4.3.2 Objective

The objective of this problem is to determine transient temperature distribution in the vicinity of two repository panels in a repository-scale simulation domain. A two-dimensional vertical slice through the repositories is to be modeled. Aspects of the code to be tested include two-dimensional Cartesian coordinates, heat-conduction-only mode, zonal heat generation, and zonal-dependent material properties. The solution domain is a region representative of anticipated PORFLO application in the BWIP program.

4.3.3 Problem Statement

Two repository panels which contain a heat-generating material are located on the same horizontal level in a layered hydrogeologic porous media. They are separated by a distance of 1063 m. The heat generation is decreasing with time from an initial value consistent with an assumed panel heat load of 17 watts/m^2 . Nine hydrogeologic layers are to be considered in the region from -842 to -1575 m below the nominal surface. The porous rock in each layer has different thermal properties, but they are constant in each layer. Water which fills the rock pores is to be treated as stationary (e.g. no groundwater flow for this conduction problem).

The initial vertical temperature gradient in the solution domain is -0.04°C/m , with the temperature of 75°C at a depth of -1575 m being the reference. The vertical boundaries are to be maintained at this gradient throughout the simulation. Horizontal boundaries are to be held constant at the initial temperature at the boundary depths.

The geometric configuration of the region of interest is presented in Figure 4.3.1. The solution domain is the same as used in subsequently more complex benchmarking problems FF-3 and MT-4, which are to include fluid flow coupled to heat transfer and radionuclide transport, respectively.

4.3.4 Models Used

The PORFLO code and the TEMPEST codes are to be used in this problem.

4.3.5 Assumptions

Assumptions made for this problem are:

- Water is present in porous rock, but no flow occurs.
- Material properties are constant, but differ in the nine layers and in the repositories.
- The repository regions are a porous, conducting material, and heat generation is uniformly distributed over their volumes.
- Heat generation is decaying with time from an initial value specified at an arbitrary time zero.
- Material in each layer has an isotropic thermal conductivity.

4.3.6 Input Specifications

Dimensions of the solution domain, layer depths, and repository locations are in Figure 4.3.1. This region is representative in size and extent to anticipated PORFLO application in the BWIP program. Initial temperature distribution in °C is

$$T(x,y) = 75 - 0.04(y + 1575) \quad (4.3.1)$$

where y is the vertical dimension measured positive upward.

No initial horizontal temperature gradient exists. The initial temperatures are to be held constant at the solution-region boundaries, as determined from Equation (4.3.1). Time-dependent heat generation rates for material in the repository volumes are listed in Table 4.3.1. The values listed are selected time points representative of repository heat release rates according to an assumed initial material volume and a panel head load of 17 watts/m².

Properties of water in the porous rock are to be assumed constant with

Density	$\rho_f = 997 \text{ kg/m}^3$
Specific heat	$c_f = 4186.8 \text{ J/kg-}^\circ\text{C}$
Thermal conductivity	$D_f = 2.05 \times 10^7 \text{ J/m-yr-}^\circ\text{C}$

The rock properties in each layer of the solution domain are presented in Table 4.3.2.

4.3.7 Output Specifications

Transient temperature distributions are to be compared at times of

$t = 50 \text{ yr}$
 $t = 500 \text{ yr}$
 $t = 5,000 \text{ yr}$
 $t = 50,000 \text{ yr.}$

Vertical temperature profiles at these times are to be compared at horizontal locations through the center of the repository banks. The locations are

$x = 2290 \text{ m}$
 $x = 4450 \text{ m}$

based on zero at the left boundary of the simulation region. Horizontal temperature distributions at these times are to be compared at vertical location

$y = -1149.5 \text{ m}$

which is through the center of the repository banks.

4.3.8 Simulation Results and Discussion

Input to the PORFLO code was set up based on the problem statement specifications. A total of 7497 nodes were included in the model, 119 in the horizontal direction and 63 in the vertical direction. Variable node spacing was used in both coordinate directions with closest spaced nodes being in the vicinity of the repositories. Maximum cell aspect ratio was 133:1. Ten material zones were defined: one for each of the nine stratigraphic layers and one for the repositories. Material properties were prescribed for each layer

(zone) as being constant. Heat generation was specified as occurring only in the zone prescribing the repositories.

Initial temperature distribution in the region was specified from input using a reference temperature of 75°C at a depth of -1575 m according to Equation 4.3.1. Initial temperatures were maintained at boundary nodes throughout the simulation. Heat generation was input according to data in Table 4.3.1. The code was operated in the heat-conduction-only mode.

Time stepping of the PORFLO simulation was controlled explicitly. To start the transient simulation, a time step of 0.05 yr was specified with a growth factor of 1.1. A maximum time step of 0.1 yr was specified over the first 5 yr. These values were varied by user specification for subsequent user-specified intervals. For the last 20,000 yr simulated, the maximum time step had been relaxed to 180 yr. A total of 951 steps were computed in reaching the 50,000 yr simulation time limit.

The TEMPEST model utilized 1476 computational cells with 36 in the horizontal direction and 41 in the vertical direction. Variable grid spacing was used with specified temperature boundaries prescribed to coincide with PORFLO boundary node positions. While PORFLO utilized a horizontal reference position of zero at the midpoint between the repositories, TEMPEST gridding places the origin for this problem at the left boundary of the simulation region as shown in Figure 4.3.1. The maximum cell aspect ratio was 100:1, and only one cell width was used to model the vertical repository width of 3 m. Both codes used 1710 m as the length of the solution domain in the third coordinate direction for determining total heat generated.

The TEMPEST code was operated in the heat-conduction-only mode. Automatic time-stepping was used throughout the total simulation time. The fully implicit energy equation solution algorithm was used with an implicit time-step factor of 100 times the explicitly stable time-step. A limiting time step of 100 yr was also specified.

Results of the two code simulations are compared in Figures 4.3.2 and 4.3.3. Vertical temperature distributions through the center of leftmost repository are in Figure 4.3.2. Horizontal temperature distributions through

the repository plane are presented in Figure 4.3.3. Because of node spacing differences, these latter results are at a depth of -1148.75 m for PORFLO and -1149.5 m for TEMPEST. While PORFLO utilizes considerably finer nodding resolution, agreement between the codes is excellent for both distributions. The third distribution, requested in output specifications for the vertical line through the center plane of the rightmost repository block, is not presented. Results in this plane were compared and were found to yield essentially the same comparison as presented in Figure 4.3.2.

The maximum temperature predicted at the center of each repository is presented in Table 4.3.3 at times of 50, 500, 5,000, and 50,000 yr. Differences are less than 1°C out of a total temperature increase of almost 100°C. Because of node-spacing differences in the models, PORFLO data are at $y = -1148.75$ m, offset from the centerplane, while TEMPEST temperatures are at repository centerline of $y = -1149.5$ m. In part, the relative small temperature differences in tabulated data are a consequence of this position difference. Differences may also be due to the functional heat generation points hit during the time-stepping process, as may occur any time a piecewise linear curve is used in a tabular form.

Agreement of temperature distributions predicted by the PORFLO and TEMPEST codes for this repository scale simulation suggests that PORFLO is predicting correctly in this geometry and solution mode. This is supported by the fact that both codes use different solution techniques and time-stepping algorithms. The results are well within expected agreement limits in light of node spacing, and hence, resolution differences in the models.

TABLE 4.3.1. Repository Heat Generation Rates as a Function of Time

<u>Time (yr)</u>	<u>Heat Generation (J/m³-yr)</u>
0	1.657 x 10 ⁸
1	1.591
2	1.537
3	1.490
4	1.448
5	1.410
6	1.376
7	1.344
8	1.315
9	1.287
10	1.261
11	1.236
12	1.212
13	1.189
14	1.167
15	1.146
20	1.049
25	9.651 x 10 ⁷
30	8.912
35	8.254
40	7.669
50	6.674
60	5.872
70	5.223
80	4.691
90	4.261
190	2.441
290	1.931
390	1.639
490	1.423
690	1.110
990	8.065 x 10 ⁶
1990	4.057
2990	3.086
3990	2.740
4990	2.531
6990	2.211
9990	1.836
19990	1.084
29990	7.188 x 10 ⁵
39990	5.145
49990	3.855
69990	2.357
99990	1.319
999990	5.584 x 10 ⁴

TABLE 4.3.2. Layer Thermal Properties

Layer No.	Rock Density (kg/m ³)	Rock Specific Heat (J/kg-°C)	Rock Thermal Conductivity (J/m-yr-°C)	Porosity
1	2780	845	5.362 x 10 ⁷	0.001
2	2400	845	5.362	0.001
3	2780	930	5.610	0.0001
4	2400	930	5.610	0.002
5	2780	930	5.610	0.0001
6	2400	930	5.610	0.001
7	2780	845	5.362	0.001
8	2780	760	5.050	0.001
9	2780	845	5.362	0.001
10 ^(a)	2780	930	5.610	0.005

(a) Repository panel

TABLE 4.3.3. Maximum Predicted Repository Temperatures

Time (yr)	<u>Left Repository</u>		<u>Right Repository</u>	
	PORFLO ^(a)	TEMPEST ^(b)	PORFLO	TEMPEST
	T(°C)	T(°C)	T(°C)	T(°C)
50	148	148.91	148	148.91
500	139	140.35	139	140.02
5,000	92.2	92.20	88.4	88.34
50,000	61.9	61.94	61.5	61.59

(a) PORFLO outputs temperatures with a D10.2 format resulting in only three digits

(b) TEMPEST outputs temperatures to F10.2 format resulting in the five digits reported.

FIGURE 4.3.1. Problem HT-3: Repository Scale Conduction Problem Geometry

PLOT FILE = /BVI/HT3/PLOTS TPLT50A TPLT500A TPLT5000A TPLT50000A
 PROBLEM HT3: T VS Z AT TIME OF 50, 500, 5,000, AND 50,000 YEARS.

FIGURE 4.3.2. Problem HT-3: Vertical Temperature Distribution Through Left Repository ($x = 2290$ m) at Times of 50, 500, 5,000, and 50,000 yr

PLOT FILE = /BWIP/HT3/PLOTS TPLT50C TPLT500C TPLT5000C TPL50000C

PROBLEM HT3: T VS X AT Z = -1149.5M, TIMES OF 50, 500, 5,000 AND 50,000 YEARS.

FIGURE 4.3.3. Problem HT-3: Horizontal Temperature Distribution Through Repository at Times of 50, 500, 5,000, and 50,000 yr

4.4 STEADY FLOW IN A REGIONAL GROUNDWATER SYSTEM

4.4.1 Problem Designation

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

4.4.2 Objective

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

4.4.3 Problem Statement

A uniformly sloped water table exists over a region in which groundwater flow is to be computed. Figure 4.4.1 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.

4.4.4 Models Used

The PORFLO code is to be used in the fluid-flow-only mode. The analytical solution is to be generated using computer mathematics library routines.

4.4.5 Analytical Solution

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

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = 0. \quad (4.4.1)$$

Boundary conditions for this problem (see Figure 4.4.1) are specified as

$$\frac{\partial h}{\partial x}(0,y) = \frac{\partial h}{\partial x}(L,y) = \frac{\partial h}{\partial y}(x,0) = 0 \quad (4.4.2)$$

along the bottom and lateral boundaries, and

$$h(x,H) = f(x) \quad (4.4.3)$$

along the top surface of the solution domain.

For an assumed linear water table, the functional form can be expressed as

$$f(x) = H + x \tan \alpha \quad (4.4.4)$$

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

$$h = \left(H + \frac{L \tan \alpha}{2} \right) - \frac{4 \tan \alpha}{L} \sum_{m=0}^{\infty} \frac{\cos(\xi_m x) \cosh(\xi_m y)}{\xi_m^2 \cosh(\xi_m H)} \quad (4.4.5)$$

where

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

Differentiating Equation 4.4.5 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

(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 (4.4.5) given here. Although not stated in the reference, it is straightforward to show that the top boundary condition (Equation 4.4.3) is satisfied by the solution over the range $0 < x < L$ while conditions of Equation 4.4.2 apply for $y = H$ at $x = 0$ and L .

$$U = - \frac{4K \tan \alpha}{L} \sum_{m=0}^{\infty} \frac{\sin(\xi_m x) \cosh(\xi_m y)}{\xi_m \cosh(\xi_m H)} \quad (4.4.6)$$

and

$$V = \frac{4 K \tan \alpha}{L} \sum_{m=0}^{\infty} \frac{\cos(\xi_m x) \sinh(\xi_m y)}{\xi_m \cosh(\xi_m H)}. \quad (4.4.7)$$

4.4.6 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.

4.4.7 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 m
Region Width	L = 1000 m
Water Table Angle	$\alpha = 1.7184$ degrees
Hydraulic Conductivity	K = 1 m/yr

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

4.4.8 Output Specifications

PORFLO 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 $x = 25$ m, 500 m, and 975 m.

These latter positions will yield data for expected symmetry comparisons.

4.4.9 Simulation Results and Discussion

The PORFLO model of this solution domain was computed in the fluid-flow-only mode. A 42 by 22 node system was used with constant spacing of $\Delta x = \Delta y = 25$ m. Zero flux conditions were specified for the hydraulic head along the bottom and lateral boundaries. Along the top surface a linear gradient was prescribed with a reference value of 500 m at left and a gradient of 0.03 m/m increasing in the positive horizontal coordinate direction.

PORFLO utilizes an asymptotic approach to steady-state solution technique which essentially involves running a transient until physical variables are no longer varying with time. For this problem, the flow equation was computed to $80,000$ yr. At this time the relative pressure change, $\Delta P/P$, was of the order of 10^{-11} , thus indicating a steady-state condition had essentially been reached. This technique is used because a direct-solution steady-state algorithm is not included in PORFLO.

Figure 4.4.2 presents the streamlines predicted for PORFLO for this flow. Streamline symmetry is evident in the code's predictions. Given the nature of the problem geometry and impressed boundary conditions, such symmetry is expected for this problem and can be argued as physically correct. Proving mathematically the symmetry of the streamlines has not been pursued. Figure 4.4.3 presents a comparison of the vertical hydraulic head distribution at horizontal locations of 37.5 , 512.5 , and 962.5 m. PORFLO results are compared to analytical solution results generated from Equation 4.4.5 at these locations, because they are closest to cell centerpoints. The stairstepped nature of the PORFLO curves is a direct consequence of PORFLO's computer output using D10.2 format. Thus, only three digits are printed. For example, computed head values of 500.5 m would be rounded on output to $5.010 + 0.2$ while 500.4 would be $5.000 + 02$ on output. The PORFLO results which are plotted were obtained from computer output, and, because of the output round-off, exhibit

the characteristic stairstepped look. The seeming discrepancy at $x = 512.5$ m is also due to this roundoff on output. The analytical solution value is 515.32 m whereas PORFLO output prints a value of $5.150 + 02$. A horizontal hydraulic distribution at the depth of 250 m is compared in Figure 4.4.4. The agreement is very good, albeit the rounding to three digits is again evident.

The predicted horizontal Darcy velocities are compared in Figure 4.4.5 for positions of $x = 25$ m, 500 m, and 975 m (these are grid face positions where Darcy velocities are computed). Results near the symmetric positions ($x = 25$ m and 975 m) are identical. Agreement at all positions is very good. The vertical Darcy velocity distribution presented in Figure 4.4.5 further shows very good agreement with the analytical distribution. Recirculation in the region is evident by the downflow on the right and upflow on the left.

The results of this simulation are very good. The agreement with the analytical solution is excellent over the solution domain. They indicate the code is predicting correctly in this mode. The only discrepancy in results is identifiable directly as caused by roundoff of results on output.

FIGURE 4.4.1. Problem FF-1: Solution Domain

FIGURE 4.4.2. Problem FF-1: Regional Groundwater Flow Streamlines

FLUID FLOW PROBLEM FF-1

FIGURE 4.4.3. Problem FF-1: Vertical Distribution of Hydraulic Head

FLUID FLOW PROBLEM FF-1

FIGURE 4.4.4. Problem FF-1: Horizontal Distribution of Hydraulic Head

FLUID FLOW PROBLEM FF1

FIGURE 4.4.5. Problem FF-1: Vertical Distribution of Horizontal Darcy Velocity

FLUID FLOW PROBLEM FF1

FIGURE 4.4.6. Problem FF-1: Horizontal Distribution of Vertical Darcy Velocity

4.5 TRANSIENT TWO-DIMENSIONAL FLOW

4.5.1 Problem Designation

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

4.5.2 Objective

The objective of this problem is to test PORFLO's computation of transient groundwater flow in a two-dimensional region. Such a flow occurs because of an initial hydraulic head distribution which is not in equilibrium.

4.5.3 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,

$$h = h_{\max} \sin \left(\frac{\pi x}{X} \right) \sin \left(\frac{\pi y}{Y} \right). \quad (4.5.1)$$

With no sources or sinks in the region, the hydraulic head in the region will asymptotically decrease with time. Boundaries of the region are maintained at constant head. Figure 4.5.1 presents a schematic of the problem. Solution of a similar problem is given by King, et al. (1981).

4.5.4 Models Used

The PORFLO code is used in a fluid-flow-only mode without thermal coupling or density disparity. Results are compared to an equivalent analytical solution developed and solved for the problem.

4.5.5 Analytical Solution

Assuming constant hydraulic conductivities ($K_{ij} = K$), no density disparity ($\delta_b = 0$), and isothermal flow ($\frac{\partial T}{\partial t} = 0$), The hydraulic head equation solved by PORFLO can be written in Cartesian coordinates

$$\frac{S_s}{K} \frac{\partial h}{\partial t} = \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}. \quad (4.5.2)$$

An analytical solution to this equation can be obtained subject to initial conditions of

$$h(x, y, 0) = h_{\max} \sin\left(\frac{\pi x}{X}\right) \sin\left(\frac{\pi y}{Y}\right) \quad (4.5.3)$$

for $0 \leq x \leq X$, $0 \leq y \leq Y$ and for boundary conditions of

$$\begin{aligned} h(0, y, t) = h(X, y, t) = h_b &= 0 \\ h(x, 0, t) = h(x, Y, t) = h_b &= 0 \end{aligned} \quad (4.5.4)$$

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 4.5.2 is

$$h(x, y, t) = h_{\max} \left[\exp\left(-\frac{\pi^2 K t}{S_s} \left(\frac{1}{X^2} + \frac{1}{Y^2}\right)\right) \sin\left(\frac{\pi x}{X}\right) \sin\left(\frac{\pi y}{Y}\right) \right]. \quad (4.5.5)$$

This solution can be readily verified by substitution into Equations (4.5.2) to (4.5.4).

Transient horizontal and vertical Darcy velocities are obtainable by differentiating Equation 4.5.5 with respect to x and y , respectively, and multiplying the result by hydraulic conductivity.

The result is

$$u = \frac{K h_{\max} \pi}{X} \left[\exp\left(-\frac{\pi^2 K t}{S_s} \left(\frac{1}{X^2} + \frac{1}{Y^2}\right)\right) \cos\left(\frac{\pi x}{X}\right) \sin\left(\frac{\pi y}{Y}\right) \right] \quad (4.5.6)$$

and

$$v = \frac{K h_{\max} \pi}{Y} \left[\exp \left(- \frac{\pi^2 K t}{S_s} \left(\frac{1}{X^2} + \frac{1}{Y^2} \right) \right) \sin \left(\frac{\pi X}{X} \right) \cos \left(\frac{\pi Y}{Y} \right) \right] \quad (4.5.7)$$

for horizontal and vertical components, respectively.

4.5.6 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.

4.5.7 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	$h_{\max} = 100 \text{ m}$

4.5.8 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 transient distributions are to be compared to analytical solution. Selected locations are to be compared to ensure predicted symmetry about the $\frac{X}{X} = \frac{1}{2}$ and the $\frac{Y}{Y} = \frac{1}{2}$ planes.

4.5.9 Simulation Results and Discussion

PORFLO input for this problem was set up utilizing a 41 by 21 node array. Equal spacing of $\Delta x = \Delta y = 50$ m was used in each direction. Thus the boundary nodes corresponded to the location of the simulation domain size of 2000 m x 1000 m. Initial velocity conditions were specified everywhere as zero. The initial pressure distribution was specified according to Equation 4.5.3. This was done using a short preprocessor program written specifically for the purpose of computing initial hydraulic heads at each node point and outputting data in a format consistent with PORFLO input requirements. This preprocessor was used because 800 initial pressure values were required.

The solution was carried out to 10,000 yr with specified equal time-step intervals of 100 yr. Flow-only solution mode was used and output was at every 2000 yr. Because of the character of the initial conditions and the solution domain, quarter-section symmetry exists.

PORFLO pressure distribution results were found to be exactly symmetric within the three digits output. Table 4.5.1 presents a comparison of head results at selected locations. Other locations also compared similarly. At the points listed in Table 4.5.1, the PORFLO results in all cases are within a rounded-off difference of the analytical solution.

Table 4.5.2 presents a similar comparison of horizontal and vertical Darcy velocities at selected points. To within the three digits output, the PORFLO code was computing symmetrically about the $x = 1000$ m plane for horizontal (U) Darcy velocities and about the $y = 500$ m plane for the vertical (V) Darcy velocities.

Graphical comparison of transient hydraulic head data are presented in Figure 4.5.2. The central location (curve 1) was a reference monitor cell. Other locations plotted were only output at 2000 yr intervals. Agreement of PORFLO results and analytical solution results is excellent. Transient Darcy velocity components are compared in Figures 4.5.3 and 4.5.4. Agreement of PORFLO and analytical results is very good. These results indicate PORFLO is accurately predicting transient pressure and flow in this geometry.

TABLE 4.5.1. Transient Pressure

Time (yr)	Analytical ^(a)	PORFLO ^(b)	Analytical	PORFLO	
	<u>h(1000,500,t)</u>	<u>h(1000,500,t)</u>	<u>h(500,500,t)</u>	<u>h(500,500,t)</u>	<u>h(1500,500,t)</u>
0	100.00	100	70.71	70.7	70.7
2,000	72.48	73.0	51.25	51.6	51.6
4,000	52.54	52.9	37.15	37.4	37.4
6,000	38.08	38.4	26.93	27.1	27.1
8,000	27.60	27.8	19.52	19.7	19.7
10,000	20.01	20.02	14.15	14.3	14.3

(a) Analytical only reported to two decimal places

(b) PORFLO output to 010.2 format results in only three digits

TABLE 4.5.2. Transient Darcy Velocities

Time (yr)	Analytical	PORFLO	Analytical	PORFLO
	<u>U(525,500,t)</u>	<u>U(525,500,t)</u>	<u>V(1000,225,t)</u>	<u>V(1000,225,t)</u>
2,000	-2.318x10 ⁻⁴	-2.35x10 ⁻⁴	-5.195x10 ⁻⁴	-5.23x10 ⁻⁴
4,000	-1.681	-1.71	-3.765	-3.79
6,000	-1.218	-1.24	-2.729	-2.75
8,000	-0.883	-0.898	-1.978	-1.99
10,000	-0.640	-0.651	-1.553	-1.45

FIGURE 4.5.1. Problem FF-2: Sinusoidal "Potential Mound" Problem Schematic

FIGURE 4.5.2. Problem FF-2: Transient Pressure

FLUID FLOW PROBLEM FF2

FIGURE 4.5.3. Problem FF-2: Transient Horizontal Darcy Velocity Component

FLUID FLOW PROBLEM FF2

FIGURE 4.5.4. Problem FF-2: Transient Vertical Darcy Velocity Component

4.6 BUOYANCY-AFFECTED FLOW IN THE VICINITY OF A REPOSITORY

4.6.1 Problem Designation

This problem is designated: Fluid Flow Problem FF-3.

4.6.2 Objective

The objective of this repository scale problem is to determine affected flow and temperature distribution in the vicinity of a pair of repository banks located in a hydrogeologic formation. The formation consists of layers of porous basalt rock. Material in the two repository banks is porous and contains heat generating material. Heat generation rates decrease with time. This benchmarking problem is representative of anticipated repository scale analysis with PORFLO.

4.6.3 Problem Statement

Two repository banks, 3-m high, are located at a median depth of -1149.5 m in a layered hydrogeologic media. The two banks are separated by a distance of 1063 m, as shown in Figure 4.6.1. The solution domain includes nine layers of material with differing hydrogeologic parameters. The depth of the solution domain ranges from -842 m to -1575 m below the surface. The horizontal distance ranges from 0 to 6570 m, as shown in the figure.

Heat generation occurs in the repository banks. The heat generation rate is uniform over the total bank volume and decreases with time. Transient decay rate, composite layer thicknesses, and hydrogeologic data for this problem are included in the Input Specifications.

Of interest in this problem is predicting the transient thermal field and buoyancy-affected flow field in the vicinity of the repositories. The initial vertical temperature gradient in the formation is $-0.04^{\circ}\text{C}/\text{m}$ with the temperature of 75°C at a depth of -1575 m being the reference. The vertical boundaries are to be maintained at this gradient throughout the simulation. Horizontal boundaries are to be held constant at the initial temperature at that depth. Initial hydraulic head is to be prescribed as a function of depth and to be maintained constant at the initial value on the boundaries.

4.6.4 Models Used

The PORFLO code and the SWENT code are to be used.

4.6.5 Assumptions

Assumptions made in this problem include:

- The horizontal hydrogeologic layers are representative composites of basalt rock; each is uniform in thickness and extent.
- Flow and energy transport in the media are two-dimensional and only a vertical slice through the media is treated.
- Boundaries are at sufficient distance from the repository banks such that Dirichlet boundary conditions are appropriate.
- A nonequilibrium initial hydraulic head distribution is maintained on the boundaries and no hydrodynamic equalization occurs prior to initial repository bank heat loading.
- Input specification parameters are representative of values for intended PORFLO application in basalt rock.

4.6.6 Input Specifications

Dimensions of the solution domain, layer depths, and repository locations are in Figure 4.6.1. Initial temperature distribution in degrees Celsius is

$$T(x,y) = 75 - 0.04(y + 1575) \quad (4.6.1)$$

where y is the vertical dimension measured positive upward from a nominal reference surface defined to be $y = 0$. The initial temperatures are to be held constant at the solution region boundaries, as determined from Equation (4.6.1). Heat generation rates in the repository volumes are listed as a function of time in Table 4.6.1. The values listed are an approximation to a realistic rate of heat generation for waste repository material with an assumed panel heat load of 17 watts/m². Reference material properties of water in the porous rock at $T = 26.85^\circ\text{C}$ are as follows:

Density	$\rho_f = 997 \text{ kg/m}^3$
Specific heat	$c_f = 4186.8 \text{ J/kg-}^\circ\text{C}$
Thermal conductivity	$D_f = 2.05 \times 10^7 \text{ J/m-yr-}^\circ\text{C}$

The rock properties in each layer of the solution domain are presented in Table 4.6.2. The hydraulic properties of each layer are given in Table 4.6.3. The initial horizontal hydraulic head gradient is $-5.0 \times 10^{-4} \text{ m/m}$. The initial vertical hydraulic gradient is $-1.0 \times 10^{-3} \text{ m/m}$. These gradients are referenced to a hydraulic head of 127.54 m at the lower left corner of the solution domain, e.g. $x = 0$, $y = -1575 \text{ m}$. These problem specifications were used to generate results presented subsequently. During this work, however, the problem parameters were changed to make them compatible with both the SWENT and PORFLO codes. Appendix B presents a discussion of the chronology and changes made during the benchmarking effort and the effect these change had on results.

TABLE 4.6.1. Heat Generation Profile

<u>Time (yr)</u>	<u>Heat Generation (J/m³-yr)</u>
0	1.657 x 10 ⁸
1	1.591
2	1.537
3	1.490
4	1.448
5	1.410
6	1.376
7	1.344
8	1.315
9	1.287
10	1.261
11	1.236
12	1.212
13	1.189
14	1.167
15	1.146
20	1.049
25	9.651 x 10 ⁷
30	8.912
35	8.254
40	7.669
50	6.674
60	5.872
70	5.223
80	4.691
90	4.261
190	2.441
290	1.931
390	1.639
490	1.423
690	1.110
990	8.065 x 10 ⁶
1990	4.057
2990	3.086
3990	2.740
4990	2.531
6990	2.211
9990	1.836
19990	1.084
29990	7.188 x 10 ⁵
39990	5.145
49990	3.855
69990	2.357
99990	1.319
999990	5.584 x 10 ⁴

TABLE 4.6.2. Layer Thermal Properties

Layer No.	Layer Thickness (m)	Rock Density (kg/m ³)	Rock Specific Heat (J/kg- C)	Rock Thermal Conductivity (J/m-yr- C)	Porosity d	Longitudinal Dispersion α_L (m)	Transverse Dispersion α_T (m)
1	427	2780	845	5.362×10^7	0.001	50.0	2.0
2	6	2400	845	5.362	0.001	50.0	2.0
3	35	2780	930	5.610	0.0001	50.0	2.0
4	32	2400	930	5.610	0.002	50.0	2.0
5	32	2780	930	5.610	0.0001	50.0	2.0
6	10	2400	930	5.610	0.001	50.0	2.0
7	71	2780	845	5.362	0.001	50.0	2.0
8	75	2780	760	5.050	0.001	50.0	2.0
9	95	2780	845	5.362	0.001	50.0	2.0
10 ^(a)	3	2780	930	5.610	0.005	50.0	2.0

(a) Repository bank

TABLE 4.6.3. Layer Hydraulic Properties

Layer No.	Horizontal Conductivity K_x (m/yr)	Vertical Conductivity K_y (m/yr)	Specific Storage S_s (1/m)
1	6.308×10^{-2}	1.892×10^{-5}	1×10^{-4}
2	6.308×10^{-2}	6.308×10^{-2}	1×10^{-4}
3	6.308×10^{-6}	1.892×10^{-5}	1×10^{-4}
4	2.839×10^{-1}	2.839×10^{-1}	1×10^{-4}
5	6.308×10^{-6}	1.892×10^{-5}	1×10^{-4}
6	2.839×10^{-1}	2.839×10^{-1}	1×10^{-4}
7	3.200×10^{-2}	2.839×10^{-5}	1×10^{-4}
8	6.000×10^{-2}	1.144×10^{-5}	1×10^{-4}
9	9.200×10^{-2}	1.200×10^{-5}	1×10^{-4}
10 ^(a)	6.308×10^{-6}	1.892×10^{-5}	1×10^{-4}

(a) Repository bank

4.6.7 Output Specifications

Transient temperature and flow distributions are to be compared at times of

t = 50 yr
t = 500 yr
t = 5,000 yr
t = 50,000 yr.

Vertical profiles of temperature and horizontal Darcy velocities at these times are to be compared at horizontal locations through the center of the repository banks. The locations are

x = 2290 m
x = 4450 m

relative to the left hand boundary of the simulation region. Horizontal temperature distributions and horizontal distribution of vertical Darcy velocity at these times are to be compared at a vertical location

y = -1149.5 m

which is the center of the repository banks.

4.6.8 Simulation Results and Discussion

Two simulations of this specified problem were run, one with the PORFLO code and one with the SWENT code. The PORFLO simulation was run by BCSR personnel, and the SWENT code was run as part of this work. An effort was made to keep the two simulations similar. This required interaction to ensure the problems were kept within each code's capabilities.

There are certain differences between the two codes, some of which are significant to this problem. One primary difference is that PORFLO solves a pressure equation written in terms of hydraulic head (Equation 2.1.1). SWENT solves a similar equation but one which is written in terms of pressure in units of Pascals. Because of this, it was necessary to convert the initial hydraulic head data to pressure for the SWENT simulation boundary conditions in advance of input. The method used is discussed in Appendix C.

SWENT has a large computer core allocation requirement. Thus, a considerably more coarse grid spacing was used in the SWENT simulation than in the PORFLO simulation to keep core requirements reasonable. This is in keeping with the benchmarking objective of using SWENT's capabilities and computing a similar, but not necessarily an identically noded PORFLO problem. Other differences exist in the code's grid structure and setup. PORFLO uses a concept wherein location of node points are defined on input. Computational control volume surfaces are then determined at the average distance between node points. SWENT, on the other hand, requires specification of computational cell widths on input and then nodes are internally determined at cell centers. This difference is important because it hinders data comparison at specified locations. With variable noding, it is not possible to match both cell center locations and cell surface locations, even if the same number of nodes and cells are used.

The SWENT simulation of this problem was computed using 36 computational cells in the horizontal direction and 41 computational cells in the vertical direction; at least two cells were included in each modeled hydrogeologic layer. The total horizontal distance modeled was 6570 m, the same as with PORFLO. The total vertical distance modeled was 733 m from a depth of -842 m to -1575 m. Variable grid spacing was used in each coordinate direction. Adjacent grid cell widths were maintained at a ratio less than 1.5. The largest cell aspect ratio was 100:1. The location and dimensions of each repository volume were maintained the same as in the PORFLO case. This provides identical heat source volumes, but in the SWENT model only one vertical cell was used to model the repository thickness of 3 m (PORFLO used two cells, 1.5 m each).

PORFLO has a user feature which SWENT does not. With PORFLO, a user can specify initial gradient distributions in both horizontal and vertical directions relative to a reference node. For SWENT, individual values of pressure and temperature must be input for each boundary cell face. A preinput program was written to prepare the 400-some odd cards required to make all these boundary specifications for SWENT. The procedure used is detailed in Appendix C. A brief summary is given here. A program was written which computed the hydraulic head distribution as a function of depth according to

specified gradients and computed temperatures as a function of depth according to Equation (4.6.1). Pressure was then computed using the relation $P = \rho g(h+z)$ where ρ is the density at temperature T , and depth, z . Depth, z , is measured positive downward in SWENT. This was done for each boundary cell. Computed values of pressure and temperature were then written to a scratch file in exactly the format required for SWENT boundary condition input. This scratch file was then merged with the model input deck using a text editor feature on the computer. In this way, pressure boundary conditions were available to nine significant digits, according to an F10.1 format. Such computation is accurate enough so that the hydraulic gradient was not lost in the magnitude of the local static pressure. (It was found that only seven significant digits available with an E10 format were not sufficiently accurate to resolve a gradient of -0.001 m/m.)

The transient heat generation in the repository volumes was input using source term specification. This was done with recurrent data sets in the input deck. A set of source term cards (two cards are required for each source cell, 15 source cells were used) was created for each time interval listed in Table 4.6.1. The procedure used was to initially type one time point set of source cards, copy that set with a text editor, change the heat source value, and copy it again. This was done for all time points. In all, over 1800 input card records were created in this manner. Because SWENT does not have linear interpolation capability in source specification, the heat generation value used over each time interval (recurrent data set) was the average of the value between adjacent time points listed in Table 4.6.1.

Except for the initial transient startup (first ten time steps), automatic time-stepping was chosen for the SWENT simulation. Parameters governing maximum time-step intervals were defaulted in all cases except maximum time-step. Beyond 15 yr, the maximum time-step allowed during the transient was limited to require at least two time-steps over each interval between heat generation time points. The code was operated in a reduced band width, direction solution method, using backward-in-space (BIS) and backward-in-time (BIT) differencing. These are default modes. There were a total of 41 recurrent data sets (time) intervals and the code took a total of 331 time steps to compute to the required 50,000 yr. The simulation took a little over 6 min of computer time to run on the CRAY-1S.

The PORFLO simulation was set up using 119 node points in the horizontal direction. In the vertical direction, 73 nodes were used. Thus, nearly twice the vertical resolution and over three times the horizontal resolution was exhibited by this node structure in comparison to the SWENT model.

The simulation region was the same, spanning a distance of 6570 m horizontally and 733 m vertically from a depth of -842 m to -1575 m (1710 m was the dimension used in both simulations for the distance in third dimension, which defined the heat generating repository volume). Boundary conditions were prescribed using PORFLO's gradient designation option. The hydraulic head was specified at a reference node at the lower left node point, and the gradients listed in input specifications were prescribed. The code internally computes appropriate boundary and initial values in each cell. This was done for temperature, too, using the node point at the lower left corner as a reference to Equation (4.6.1).

Temperature distribution results computed with PORFLO and SWENT were in very good agreement, as shown in Figures 4.6.2 and 4.6.3. For the specified thermal properties in this problem, thermal energy transport is conduction-dominated. The distributions are very similar to those computed in the conduction-only mode in problem HT-3 (Section 4.3). The maximum temperatures (predicted at the center of the leftmost repository) are compared in Table 4.6.4. Because of nodding differences, PORFLO results are at a depth of -1148.75 m, while SWENT results are at a depth of -1149.5 m.

Per Section 4.6.7, predicted horizontal component of Darcy velocity is to be compared at two vertical planes. The first plane is to be vertical through the center of the leftmost repository panel ($x = 2290$ m). Because the SWENT model used coarser nodding, SWENT results computed at a cell face nearest this plane are used. These are at horizontal location $x = 2365$ m. PORFLO results used for comparison are at $x = 2290$ m. The second vertical plane of comparison is to be at the rightmost end of the right repository. This plane is horizontal position $x = 4925.5$ m, and is the same for both SWENT and PORFLO models.

TABLE 4.6.4. Comparison of Maximum Repository Temperatures

Time (yr)	Problem HT-3		Problem FF-3	
	PORFLO	TEMPEST	PORFLO	SWENT
50	148°C	148.91°C	148°C	150.1°C
500	139°C	140.35°C	139°C	140.0°C
5,000	92.2°C	92.20°C	92.1°C	92.0°C
50,000	61.9°C	61.94°C	61.7°C	62.1°C

Figure 4.6.4 presents the vertical distribution of the horizontal of Darcy velocity at times of 50, 500, 5,000, and 50,000 yr at the plane of $x = 2290$ m. Predicted velocities largely exhibit good agreement although certain discrepancies exist. The greatest discrepancy occurs at 50 yr. SWENT results show an almost opposite flow characteristic from the PORFLO results with velocity being negative or to the left. This occurs particularly in the region where heat has penetrated up to this time (compare temperature at 50 yr, Figure 4.6.2 to regions of negative flow). By 500 yr, the negative flows predicted by SWENT have turned around and are in excellent agreement with PORFLO's results over the whole plane. Similarly, good agreement carries through to 50,000 yr. By this time, temperature distribution has nearly returned to initial conditions and flow is nearly at equilibrium with boundary conditions, e.g., buoyancy effects are no longer significant. The way the two codes treat one physical model parameter and its effect on negative velocities predicted by SWENT is addressed subsequently in this section.

As a check on results, horizontal Darcy velocity at several locations was calculated using a hand calculator. In the lowest material region, agreement between SWENT and PORFLO velocities were within 2 percent of hand calculated values determined from impressed boundary conditions. The velocities in layer 4 (which has the highest hydraulic conductivity and hence the greatest Darcy velocity) were within 5 percent of the hand calculated values. Thus both codes appear to be predicting correct equilibrium flow in the absence of buoyancy effects.

Vertical distribution of horizontal Darcy velocity at the second plane of comparison ($x = 4925.5$ m) is presented in Figure 4.6.5. With the exception of results at 50 yr, agreement between SWENT and PORFLO is excellent. At 50 yr, PORFLO is predicting a counterdirectional flow in layer 4. This is indicative of a recirculation caused by buoyancy effects. SWENT also predicts a similar counterdirectional flow in this layer, but it does not become evident until later in time.

Comparison of horizontal distribution of vertical component of Darcy velocity is made at one plane. This is at depth $y = -1148$ m which is the top surface of the material region defining the repository panels. This plane is the same in both SWENT and PORFLO models.

Comparison of predicted vertical Darcy velocities through the plane defined by the top of the repository volumes is made in Figure 4.6.6. Again the largest discrepancy appears at 50 yr where SWENT predicts a maximum (upflow) velocity of about 11×10^{-6} m/yr and PORFLO predicts a value of about 6×10^{-6} . Results at later times, percentage-wise, are in much better agreement. At 50,000 yr, where buoyancy effects are nearly decayed away, excellent agreement is found. Based on the impressed vertical hydraulic gradient of -0.001 m/m, a hand calculation of one velocity near the right end of the domain was made. Velocities predicted by SWENT and PORFLO were found to agree within about 7 percent of this theoretical value.

As discussed in more detail in Appendix B, both SWENT and PORFLO computations presented here are the result of several modeling perturbations. Because largest discrepancies occurred at 50 yr, several investigative simulations were run with SWENT to a time of 50 yr. Sequentially, these included:

- The solution algorithm selected was changed to CIT/CIS while maintaining the default value of one outer iteration loop. Changing from BIT/BIS to CIT/CIS resulted in approximately 10 percent variation in certain velocities.
- The CIT/CIS algorithm was selected with a minimum of two outer loop iterations.

- The BIT/BIS algorithm was selected and a maximum time-step size was restricted to require at least four time steps over each recurrent data set.
- Rock compressibility was set to $1 \times 10^{-15}/\text{Pa}$ for the BIS/BIT case to determine if a pressure-dependent variation in porosity was being effected.
- Pressure boundary conditions on corner cells were switched to the alternate surface.
- The coefficient of thermal expansion of water was decreased.

Forcing two outer iteration loops had the effect of reducing converged (maximum) mass balance error from 0.04 percent to 0.005 percent. Predicted flow velocities were largely unaffected. None of these investigations had sufficient cause to explain the large vertical velocity differences (Figure 4.6.6 for example). Changing the coefficients of thermal expansion, however, did.

SWENT calculates fluid density based on a linearized expression

$$\rho = \rho_R (1 + C_P (P - P_R) - C_T (T - T_R)). \quad (4.6.2)$$

where ρ_R , P_R , and T_R are reference density, pressure, and temperature, respectively. C_P and C_T are constant coefficients defined as compressibility of water and coefficient of thermal expansion, respectively. PORFLO computes water density based on local ambient temperature from coded water property data. It does not assume the coefficient of thermal expansion is constant. It neglects the compressibility of water.

In the SWENT results presented herein (Figures 4.6.4 to 4.6.6), C_T was assumed to be $0.00075/^\circ\text{C}$. This value was an average based on the functional dependency computed by PORFLO over the temperature range of this simulation according to BCSR personnel running the PORFLO code^(a).

(a) Niall Kline, personal communication.

Computed SWENT results using $C_T = 0.0005/^\circ\text{C}$, a value more consistent with low pressure water density data (Ekert and Drake, 1972, p. 777) are presented in Figure 4.6.7. The three graphs included in the figure correspond directly to results in Figures 4.6.4a to 4.6.6a. The most significant observation is in the horizontal distribution of vertical Darcy velocity. The peak vertical velocity has been reduced from about 11×10^{-6} m/yr to about 7×10^{-6} m/yr and is in much better agreement with PORFLO results. Horizontal Darcy velocities have correspondingly been shifted in the direction of better agreement with PORFLO. These results indicate that a basic physical modeling difference in the two codes might explain observed flow field differences. Changing C_T had the effect of improving results. Other physical parameters, or the way they are treated in the codes, which have not been investigated here, may also cause the observed discrepancies. It is also possible that resolution effect of node structure may be significant. Additional work is required to answer these questions.

FIGURE 4.6.1. Problem FF-3: Repository Flow and Heat Transfer Problem Geometry

FIGURE 4.6.2. Problem FF-3: Vertical Temperature Distribution Comparison at 50, 500, 5,000, and 50,000 yr

FLUID FLOW PROBLEM FF3

PLOT FILE=/BWIP/FF3/PLOTS TPLTALLC - T VS X AT Z=-1149.5M, TIME=50 TO 50000YRS.

FIGURE 4.6.3. Problem FF-3: Horizontal Temperature Distribution Comparison at 50, 500, 5,000, and 50,000 yr

FIGURE 4.6.4. Problem FF-3: Vertical Distribution of Horizontal Darcy Near Center of Left Repository Panel at Times of a) 50 yr, b) 500 yr, c) 5,000 yr, and d) 50,000 yr

FIGURE 4.6.5. Problem FF-3: Vertical Distribution of Horizontal Darcy Velocity at the Right End of the Rightmost Repository at Times of a) 50 yr, b) 500 yr, c) 5,000 yr, and d) 50,000 yr

FIGURE 4.6.6. Problem FF-3: Horizontal Distribution of Vertical Darcy Velocity at times of a) 50 yr, b) 500 yr, c) 5,000 yr and d) 50,000 yr

FIGURE 4.6.7. Problem FF-3: Darcy Velocity Results at 50 yr with $C_T = 0.0005/^\circ\text{C}$. a) U-Darcy at $x = 2290$ m, b) U-Darcy at $x = 4925$ m, and c) V-Darcy at $y = 11.48$ m

4.7 TRANSIENT RADIONUCLIDE TRANSPORT IN A ONE-DIMENSIONAL FLOW FIELD

4.7.1 Problem Designation

This problem is designated: Mass Transport Problem MT-1.

4.7.2 Objective

The objective of this problem is to test calculation of radionuclide transport with the PORFLO code in a groundwater flow. The flow is constant and unidirectional. Radionuclide transport is transient. Retardation and decay are neglected. Two cases are to be simulated: one for a short simulation distance and one for a long distance.

4.7.3 Problem Statement

The problem is to compute the transient advection of the radionuclide in groundwater flow subject to a step change in radionuclide concentration boundary condition. Flow is unidirectional in a uniform porous medium. Figure 4.7.1 presents a schematic of the problem.

The analytical solution to this problem may be formulated the same as heat transfer problem HT-2 (Section 4.2). Simulations are to be conducted over similar domain and coordinate directions. In addition, the simulation is to be conducted over a length of 10,000 m for a time period of 25,000 yr to test length and time-scale effects of discretization.

4.7.4 Models Used

The PORFLO code in the radionuclide-transport-mode-only is used to compute the transient distribution. Mathematical library routines are used to compute the complementary error function in the analytical solution. Results from the T3D code are also used for a secondary computer code comparison over the longer distance. These latter results were provided by Rockwell/BWIP.

4.7.5 Analytical Solution

PORFLO radionuclide transport is modeled using a transport equation for concentration including sources (generation) and sinks (retardation, decay, sorption). For the present problem, this transport equation may be reduced to

$$\frac{\partial C}{\partial t} + v \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} \quad (4.7.1)$$

by assuming no sources or sinks and defining

$$v = \frac{U}{R_d \phi} \quad (4.7.2)$$

and

$$D = (D_m + \frac{\alpha_L U}{\phi}) \frac{1}{R_d} \quad (4.7.3)$$

Subject to the initial condition

$$\text{for } t = 0, C = C_0 = 0 \text{ for all } x \quad (4.7.4)$$

and the boundary conditions:

$$\begin{aligned} \text{for } x = 0, C &= C_1 \quad \text{for all } t \\ \text{for } x = \infty, C &= C_0 = 0 \text{ for all } t, \end{aligned} \quad (4.7.5)$$

the solution to Equation (4.7.1) is identical to that of Equation (4.2.1) and is given by

$$C = \frac{C_1}{2} \left[\operatorname{erfc} \left(\frac{x-vt}{2\sqrt{Dt}} \right) + \exp \left(\frac{vx}{D} \right) \operatorname{erfc} \left(\frac{x+vt}{2\sqrt{Dt}} \right) \right]. \quad (4.7.6)$$

4.7.6 Assumptions

Assumptions made for simulation of this problem are:

- The physical source size is small, relative to the problem domain and is introduced on a time scale which is short, relative to the transient time of interest and, hence, it may be assumed to be a step change in time in the problem solution.
- The radionuclide has a long half-life ($\sim 10^9$ yr) and its decay is negligible, relative to the transport of the problem.
- No retardation occurs.
- The infinite analytical solution domain can be approximated by a finite numerical solution domain. The solution is thus assumed to be valid only until a nonnegligible concentration is predicted at 0.9 of the total domain length.

4.7.7 Input Specifications

To ascertain the correctness of the radionuclide transport equation solution, two cases are to be run. In case 1, hydrologic and flow parameters are:

Porosity	$\phi = 0.001$
Darcy velocity	$u = 0.03$ m/yr
Retardation factor	$R_d = 1.0$
Half-life	$T_{1/2} = 10^9$ yr
Molecular diffusion coefficient	$D_m = 0.03$ m ² /yr
Longitudinal dispersion length	$\alpha_L = 2$ m.

For these conditions, the following may be computed for the analytical solution:

Advection velocity	$v = 30$ m/yr
Dispersivity	$D = 60$ m ² /yr.

The solution domain is to be 1000 m for this case.

For case 2, the following parameters are to be used so that PORFLO calculations may be directly compared to both the analytical solution and to simulation results of the T3D code. The parameters for this case are:

Porosity	$\phi = 0.01$
Darcy velocity	$u = 3.15 \times 10^{-3} \text{ m/yr}$
Retardation factor	$R_d = 1.0$
Half-life	$T_{1/2} = 10^9 \text{ yr}$
Molecular diffusivity	$D_m = 0.03 \text{ m}^2/\text{yr}$
Longitudinal dispersion length	$\alpha_L = 50 \text{ m.}$

For these, the analytical solution parameters can be determined as

Advection velocity	$v = 3.15 \times 10^{-1} \text{ m/yr}$
Retarded dispersivity	$\theta = 15.75 \text{ m}^2/\text{yr.}$

The total solution domain is to be 10,000 m for this case.

4.7.8 Output Specifications

Radionuclide transport is to be computed for two cases in this test problem as follows:

- Case 1. Compute radionuclide distribution at 5 and 10 yr over the solution domain of 1000 m in the horizontal coordinate direction. These results are to be compared to the analytical solution.
- Case 2. Compute the radionuclide distribution at 5-, 10- and 20×10^3 yr over the solution domain of 10,000 m in the horizontal coordinate direction. These results are to be compared to the analytical solution and results computed with the T3D code which were provided by Rockwell/BWIP.

4.7.9 Simulation Results and Discussions

The PORFLO code was utilized to simulate the problem for the first case. With a domain length of 1000 m, 41 axial nodes were used with constant node spacing of $\Delta x = 25 \text{ m.}$ In the transverse direction, four nodes were used with zero transverse flux specified at the boundaries to model the infinite transverse dimension. The step-change boundary condition was modeled with a specified boundary value at the boundary node, $x = 0$, for times greater than 0. For this node spacing, the maximum cell Pe was 12.49. Subsequently, a second simulation of this case was rerun which resulted in a maximum cell Pe of 0.9995.

For case 2, 261 axial nodes were used to cover the solution domain of 10,000 m. Over the first 3000 m, $\Delta x = 25$ m, while $\Delta x = 50$ m was used beyond 3000 m. For both cases, first-order differencing was selected while the code was operating in the concentration-only mode.

Results for case 1 are presented in Figure 4.7.2. For the coarser node simulation, where $Pe = 12.49$, results were not in very good agreement with the analytical solution. The diffusive character of the first-order differencing was causing too large a dispersive effect. The subsequently renoded case resulted in $Pe = 0.9995$. Excellent agreement occurs for this latter simulation.

The analytical solution for this problem was computed using library routines for the complementary error function. The accuracy of the coding was ensured by two independent reviewers. Results were computed at conditions given by Ward et al. (1983) for his conditions and were found to agree with his analytical and SWIFT code calculations. This effort further ensured the correctness of the analytical solution results after first identifying the differences between the PORFLO case of $Pe = 12.49$.

One observation is worth noting. When the identity

$$\text{erfc}(\xi) = 1 - \text{erf}(\xi) \quad (4.7.7)$$

was used in the analytical solution, incorrect results were obtained with this problem. This is because of the product of $\exp(\xi)$ and $\text{erfc}(\xi)$ in the second term in solution (Equation 4.7.6). This term is the product of a very large number [$\exp(\xi)$] and a very small number [$\text{erfc}(\xi)$]. If the identity of Equation (4.7.7) is used, then the significance of this product is lost in the subtraction and the coded analytical solution can be significantly in error beyond the distance where $x = vt$.

Results for case 2 are presented in Figure 4.7.3. Selected results are also tabulated for this case in Table 4.7.1. PORFLO, T3D, and analytical solution results are presented. Agreement between the PORFLO results is very good over a majority of the penetration distance of the nuclide concentration through the solution domain. Largest discrepancy is at the lower concentrations occurring at the extremity of the penetration front.

These results indicate that PORFLO is capable of accurately simulating radionuclide transport under the conditions of constant advection velocity, without decay or retardation. Particular attention, however, has to be paid to noding and the associated Pe . In this problem, PORFLO was specifically operated in a first-order differencing mode, although higher order differencing modes may be selected in running PORFLO. This is the mode the code switches to if second-order differencing is chosen and maximum cell Pe number exceeds a value of one^(a) during the simulation. As these results indicate, significant errors can arise for a simple problem. When particular attention is paid to the accuracy dependency of the differencing scheme and node spacing, acceptable results are predicted with PORFLO.

(a) Kline, et al. 1983, p. 43. According to Budhi Sagar, personal communication, the switch occurs at a value of $Pe = 2$.

TABLE 4.7.1. Problem MT-1: Comparison of PORFLO, T3D, and Analytical Results for 10,000 m Solution Domain

x(m)	PORFLO	Time (5,000 yr)		x(m)	PORFLO	Time (20,000 yr)	
		T3D	Analytical			T3D	Analytical
0	1.000	1.000	1.000	0	1.000	1.000	1.000
400	0.999	0.974	0.999	3500	1.000		1.000
500	0.998	0.974	0.999	4000	0.999	0.964	0.998
600	0.996		0.996	4500	0.994		0.989
700	0.992		0.992	5000	0.961	0.929	0.957
800	0.984		0.974	5500	0.857		0.861
900	0.970	0.964	0.970	6000	0.655	0.643	0.674
1000	0.947	0.925	0.948	6500	0.409		0.428
1200	0.863	0.831	0.864	7000	0.205	0.203	0.208
1400	0.716	0.676	0.719	7500	0.0834		0.0740
1600	0.521	0.487	0.526	8000	0.0280	0.024	0.0188
1800	0.324	0.302	0.327	8500	0.0078		0.0033
2000	0.160	0.163	0.168	9000	0.0020		0.0004
2200	0.0732	0.076	0.070				
2400	0.0265	0.031	0.024				
2600	0.00810	0.011	0.0063				
2800	0.00211	0.004	0.0013				
3000	0.0004	0.001	0.0002

FIGURE 4.7.1. Problem MT-1: Solution Domain Schematic

MASS TRANSFER PROBLEM MT1

FIGURE 4.7.2. Problem MT-1: Transient Concentration Distribution for 1000 m Solution Domain

FIGURE 4.7.3. Problem MT-1: Transient Concentration Distribution for 10,000 m Solution Domain

4.8 TWO-DIMENSIONAL DISPERSION OF RADIONUCLIDES IN UNIDIRECTIONAL FLOW

4.8.1 Problem Designation

This problem is designated: Mass Transport Problem MT-2.

4.8.2 Objective

The objective of this problem is to test two-dimensional radionuclide transport with the PORFLD code in a unidirectional constant groundwater flow. Longitudinal and tangential dispersivities are unequal. Results are to be compared to an analytical solution for the case of a finite-length line source which is small, relative to the problem domain.

4.8.3 Problem Statement

Groundwater flow occurs in a horizontal region bounded by impermeable boundaries above and below. The flow is constant and unidirectional. Located in the layer is a source of radionuclide. The source size is small, relative to the thickness of the layer and the length of the region of interest. The source is centrally located between the impermeable walls. The half-life of the radionuclide is long ($\sim 10^{20}$ yr) and its decay is to be neglected. The problem is to determine the concentration of the radionuclide subject to dispersion in both the longitudinal and transverse directions. Buoyancy due to heat generation of the radionuclide is to be neglected. An analytical solution for this problem is obtainable. Figure 4.8.1 presents a schematic of the problem and solution domain.

4.8.4 Models Used

The PORFLO code is used in the mass-transport-only mode. Both longitudinal and transverse dispersion are modeled in a two-dimensional coordinate system which exhibits constant, unidirectional flow in the longitudinal coordinate direction. The analytical solution for this problem is derivable. It is solved using computer mathematics library routines for sinusoidal and complementary error functions which occur in the analytical solution.

4.8.5 Analytical Solution

The analytical solution has been developed and the solution has been presented by Bruch and Street (1967). The problem considered is illustrated in Figure 4.8.1 and is stated as follows.

One-dimensional groundwater flow occurs in a horizontal layer defined by the region

$$-h_1 \leq y \leq h_1$$

and

$$x \geq 0.$$

The groundwater velocity is v and is constant and uniform in the region. A radionuclide source occurs at the origin, $x = 0$, over the symmetrically located distance

$$-h_s \leq y \leq h_s.$$

The boundaries at $y = \pm h_1$ are uniform and impermeable. It follows that concentration gradients $y = \pm h_1$ are zero. Due to symmetry, concentration gradient $dC/dy = 0$ at $y = 0$. Thus, the problem only needs be solved for $0 \leq y < h_1$. With the concentration bounded at $x = \infty$, the problem is an initial boundary value problem governed by the differential equation

$$\frac{\partial C}{\partial t} + v \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} \quad (4.8.1)$$

for times

$$t > 0$$

over the region

$$x > 0$$

$$0 \leq y < h_1.$$

By defining

$$v = \frac{U}{R_d \phi} \quad (4.8.2)$$

and

$$D_x = D_{mx}/R_d = (D_m + \frac{\alpha_L U}{\phi}) \frac{1}{R_d} \quad (4.8.3)$$

$$D_y = D_{my}/R_d = (D_m + \frac{\alpha_T U}{\phi}) \frac{1}{R_d}, \quad (4.8.4)$$

the radionuclide transport equation solved by PORFLO is reducible to the analytically solvable Equation (4.8.1).

Initial conditions for the analytical problem are stated as

$$C(x,y,0) = 0 \text{ for } 0 \leq y < h_1, x > 0. \quad (4.8.5)$$

Boundary conditions are

$$\begin{aligned} C(0,y,t) &= C_1 \text{ for } 0 \leq y \leq h_s \\ &= 0 \text{ for } h_s < y < h_1 \end{aligned} \quad (4.8.6)$$

$$\frac{\partial C(x,0,t)}{\partial y} = 0 \text{ for } x \geq 0, t > 0 \quad (4.8.7)$$

$$\frac{\partial C(x,h_1,t)}{\partial y} = 0 \text{ for } x \geq 0, t > 0 \quad (4.8.8)$$

and $|C(\infty,y,t)|$ is bounded.

The problem is solved using separation of variables after decomposing it into a steady and unsteady problem. The solution is:

$$\begin{aligned} C(x,y,t) &= \frac{C_1 h_s}{2 h_1} \left[\operatorname{erfc} \left(\frac{x-vt}{2 \sqrt{D_x t}} \right) + \exp \left(\frac{vx}{D_x} \right) \operatorname{erfc} \left(\frac{x+vt}{2 \sqrt{D_x t}} \right) \right] \\ &+ \frac{1}{2} \sum_{n=1}^{\infty} (F_n \cos \frac{n\pi}{h_1} y) \exp \left[\frac{1}{2} \left(\frac{v}{D_x} - J_n \right) x \right] \operatorname{erfc} \left(\frac{x - J_n D_x t}{2 \sqrt{D_x t}} \right) \\ &+ \frac{1}{2} \sum_{n=1}^{\infty} (F_n \cos \frac{n\pi}{h_1} y) \exp \left[\frac{1}{2} \left(\frac{v}{D_x} + J_n \right) x \right] \operatorname{erfc} \left(\frac{x + J_n D_x t}{2 \sqrt{D_x t}} \right) \end{aligned} \quad (4.8.9)$$

where

$$F_n \equiv \frac{2C_1}{\pi n} \sin \frac{n\pi}{h_1} h_s \text{ for } n = 1, 2, 3 \dots \infty \quad (4.8.10)$$

and

$$J_n \equiv \left[\frac{v}{D_x} + \left(\frac{2n\pi}{h_1} \right)^2 \frac{D_x}{v} \right]^{1/2}. \quad (4.8.11)$$

4.8.6 Assumptions

Assumptions made in solution of this problem include:

- The PORFLO solution domain is finite and the simulation is only valid until a nonnegligible concentration is predicted at 0.9L.
- Material properties are uniform in the solution domain, except that total lateral and transverse diffusion coefficients, D_x and D_y , respectively, are unequal.
- Flow is unidirectional and constant.
- Buoyancy is neglected.
- Radionuclide decay is neglected.
- No retardation occurs.

4.8.7 Input Specifications

Input parameters required for the PORFLO simulation problem are:

Fluid density	$\rho_f = 1000 \text{ kg/m}^3$
Rock density	$\rho_s = 2780 \text{ kg/m}^3$
Porosity	$\phi = 0.001$
Horizontal Darcy velocity	$U = 5.2 \times 10^{-4} \text{ m/yr}$
Lateral Darcy velocity	$V = 0$
Retardation factor	$R_d = 1.0$
Decay factor	$\lambda = 0.0$
Longitudinal dispersion length	$\alpha_L = 192.304 \text{ m}$
Tangential dispersion length	$\alpha_T = 19.227 \text{ m}$
Molecular diffusivity	$D_m = 0.002 \text{ m}^2/\text{yr}$

From these parameters, the following are determined, as required, for the analytical solution:

Advection velocity	$v = 0.52 \text{ m/yr}$
Longitudinal dispersion coefficient	$D_x = 100 \text{ m}^2/\text{yr}$
Transverse dispersion coefficient	$D_y = 10 \text{ m}^2/\text{yr}$

The problem solution domain is defined as

Source width	$h_s = 20 \text{ m}$
Layer depth	$h_1 = 200 \text{ m}$
Longitudinal distance	$L = 5000 \text{ m}$

4.8.8 Output Specifications

Transient concentrations in the solution domain are to be computed at times of 25, 50, and 100 yr. PORFLO results are to be compared to analytical solution results at these times. The transient distributions as a function of longitudinal distance from the source along the symmetry centerline are to be compared to analytical results along the centerline and at $y = 25 \text{ m}$. Transverse distributions are to be compared at a representative axial distance.

4.8.9 Simulation Results and Discussion

PORFLO was used to model the problem as stated. In the horizontal direction, 160 nodes were used. Equal spacing of $\Delta x = 25 \text{ m}$ was used to a distance of 3000 m and, thereafter, equally spaced nodes of $\Delta x = 50 \text{ m}$ were used. In the transverse direction, 40 nodes, equally spaced at $\Delta y = 10 \text{ m}$, were used. In the transverse direction, the PORFLO model was set up to span a total width with boundary nodes at -195 m and $+195 \text{ m}$. Modeling both sides of the channel was done to ascertain if the symmetry in the problem was correctly predicted. Results showed exact symmetry to the significance of output digits. PORFLO was operated in the concentration-only mode with first-order differencing.

A comparison of PORFLO and analytical results at 25, 50, and 100 yr is made. Figure 4.8.2 presents the axial concentration distribution along the centerline, $y = 0$. Agreement of results is very good. Figure 4.8.3 presents a similar distribution at a lateral distance of 25 m from the centerline. This position is 5 m beyond the half width of the source. PORFLO and analytical results are in very good agreement. Deviations are a direct result of noding resolution that is insufficient to resolve the boundary condition discontinuity at $x = 0, y = 20 \text{ m}$. The lateral distributions at $x = 100 \text{ m}$ are also in very good agreement as presented in Figure 4.8.4.

Based on the good agreement of these results, it can be concluded that the PORFLO concentration-only-mode is computing accurately and correctly for this case. The longitudinal and transverse dispersion lengths differed by a factor of 10 and presented no obvious problem to the solution.

FIGURE 4.8.1. Problem MT-2: Solution Domain Schematic

MASS TRANSPORT PROBLEM MT2

FIGURE 4.8.2. Problem MT-2: Axial Centerline Concentration Distribution for 25, 50, and 100 yr

MASS TRANSPORT PROBLEM MT2

FIGURE 4.8.3. Problem MT-2: Axial Concentration Distribution at $y = 25$ m for 25, 50, and 100 yr

MASS TRANSPORT PROBLEM MT2

PLOT FILE=/BWIP/MT2/PLOTS YPLTD100X100 - MT2: C VS Y AT X=100M, T=25,50,100 YRS.

FIGURE 4.8.4. Problem MT-2: Lateral Concentration Distribution at $x = 100$ m for 25, 50, and 100 yr

4.9 ONE-DIMENSIONAL RADIONUCLIDE TRANSPORT WITH DECAYING SOURCE

4.9.1 Problem Designation

This problem is designated: Mass Transport Problem MT-3.

4.9.2 Objective

The objective of this problem is to test PORFLO's capability to model radionuclide transport with a decaying source in a unidirectional constant groundwater flow. Radionuclide decay and retardation effects are to be included. Results are to be compared to SWENT code predictions for a similar problem.

4.9.3 Problem Statement

A repository is situated in a constant unidirectional groundwater flow in a porous rock medium. At arbitrary time $t = 0$, a decaying radionuclide begins to be leached into the groundwater flow. The nuclide is subject to advection, dispersion, and sorption. Retardation which results from the sorption is constant in time and space. Figure 4.9.1 presents a schematic of the problem.

The unidirectional flow is bound by theoretically impermeable layers above and below. The solution domain is 10,000 m long with the source region spanning the 15-m wide layer and is 75 m long. The center of the radionuclide source region is located 1000 m from the left boundary of the solution domain of interest. The radionuclide source strength decreases exponentially in time. The material's half life is 1000 yr.

4.9.4 Models Used

The PORFLO and SWENT codes are to be used in this benchmarking problem.

4.9.5 Assumptions

- Flow and transport are one-dimensional.
- Hydrogeologic parameters are constant.
- The radionuclide containment is present in trace quantity, and its presence and decay heat do not affect the flow.

4.9.6 Flow Specifications

Parameters required for PORFLO and SWENT code solution of the modeled problem are:

Darcy velocity	$u = 0.003 \text{ m/yr}$
Rock density	$\rho_s = 2780 \text{ kgm/m}^3$
Fluid density	$\rho_f = 1000 \text{ kg/m}^3$
Porosity	$\phi = 0.001$
Longitudinal dispersion length	$\alpha_L = 50 \text{ m}$
Molecular diffusivity	$D_m = 0.0$
Sorption coefficient	$K_d = 2.5 \times 10^{-7} \text{ m}^3/\text{kg}$
Half-life	$T_{1/2} = 1000 \text{ yr}$

The model region parameters are:

Solution domain length	$L = 10,000 \text{ m}$
Solution domain width	$W = 15 \text{ m}$
Source length from origin	$L_s = 1000 \text{ m}$
Source volume	$V = 1125 \text{ m}^3$

Transient radionuclide source strength is given in Table 4.9.1. Values listed are a piecewise linear approximation to an exponential decay, relative to an assumed initial value of 1 mg/liter (of total volume) per year.

4.9.7 Output Specification

PORFLO-computed radionuclide distribution in the solution domain is to be compared to SWENT simulation results at times of 500, 1,000, 2,000, and 5,000 yr.

4.9.8 Simulation Results and Discussion

The PORFLO model of this problem was set up using 261 longitudinal nodes and 4 transverse nodes. A zero flux boundary condition was specified on the transverse nodes to model the impermeable layers. The nodes were spaced so as to maintain the width between the impermeable layers at 15 m, as the problem states. In the longitudinal direction, nodes were equally spaced at $\Delta x = 25 \text{ m}$ over the first 3000 m and $\Delta x = 50 \text{ m}$ beyond there. The total simulation distance was 10,000 m. Mass source release rates were specified on

input in tabulated form according to Table 4.9.1. The source injection was over the 75-m distance symmetrically located around the longitudinal distance of 1000 m as stated in the problem. The solution mode chosen was the standard central differencing option, with switch over to donor cell differencing for cell Peclet numbers greater than one.

Constant time-step intervals of 10 yr were specified for use during the first 3000 yr. Thereafter, a maximum step of 15 yr was specified. A total of 410 steps was taken in reaching the 5000-yr simulation time.

For initialization, U-Darcy was specified as 0.003 m/yr everywhere, while all other variables were zeroed. The code was run in a concentration-only mode for this problem.

A SWENT code model was set up using 401 longitudinal nodes with one lateral and one transverse node. The cell width in the lateral direction was taken as unity, and in the transverse (vertical) direction it was specified as 15 m. In the longitudinal direction, equal node spacings of 25 m were specified, except that the first cell was halved so the SWENT node locations exactly matched PORFLO's over the first 3000 m. As a result the source location and volume were exactly matched in both models.

For the SWENT model, source cells were used for both injection of fluid and radionuclide. In the first cell next to the leftmost boundary ($x = 0$), a mass injection (source cell) was specified. The fluid injection rate was the amount required to obtain a U-Darcy velocity through the channel of 0.003 m/yr. Steady-state flow solution option was selected. At the rightmost boundary, an aquifer influence function boundary condition was specified which provided an outflow path for the injection fluid.

The radionuclide source cells were specified to directly correspond to the location of PORFLO source cells at the distance of 1000 m. Recurrent data sets were used to input the source strengths listed in Table 4.9.1. The source rate over each interval (recurrent data set) was taken as the average value between adjacent time points. Thus, a stair-stepped approximation to the piecewise linear table values was used. The effect of this stairstepping is present in the results as discussed subsequently.

PORFLO^(a) and SWENT model results are included in Figures 4.9.2 and 4.9.3. Predicted longitudinal distributions are presented for times of 500, 1000, 2000, and 5000 yr over the simulation distance of 10,000 m. Results are presented in both linear and semi-log plots to show large variations which occur over the distance with time. (Symbols identifying the curves are only drawn at each 10th node point in the figures.) Agreement between the SWENT and PORFLO results is very good at all times.

PORFLO results show a less dispersive effect upstream than does SWENT, and a sharper fall-off in the downstream direction. This may be due to numerical procedures. PORFLO computed using central differencing and SWENT computed in the backwards-in-space, backwards-in-time direct solution mode. At 5000 yr, there is a noticeable waviness to the SWENT results. This is a direct consequence of the stairstepped source injection curve. The concentration predicted at the source location is in good agreement at all times.

The agreement of these results indicates that features tested in PORFLO are working correctly. These include mass (source) injection, radionuclide decay, and retardation. When compared to SWENT results as a basis, PORFLO predicts acceptably accurate radionuclide transport in this operating mode.

(a) An error in PORFLO was encountered in simulating this problem. The error was one in which the decay source term was not multiplied by cell volume. The error was corrected for computation of results presented in this problem and also problems MT-1, MT-2, and MT-4. These latter problem results were unaffected, however, because decay was neglected in each of them.

TABLE 4.9.1. Transient Radionuclide Source Profile

Time (yr)	$\dot{m}$ (mg/liter-year)
0	1.00
74	0.95
152	0.90
235	0.85
322	0.80
415	0.75
515	0.70
621	0.65
737	0.60
863	0.55
1000	0.50
1322	0.40
1737	0.30
2322	0.20
3322	0.10
4322	0.05
6644	0.01

FIGURE 4.9.1. Unidirectional Flow with Radioactive Source Problem Schematic

MASS TRANSFER PROBLEM MT3

PLOT FILE = /BWIP/MT3/PLOTS CPLTMT3A - CONC VS X AT T = 500, 1000, 2000, 5000YR.

FIGURE 4.9.2. Problem MT-3: Transient Radionuclide Distributions

MASS TRANSFER PROBLEM MT3

PLOT FILE = /BWIP/MT3/PLOTS CPLTMT3A - CONC VS X AT T = 500, 1000, 2000, 5000YR.

FIGURE 4.9.3. Problem MT-3: Transient Radionuclide Concentration Distributions

4.10 RADIONUCLIDE TRANSPORT IN BUOYANCY AFFECTED FLOW IN THE VICINITY OF A REPOSITORY

4.10.1 Problem Designation

This problem is designated: Mass Transport Problem MT-4.

4.10.2 Objective

The objective of this problem is to determine radionuclide transport in flow in the vicinity of a pair of repository banks located in a layered hydrogeologic formation. The formation consists of modeled composite layers of basalt rock. Material in the repository banks is porous and contains a material which exhibits a decreasing heat generation rate with time. A radionuclide source occurs during a span of 8150 years over the period from 1050 to 9200 yr. Except for the radionuclide source and resulting transport, this problem is the same as Fluid Flow Problem FF-3.

4.10.3 Problem Statement

Two repository banks are located at a depth of -1149.5 m in a hydrogeologic layered media. The two banks are separated by a distance of 1063 m as shown in Figure 10.1. The solution region of interest includes nine composite layers of material with differing hydrogeologic parameters. The depth of the solution domain of interest ranges from -842 m to -1575 m below the surface. The horizontal distance spans a length of 6570 m as shown in the figure.

Heat generation occurs in the repository banks. The generation is uniform over the repository bank volume and decreases with time. Transient decay rate, composite layer thickness, and hydrogeologic data for this problem are included in the input specifications and are the same as in problem FF-3 with the addition that a radionuclide (I^{129} with $T_{1/2} = 1.59 \times 10^7$ yr) is released over the time span from 1050 to 9200 yr.

Of interest in this problem is predicting the transient radionuclide distribution in the buoyancy-affected flow field. The initial vertical temperature gradient in the formation is -0.04°C/m with the temperature of 75°C at a depth of -1575 m being the reference. The vertical boundaries are to be maintained at this gradient throughout the simulation. Horizontal boundaries

are to be held constant at the initial temperature at that depth. Initial hydraulic head is to be prescribed on each boundary and will be maintained constant on the boundary.

4.10.4 Models Used

The PORFLO code and the SWENT code are to be used. The problem is modeled the same as problem FF-3 (Section 4.6) with the addition of the radionuclide source.

4.10.5 Assumptions

Assumptions made in this problem include:

- The horizontal hydrogeologic layers are composites and are uniform in thickness and extent.
- Flow and energy transport in the media are two-dimensional and only a vertical slice through the media is treated.
- Boundaries are at a sufficient distance from the repository banks, such that the prescribed boundary conditions are constant.
- A nonequilibrium initial hydraulic head distribution is maintained on the boundaries and no hydrodynamic equalization occurs prior to initial repository bank heat loading.
- Heat generation is only accounted for in the repository volume.

4.10.6 Input Specifications

Dimensions of the solution domain, layer depths, and repository locations are in Figure 10.1. The initial temperature distribution is

$$T(x,y) = 75 - 0.04(y + 1575) \quad (4.10.1)$$

where y is the vertical coordinate direction measured positive upward. The initial temperatures are to be held constant at the solution region boundaries as determined from Equation (4.10.1). Transient heat generation rates in the repository volumes are listed in Table 4.10.1. Reference material properties of water in the porous rock are:

Density	$\rho_f = 997 \text{ kg/m}^3$
Specific heat	$c_f = 4186.8 \text{ J/kg-}^\circ\text{C}$
Thermal conductivity	$D_f = 2.05 \times 10^7 \text{ J/m-yr-}^\circ\text{C}$
Molecular diffusivity	$D = 0.02 \text{ m}^2/\text{yr}$

The rock properties in each layer of the solution domain are presented in Table 4.10.2. The hydraulic properties of each layer are given in Table 4.10.3. The initial hydraulic gradient is $-5 \times 10^{-4} \text{ m/m}$ in the horizontal direction and $-1 \times 10^{-3} \text{ m/m}$ in the vertical direction, relative to a hydraulic head of 127.54 m at the lower left-hand corner of the solution domain. The radionuclide release rate is given in Table 4.10.4. The tabulated values represent a piecewise linear release rate curve. The radionuclide transported is to be I^{129} which has a half-life of $1.59 \times 10^7 \text{ yr}$.

TABLE 4.10.1. Heat Generation Decay

Time (yr)	Heat Generation (J/m ³ -yr)
0	1.657 x 10 ⁸
1	1.591
2	1.537
3	1.490
4	1.448
5	1.410
6	1.376
7	1.344
8	1.315
9	1.287
10	1.261
11	1.236
12	1.212
13	1.189
14	1.167
15	1.146
20	1.049
25	9.651 x 10 ⁷
30	8.912
35	8.254
40	7.669
50	6.674
60	5.872
70	5.223
80	4.691
90	4.261
190	2.441
290	1.931
390	1.639
490	1.423
690	1.110
990	8.065 x 10 ⁶
1990	4.057
2990	3.086
3990	2.740
4990	2.531
6990	2.211
9990	1.836
19990	1.084
29990	7.188 x 10 ⁵
39990	5.145
49990	3.855
69990	2.357
99990	1.319
999990	5.584 x 10 ⁴

TABLE 4.10.2. Layer Thermal Properties

Layer No.	Layer Thickness (m)	Rock Density (kg/m ³)	Rock Specific Heat (J/kg- C)	Rock Thermal Conductivity (J/m-yr- C)	Porosity d	Longitudinal Dispersivity α_L	Transverse Dispersivity α_T
1	427	2780	845	5.362×10^7	0.001	50.0	2.0
2	6	2400	845	5.362	0.001	50.0	2.0
3	35	2780	930	5.610	0.0001	50.0	2.0
4	32	2400	930	5.610	0.002	50.0	2.0
5	32	2780	930	5.610	0.0001	50.0	2.0
6	10	2400	930	5.610	0.001	50.0	2.0
7	71	2780	845	5.362	0.001	50.0	2.0
8	75	2780	760	5.050	0.001	50.0	2.0
9	95	2780	845	5.362	0.001	50.0	2.0
10 (a)	3	2780	930	5.610	0.005	50.0	2.0

_____ m
 (a) Repository bank

TABLE 4.10.3. Composite Layer Hydraulic Properties

Layer No.	Horizontal Conductivity K_x (m/yr)	Vertical Conductivity K_y (m/yr)	Specific Storage S_s (1/m)
1	6.308×10^{-2}	1.892×10^{-5}	1×10^{-4}
2	6.308×10^{-2}	6.308×10^0	1×10^{-4}
3	6.308×10^{-6}	1.892×10^{-5}	1×10^{-4}
4	2.839×10^{-1}	2.839×10^0	1×10^{-4}
5	6.308×10^{-6}	1.892×10^{-5}	1×10^{-4}
6	2.839×10^{-1}	2.839×10^0	1×10^{-4}
7	3.200×10^{-2}	2.839×10^{-5}	1×10^{-4}
8	6.000×10^{-2}	1.144×10^{-5}	1×10^{-4}
9	9.200×10^{-2}	1.200×10^{-5}	1×10^{-4}
10(a)	6.308×10^{-6}	1.892×10^{-5}	1×10^{-4}

(a) Repository bank

TABLE 4.10.4. Radionuclide Release Rate

Time (yr)	Release Rate (mg/L-yr)
0.0	0.0
1050.0	0.0
5100.0	1.57×10^{-4}
9200.0	0.0
1000000.0	0.0

4.10.7 Output Specifications

Transient radionuclide distributions are to be compared at times of

$t = 5,000$ years

$t = 50,000$ years.

Vertical radionuclide profiles at these times are to be compared at horizontal locations through the repository banks. The locations are

$x = 2290$ m

$x = 4850$ m.

Horizontal radionuclide distributions at these times are to be compared at vertical location

$y = -1149.5$ m

which is through the center of the repository banks.

4.10.8 Simulation of Results and Discussions

The PORFLO and SWENT models of this problem were set up and run the same as problem FF-3 (Section 4.6). Temperature and velocity distribution results are thus the same, because the radionuclide is treated as a passive scalar. There is no direct coupling effect between the radionuclide and the fluid flow or heat transfer solution. For that reason, the flow and thermal field results and discussion presented in Section 4.6.8 are directly applicable to this problem and are not repeated here. Results and discussion presented herein are limited to those directly related to the radionuclide transport aspects of the problem.

In the PORFLO simulation, the radionuclide source in the repository volumes was input as a five point time table (Table 4.10.4). During the solution, the source was linearly interpolated between these table-time points. Time-step increments over the source release time from 1050 to 9200 yr was allowed to incrementally increase. Initially the maximum time step was specified as 10 yr. By 5000 yr it had been extended a maximum of 50 yr and by the end of the simulation time of 50,000 yr, it had been extended to 180 yr. A total of 920 time-steps were computed over the simulation.

The SWENT code does not have linear interpolation capability in its source cell specifications. Computations are performed with recurrent data sets and a

new set must be input for each time point of tabulated data desired during a simulation. For that reason, the linear source release rate was broken into 20 equal 400 yr intervals and one 150 yr interval at the end of the release. A recurrent data set was specified with a constant source release strength specified over each interval. The value specified was taken as the average value between two points in the linear release curve at the beginning and end of each interval. In this way, the total release could be reasonably well approximated. Over 2400 input cards were required to model the total simulation from 0 to 50,000 yr. Automatic time-stepping was used throughout and a total of 331 time steps were computed. The default direct solution method with BIS/BIT differencing mode was used.

Several points concerning predicted concentration results must be made. SWENT computes radionuclide concentration as a dimensionless mass fraction quantity. To convert it to the same units as PORFLO's mg/liter of total volume, postprocessing of the SWENT results was necessary. This was done during the plotting preparation. As discussed in Appendix A, SWENT data for plotting was obtained by reading restart files. The dimensionless quantity C in kgm/kgm was obtained and reference density was then used to convert the concentration data to PORFLO's units. Because water density was close to 10^3 kgm/m³, the total conversion factor was nearly 10^6 which provided a convenient check on the units conversion made during plot preparation.

Vertical and horizontal distributions of radionuclide concentration are compared at times of 5,000 and 50,000 yr. The former time is near the maximum point of the source release time (Table 4.10.4).

Figure 4.10.2 presents comparison of predicted distribution in the vertical coordinate direction from depths of -1000 to -1300 m. The horizontal location of this plane is through the center of the leftmost repository. The same results are also plotted in a semi-log form in the figure. At 5,000 yr, SWENT and PORFLO predict very similar concentration distributions. The maximum concentration predicted at this plane is 32.7 mg/liter by PORFLO and 25.9 mg/liter by SWENT. The semi-log plot shows that at 5,000 yr, both codes are predicting similar distributions in the layers immediately above and below

the repository layer. PORFLO predicts more sharply decreasing concentrations at distances farther removed. At 50,000 yr, predicted distributions show some variance. SWENT is predicting considerably higher concentrations. The character of the SWENT results seem to imply a much more diffusive distribution than PORFLO which may result from the coarser noding.

Figure 4.10.3 present similar results but of a vertical distribution near the righthand end of the rightmost repository. The horizontal coordinate position is $x = 4850$ m for these results. Both codes have a cell-centered node point at this location. Again, the two codes show very good agreement at 5,000 yr, while significant variations occur at 50,000 yr. Agreement at 5,000 yr is further supported by the horizontal distribution in Figure 4.10.4. These results are through a horizontal plane located at the top of the repository blocks at $y = -1148$ m.

The SWENT results exhibit two discernible characteristics. One is that at 5,000 yr, near the peak of the source release, the predicted concentrations are less than corresponding PORFLO results. This is probably due to the greater vertical Darcy velocity predicted by SWENT (see Figure 4.6.6). This would tend to effect more advection of material out of the repository panels and into adjacent layers. The second characteristic is that the SWENT model is considerably more coarse, e.g., less nodes. This would effect more averaging and exhibit more diffusive results. This characteristic is exhibited by the uniformly dispersed SWENT results at 50,000 yr.

The PORFLO model was run using a differencing option, according to the users manual, which is CIS for $Pe \leq 2$ and doner cell for $Pe > 2$ ^(a). For this simulation, maximum Pe was typically 9, which indicates the flow is advection dominated. Problem MT-1 (Section 4.7) indicated that at Pe numbers of this magnitude, significant inaccuracies could develop. SWENT would be even more so, again because of the coarseness of noding.

(a) Users manual indicates switch at $Pe = 1$. According to Budhi Sagar, personal communication, the switch is coded to occur at $Pe = 2$.

A direct conclusion concerning acceptability of PORFLO for computation in this mode cannot be made. While certain supporting arguments suggest PORFLO is predicting more justifiable results than SWENT for this problem, significant deviations between results exist. More confirmed explanation for these deviations must be obtained before a direct acceptability conclusion can be reached for PORFLO's application to repository-scale radionuclide transport.

One other point must be made. It is important that PORFLO be operated within time step and node space guidelines suggested in the users' manual. During this work, it was also determined that there is an additional limitation to PORFLO's use on the PRIME 750 computer which is not documented. As discussed in Appendix B, nonphysical negative concentrations were predicted by PORFLO for this case when hydraulic conductivities in two adjacent layers was on the order of 10^{-9} . While this was the symptom, it was not the total cause. The problem was traced to one of machine roundoff. The PRIME 750 computer loses accuracy when differencing numbers on the order of 10^{15} . Occurrence of such numbers is thus not only related to hydraulic conductivity but also to a more complicated dependency on number of nodes, spacing, etc. A newer version of PORFLO purportedly is to alleviate this problem^(a).

(a) Budhi Sagar, personal communication.

FIGURE 4.10.1. Problem MT-4: Repository Radionuclide Couple Flow and Heat Transfer with Radionuclide Transport Solution Domain

FIGURE 4.10.2. Problem MT-4: Vertical Distribution of Radionuclide Concentration for a) linear and, b) semi-log plot at $x = 2290$ m

FIGURE 4.10.3. Problem MT-4: Vertical Distribution of Radionuclide Concentration for a) linear and, b) semi-log plot at $x = 4850$ m

FIGURE 4.10.4. Problem MT-4: Horizontal Distribution of Radionuclide Concentration

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APPENDIX A
SWENT CODE MANIPULATIONS

APPENDIX A

SWENT CODE MANIPULATIONS

The SWENT computer code (CIN: 400--01C-02) was used in this work. The steps and procedures used to put it up on the CRAY computer at Los Alamos National Laboratory (LANL) are reported in this appendix.

A card deck file of the SWENT code was obtained via a file transfer from the PNL Water and Lands VAX-11/780 to the PNL-B-VAX-11/780. The file was obtained from Steve Yabusaki who had obtained it from ONWI. The file was dated February 1983. Twelve standard test problem input and output files also originally obtained from ONWI were similarly transmitted to the B-VAX. The card deck file was then transmitted via XNET from the B-VAX to the X-machine, a CRAY-1S, at LANL. Several steps were taken to get it to compile and run on the CRAY, which uses the CTSS operating system.

First, an attempt was made to compile the card deck directly; this failed. There were six FORTRAN errors in the compilation. A check of the coding at the location of these errors was made against the microfilm listing of SWENT (400--01C-02) included in the Users' Manual (INTERA, 1983). The errors were also found to exist in the microfilmed listing. The errors were obvious incorrect coding errors.

Once the errors were identified, the original card deck file was manipulated to put it into a form which was compatible with HISTORIAN. HISTORIAN is software used for making coding changes while maintaining traceability. This software is widely used and available on LANL computers. Manipulations of the card deck file were done with the FRED file text editor. They only involved editing changes to make the file compatible with a HISTORIAN creation run. No coding changes were made up to this point.

Once the original card deck file was in the correct form, a HISTORIAN creation run was made. This creates a file which can be selectively corrected while maintaining strict traceability. With this file, the six FORTRAN errors previously identified were corrected in a HISTORIAN correction run. This run created a version of SWENT with no compilation errors. The next step was to

run standard test problem inputs to confirm that the code was computing correctly. To do this, one more correction run with HISTORIAN had to be made.

This latter correction run was required to set the blank COMMON variable, G, at a length sufficient to satisfy problem requirements. This was in accordance with redimensioning documentation in the code's users' manual. Once this last correction run was made, nine standard test problem input cases were run. Computed results were compared to output listings of the problems as originally distributed by ONWI with the code. In all nine cases, results with the present code were all but identical to original results. Differences did occur, but they are the type of differences expected when computer codes are run on different computers. At relatively few locations, differences in computed numbers were found to be one or two digits different in the fourth, fifth, and most typically the sixth significant digit.

This newly created version of SWENT was used throughout this work. The only modification that had to be made was to redimension the blank COMMON variable G for the large problems. This is strictly in accordance with stated requirements for redimensioning (INTERA, 1983).

One other adjustment was made to SWENT after completion of a given run. This was to obtain data for computerized plotting. To do this, selective HISTORIAN correction runs were made. The object of these runs was to produce an executable file which would do nothing more than read a restart file (dumped during simulation runs previously performed) and selectively write data to be plotted to a scratch file. No actual computation or execution was ever performed with these modified code versions. In fact, the selective plot coding was incorporated in such a way that the code would terminate a run prior to execution when only plot data was desired. In each case, data in the scratch file, prior to plotting, was compared to output listings to confirm that the correct data had been obtained from the restart file.

For traceability, all files, correction sets, creation and correction runstreams, and data files were stored on the Common File System (CFS) at LANL. A directory was set up under the name 8WIP. A subdirectory for the SWENT program and one for each problem was also set up. In this way, files

pertinent to each problem in the problem set could be kept logically separate. Plot files were also kept in separate subdirectories for each problem. The data file name was included on each plot generated to maintain traceability.

APPENDIX B

BENCHMARKING PROBLEMS FF-3 AND MT-4 DEVELOPMENT
CHRONOLOGY AND DISCUSSION

APPENDIX B

BENCHMARKING PROBLEMS FF-3 AND MT-4 DEVELOPMENT CHRONOLOGY AND DISCUSSION

The repository-scale benchmarking problems FF-3 (Section 4.6) and MT-4 (Section 4.10), as presented in the body of this report, were developed in their reported form through cooperative interaction between BCSR personnel running the PORFLO code and PNL personnel running the SWENT code. Changes to the originally developed problem were made. Changes were made for three principal reasons:

- SWENT does not have certain modeling capabilities which PORFLO has.
- The objective of the problems was to simulate relatively similar modeled problems.
- PORFLO computed nonphysical results for certain hydraulic conductivity parameter specifications.

The purpose of this appendix is to present the chronology of the development of benchmarking problems FF-3 and MT-4 and to discuss differences between SWENT and PORFLO. These differences occur both as model setup capabilities (input) and physical modeling approach of each code.

B.1 PROBLEM STATEMENT DEVELOPMENT

The objectives of benchmarking problems FF-3 and MT-4 were to test basic modeling capabilities of PORFLO for repository-scale analysis. The solution domain and physical parameters were to be typical of intended application within BWIP. As such, Rockwell/BWIP and BCSR personnel provided the general problem basis and problem parameters for development of the problem statements. Problem MT-4 was to be identical to FF-3 except that radionuclide transport was to be computed along with the coupled flow and heat transfer. Because of this similarity in the two problems, FF-3 is discussed in depth, while MT-4 is treated as a rather straightforward extension to that problem.

Major differences occur between the problem as it was originally stated and as reported in Section 4.6. These include (basically in the order in which they impacted changes to the problem statement):

- dispersion lengths
- specific storage terms
- impressed vertical hydraulic gradient
- specified hydraulic conductivities

The impact of each of these and resulting changes to the problem are discussed below.

The original intention was to utilize lateral and transverse dispersion lengths (α_L and α_T , respectively) which were different in each composite layer and have values typical of the composite basalt layer modeled. These are values as listed in Table B.1. PORFLO has the capability to treat these. However, it was determined during model setup that the version of SWENT used in this work does not have the capability to prescribe differing α_L and α_T values on input for differing rock types. Internally, the SWENT code is programmed to handle differing α_L and α_T values, but no input mechanism is available. Thus to keep the problem within the capabilities of both the PORFLO and SWENT codes, representative constant flow top values of $\alpha_L = 50$ m and $\alpha_T = 2$ m were chosen for simulation of this problem, as listed in Table 4.6.2. In doing so, this feature of PORFLO was eliminated from testing.

PORFLO has the capability of specifying, on input, values of specific storage (Equation 2.1.1). SWENT does not have specific storage as a parameter directly in its solved pressure equation. Rather, it maintains porosity and density inside differentials and allows each to be functional formulations of input parameters, such as compressibility of water, C_w , and compressibility of rock, C_s . The definition of specific storage is

$$S_s = \rho g (\phi C_w + C_s). \quad (B.1)$$

SWENT allows the user to input the compressibility of water, C_w , and the compressibility of the solid, C_s . On input, however, the user is only allowed to specify one value of C_s . Thus, in terms of Equation (B.1), only one realistic value of specific storage may be modeled, independent of the number of rock types in the simulation. Although the compressibility of water occurs in the definition, along with porosity, this product is typically on the order of $4.4 \times 10^{-10} \phi$ (Pa^{-1}) where $C_w = 4.4 \times 10^{-10} \text{ Pa}^{-1}$ (CRC, 1980). Furthermore, the compressibility of basalt is on the order of $C_s = 4 \times 10^{-15} \text{ Pa}^{-1}$ (NRC, 1981). With these values, it was not possible to model the specific storage values as stated in Table B.1. To keep the problem within capabilities of both codes, it was thus assumed that only one value of specific storage occurs for all rock layers. The value chosen was $S_s = 0.0001 \text{ m}^{-1}$ at reference conditions for PORFLO. This resulted in the use of $C_s = 1.04 \times 10^{-8} \text{ Pa}^{-1}$ for SWENT.

A synergistic effect of attempting to model equivalent specific storage between the two codes results from this approach. SWENT assumes that pore volume is a function of local pressure:

$$\phi = \phi_R (1 + C_s (P - P_R)) \quad (\text{B.2})$$

where ϕ_R is a reference porosity specified for each layer. With a compressibility of rock specified as $1.04 \times 10^{-8} \text{ Pa}^{-1}$, the local porosity may vary by as much as 15 percent because (hydrostatic) pressures at depths in this problem may be as high as $1.5 \times 10^7 \text{ Pa}$. This would occur, for example, if the reference pressure were taken as atmospheric ($1.013 \times 10^5 \text{ Pa}$) which might be the case simply because reference pressure is also used in water density correction, and water properties at atmospheric pressure are readily available in literature. To circumvent this effect, reference pressure in the SWENT model was taken as the hydrostatic head at the depth of $y = -1575 \text{ m}$ which is the lower boundary of the solution domain. This does not eliminate pore compressibility but it reduces its effect.

Another variation in the problem statement was also made. This has to do with the prescribed head gradients listed in Table B.2. These data were originally provided, as listed, by Rockwell/BWIP and correspond basically to borehole RRL-2 head data. The value of hydraulic head at a depth of -892 m was stated as 125.57 m with a gradient of +0.013 m/m above this depth. After both SWENT and PORFLO simulations had been run, it was determined that the value of 125.57 m was an incorrect extrapolation of the gradient above -1028 m. The correctly extrapolated "head at depth" value is

$$\begin{aligned} h(-892) &= h(-1028) - 0.015(y+1028) \\ &= 126.98 - 0.015(-892 + 1028) \\ &= 124.94 \text{ m} \end{aligned}$$

Because of differences in PORFLO and SWENT gridding for the problem, this "head at depth" value resulted in considerably different hydraulic gradient distributions in the upper region of the simulation. Furthermore, it was determined that because of noding differences, the two codes could not be run with the same vertical head gradient distribution unless a single gradient over the whole region were used or node points were matched exactly at depths where gradient changes occurred. It was concluded that a single gradient of $\Delta h/\Delta z = -0.001 \text{ m/m}$ relative to $h = 127.54 \text{ m}$ at -1575 m would be used. Two simulations of this problem as specified were run after these changes had been made. The PORFLO simulation was run by Rockwell/BWIP personnel and the SWENT code was run as part of this work. Results computed with the constant dispersion vertical hydraulic gradient of $-1 \times 10^{-3} \text{ m/m}$, and constant specific storage assumptions are included herein because they are pertinent to the experience gained in running the SWENT code for these benchmark tests.

Figure B.1 presents a comparison of the predicted horizontal component of Darcy velocity as a function of depth at a selected time of 50 yr. The location of the PORFLO results is at a distance of 2290 m from the left boundary. The SWENT results are at 2365 m from the left boundary due to differences in node spacing. Maximum horizontal Darcy velocities predicted by SWENT are as much as 50% lower than those predicted by PORFLO. This difference is not attributable to the position difference because little gradient in horizontal Darcy velocity occurs over the central length of the repository block.

TABLE B.1. Problem Parameters

Layer No.	Horizontal Conductivity K_x (m/yr)	Vertical Conductivity K_y (m/yr)	Specific Storage S_s (1/m)	Longitudinal Dispersion Length α_L	Transverse Dispersion Length α_T
1	6.308×10^0	1.892×10^{-5}	1.0×10^{-3}	2.0	0.2
2	6.308×10^0	6.308×10^0	1.0×10^{-4}	50.0	2.0
3	6.308×10^{-6}	1.892×10^{-5}	2.3×10^{-7}	2.0	0.2
4	2.839×10^1	2.839×10^0	1.0×10^{-4}	100.0	2.0
5	6.308×10^{-6}	1.892×10^{-5}	2.3×10^{-7}	2.0	0.2
6	2.839×10^0	2.839×10^0	1.0×10^{-4}	50.0	2.0
7	3.200×10^0	2.839×10^{-5}	1.0×10^{-3}	2.0	0.2
8	6.000×10^{-2}	1.144×10^{-5}	1.0×10^{-3}	2.0	0.2
9	9.200×10^{-1}	1.200×10^{-5}	1.0×10^{-3}	2.0	0.2
10(a)	6.308×10^{-6}	1.892×10^{-5}	1.0×10^{-4}	2.0	0.2

(a) Repository bank

TABLE B.2. Hydraulic Gradient

Depth (m)	Proposed		As Simulated	
	Hydraulic Head (m)	Gradient Above Depth (m/m)	Hydraulic Head (m)	Gradient Above depth (m/m)
-1575.0	127.54	-0.001	127.54	-0.001
-1028.0	126.98	-0.015		
-892.0	125.57 (124.94)(a)	+0.013		

(a) Correct extrapolation value

The basic horizontal flow distribution is in good agreement. In layer 4, which spans a depth from -1132 m to -1166 m and is a composite model of basalt layer GR-9FR, the hydraulic conductivity is an order of magnitude greater than that modeled in other layers. This difference results in much larger horizontal flow in this layer. The variation in velocity in this region is similar between PORFLO and SWENT and is a result of the temperature-dependence of hydraulic conductivity. The large difference in maximum velocity is directly attributable to an incorrectly specified reference temperature in the SWENT model. As a result, temperature dependent hydraulic conductivities were largely different. This points directly to a caution that for both codes to be expected to yield similar flow results, similar reference conditions must be specified.

PORFLO uses an expression for the hydraulic conductivity at node (i,j) at time-step $l+1$, based on data at time-step l (see Kline, et al. 1983, Equation 37, p. 30):

$$K_{i,j}^{l+1} = K_{i,j}^l \exp \left(\frac{s}{T_R + T_C} \cdot \frac{T_{i,j}^l - T_R}{T_{i,j}^l + T_C} \right) \quad (B.3)$$

where T_R is a reference temperature ($T_R = 26.85^\circ\text{C}$), T_C is a critical temperature for the fluid ($T_C = 273.15^\circ\text{C}$), and s is the viscosity exponent ($s = 1436^\circ\text{C}$). Dropping the (i,j) subscripts for convenience, this expression may be rewritten in terms of the initial hydraulic conductivity as

$$K^{l+1} = K^0 \exp \left(\left(\frac{s}{T_R + T_C} \right) \sum_{n=0}^l \left(\frac{T_n - T_R}{T_n + T_C} \right) \right) \quad (B.4)$$

where the subscript, n , refers to time-step.

By comparison, based on information in the users' manual, SWENT modifies the hydraulic conductivity based on user input parameters to describe the fluid properties. Thus, density is determined as

$$\rho = \rho_R (1 - C_T(T - T_R) + C_W (P - P_R)) \quad (B.5)$$

and viscosity as

$$\mu = \mu_R \exp \left(\frac{1}{T_R} - \frac{1}{T} \right) \quad (B.6)$$

where the reference quantities ρ_R , μ_R , T_R , P_R , and the parameters C_T and C_W are user input. Using the hydraulic conductivity definition, the corresponding temperature-dependent hydraulic conductivity would be

$$K^{l+1} = K^0 (1 - C_T (T_l - T_R) + C_W (P - P_R)) \cdot \exp \left(\frac{T_l - T_R}{T_l T_R} \right) \quad (B.7)$$

The expressions used in PORFLO (Equation B.4) and SWENT (Equation B.7), while similar, may not be exactly the same. No effort was made in this work to quantify the difference in these expressions, but differences in them could lead to differences in predicted Darcy velocities. For example, in Figure B.1, both codes predict characteristically similar horizontal Darcy velocities in layer 4 between depths of -1132 to -1166 m. Near the bottom of the layer, where temperatures are higher, hydraulic conductivities are increased and higher Darcy velocities result. Both codes exhibit this feature, although the absolute magnitude of the peak is different because reference temperatures were different in each model. Results presented herein were for the tabulated viscosity data case.

Figure B.2 presents comparison of predicted vertical components of Darcy velocity as a function of horizontal position. The depth at which this comparison is made is -1148 m, the top surface of the respository volumes. Grid surface locations are the same in both models at this depth. Observed

differences in Darcy velocity deviations determined to be the result of two factors. One was that SWENT uses a constant coefficient of thermal expansion for water specified on input ($\beta_T = 7.5 \times 10^{-4}/^{\circ}\text{C}$ was used). PORFLO computes $\beta_T(T)$ as a material property and, over the temperatures in the reference cell just above the right most repository, it varied from 6.6 to $8.8 \times 10^{-4}/^{\circ}\text{C}$ during the transient. Differences in this value results in differing temperature-dependent densities which directly affect buoyancy coupling and hence Darcy velocities.

Additional, but less dramatic, differences were attributable to mass balance criteria. SWENT uses one of three sequentially restrictive convergence criteria on mass balance. They are based on the supposition that mass must be conserved. In the basic default mode, the least restrictive criterion is that $\Delta\rho_T/\rho_R$ must be less than 0.1%, where $\Delta\rho_T$ is the temperature-dependent density change. For the present problem a temperature change of 1.4°C would cause violation of this criterion. In conjunction, large aspect-ratio cells can lead to significant deviations in the small (in magnitude) vertical Darcy velocities.

One aspect of the predicted vertical distribution of Darcy velocity also deserves discussion. The SWENT code predicted a net downward flow at the repository plane at the depth of -1148 m. This was evident at all times. This was particularly evident at 50,000 yr where the buoyancy effect of repository heating is no longer significant. The downward velocity occurs in spite of the decreasing head gradient ($\Delta h/\Delta z = -0.001 \text{ m/m}$) impressed from the bottom to the top of the solution domain.

In an attempt to determine the cause of this predicted downflow, several isothermal simulations were computed, with SWENT, out to a time of 50 yr. Heat generation in the repository blocks was eliminated and only the flow equation was solved. These isothermal simulations were computed in both CIT/CIS and BIT/BIS differencing modes and used both the direct and L2SOR solution methods available in SWENT. To ensure mass balance, the minimum number of iterations per time-step was increased from a default minimum of 1 to 3. One case was even run with a different grid spacing of the top three cells in the solution

domain. In each of these isothermal test cases, the results were the same; net downflow resulted.

The occurrence of the net downflow was determined to be caused by inconsistent specification of pressure boundary conditions. The inconsistency stemmed from not including compressibility of water in determining density of water in the conversion from hydraulic head to pressure. Because of the importance of this effect in this problem, specific details of the final procedure developed for specifying and testing the SWENT code model pressure boundary conditions is presented separately in Appendix C.

The summary conclusion, based on the predicted flow field data, was that PORFLO and SWENT results were in reasonably good agreement and results differences were explainable. In problem MT-4, a radionuclide source was added to the problem. Because radionuclide transport is treated as passive, predicted flow and temperature fields for problem MT-4 were identical to computed FF-3 results. However, concentration distribution results predicted by PORFLO for problem MT-4 were nonphysical, as discussed subsequently.

Figures B.3 and B.4 are vertical concentration distributions at a time of 5,000 yr. Agreement between SWENT and PORFLO data appears to be reasonably good at this time, as do the horizontal distribution shown in Figure B.15. At 50,000 yr, however, PORFLO predicts negative concentrations (Figure B.6) which are totally nonphysical.

After these results were initially reported, Rockwell/BWIP and BCSR personnel analyzed them and concluded that PORFLO was not predicting a sufficiently accurate flow balance to conserve mass and, hence, incorrectly predicted radionuclide transport. This resulted in the negative, nonphysical radionuclide concentrations. BWIP determined that the basis of the problem was numerical precision on the PRIME computer, on which PORFLO was computing. The symptom was identified when the ratio of hydraulic conductivities in adjacent layers was near the limit of 10^{-8} , as they were between layers 2 and 3 (Table B.1). Inaccurate flow field predictions resulted which subsequently led to inaccurate radionuclide concentrations. Rockwell/BWIP personnel identified this inaccuracy as a problem which limits the applicability of PORFLO, and are reportedly in the process of alleviating it.

The final results presented in Section 4.6 and 4.10 of this report were obtained by redefining hydraulic conductivities (compare Table B.1 and Table 4.6.4). As discussed in Section 4.10, more realistic concentration distributions resulted, but SWENT flow field results changed drastically, particularly at early times. Unfortunately these problems are benchmark problems, and are too complex for an analytical solution. Thus a simple and precise measure of accuracy in either code cannot be made.

PLOT FILE = /BWP/FF3/PLOTS UPLT50RS

PROBLEM FF3: U-DARCY VS Z AT X = 2230M, TIME = 50 YEARS.

FIGURE B.1. Problem FF-3: Vertical Distribution of Horizontal Darcy Velocity at 50 yr

PLOT FILE = /BWIP/FF3/PLOTS WPLT5005

PROBLEM FF3: W-DARCY VS X AT Z = -1148M, TIME = 50YRS.

FIGURE B.2. Problem FF-3: Horizontal Distribution of Vertical Darcy Velocity at 50 yr

PLOT FILE = /BWIP/MT4/PLOTS CPLT5000A

PROBLEM MT4: C VS Z AT X = 2290M, TIME = 5000 YEARS.

FIGURE B.3. Vertical Distribution of Radionuclide Concentration at $x = 2290$ m at 5,000 and 50,000 yr

LOT FILE = BWIP/MT4/PLOTS CPLT5000A
 PROBLEM MT4: C VS Z AT X = 2290M, TIME = 5000 YEARS.

FIGURE B.4. Semi-Logarithmic Plot of Radionuclide Concentration Comparison at $x = 2290$ m at 5,000 yr

FIGURE B.5. Horizontal Distribution of Radionuclide Concentration through the Repositories at $y = -1149.5$ m at 5,000 yr

PLOT FILE = /BWIP/MT4/PLOTS CPLT500000

PROBLEM MT4: C VS X AT Z = -1149.5M, TIME = 50000 YEARS.

FIGURE B.6. Horizontal Distribution of Radionuclide Concentration through the repositories at $y = -1149.5$ m at 50,000 yr

APPENDIX C

PRESSURE BOUNDARY CONDITION SETUP FOR SWENT

APPENDIX C
PRESSURE BOUNDARY CONDITION SETUP FOR SWENT

The procedure developed to prescribe pressure boundary conditions for the SWENT code for use with problems FF-3 and MT-4 is detailed here. This procedure was developed during investigation of anomolous net downward flow occurring in earlier SWENT models of the problems. The cause of the net downward flow was identified as being due to omission of compressibility of water in calculating density of water during setup of pressure boundary conditions. When this factor was included, net negative flows were eliminated.

Steps in procedure include the following:

1. Pressure at level $y = -1575$ was hand calculated assuming a constant density hydrostatic distribution:

$$P = \rho g y$$

where ρ is taken as the reference density. This pressure was input to SWENT as PRESSR and PINIT on cards IP-1 and C-1, respectively.

2. SWENT was run with no pressure boundary conditions specified using the steady-state mode (NCALL = 4, card SW-3). This is a null calculation during which SWENT computes an initial pressure distribution. The computed distribution was written to the output file just before line 102 in subroutine PRINT1 with the following:

```
DO 73 K = 1,NZ
M = (K-1)*NX+1
WRITE(6,9001) M,P(M)
9001 FORMAT(I5,1PE20.13)
73 CONTINUE
```

3. A scratch file called INPRES was created using a text editor. The first card of the file contains the number of horizontal and vertical cells, NX

and NZ, respectively, followed by cards defining the cell dimensions (cards ID-2 and ID-6 of SWENT input file). Following these were cards containing initial pressure distribution computed by SWENT written out in step 3.

4. A program called PRESRC was run. This program reads data from file INPRES, and creates input cards IC-6-1 and IC-6-2 in the format required by SWENT for specifying pressure boundary conditions. These cards are contained in a file called OUTPRES.
5. The correctly formatted cards IC-6-1 and IC-6-2 are merged with the SWENT input file. Card IC-5 is changed to define constant pressure boundary conditions (IAQ=4) and cards IC-6BL and IC-8BL are added behind the last IC-6-2 card.
6. SWENT was run again, but this time with constant pressure boundary conditions specified. This is again a null problem because pressure boundary conditions are balanced and provided a check on their setup.
7. Appropriate hydraulic gradients required for the problem are specified on card 1 of the INPRES file. PRESRC was run again to create SWENT input cards IC-6-1 and IC-6-2. This time the pressures represent values corresponding to appropriate impressed hydraulic gradients.
8. SWENT input cards IC-6-1 and IC-6-2 on file OUTPRES are again merged with the SWENT input file (replacing previous cards). SWENT is run in the steady-state mode and Darcy velocities calculated. The correctness of the specified hydraulic gradients are checked by hand calculations of

$$U = - K_x \frac{dh}{dx}$$

and

$$V = - K_y \frac{dh}{dy},$$

where K_x and K_y are horizontal and vertical hydraulic conductivities, respectively, and dh/dx and dh/dy are the impressed hydraulic gradients as input on card 1 of the file INPRES.

The above procedure was initially checked and verified on a simpler 10 by 10 test problem. It was run in both areal and vertical planes. For the latter, if compressibility of water is not included in determining water density in setting up pressure boundary conditions, SWENT will compute a net (nonzero) Darcy velocity proportional to the compressibility of water and the hydrostatic pressure gradient.

Included hereafter are listings of the program PRESRC, a sample INPRES file and a sample OUTPRES file. In PRESRC, both local temperature and compressibility of water are included in determining density as

$$\rho = \rho_0 (1 + C_W (P - P_R) - C_T (T - T_R)).$$

In this expression, the pressure P is the total local pressure. This is the sum of the initial pressure computed by SWENT and the local hydraulic head.

SAMPLE INPRES FILE

36	41	-.0005	0.	-.001				
	400.	300.	300.	300.	191.	172.5	149.	ID-2
150.667	150.667	150.667	150.667	150.667	150.667	150.667	150.667	ID-2
150.667	150.667	149.	191.	128.	127.	128.	128.	ID-2
191.	149.	149.	149.	149.	149.	149.	149.	ID-2
149.	149.	172.5	191.0	247.	350.	350.	350.	ID-2
370.								ID-2
51.3	43.65	44.	31.	20.	20.	14.	14.	ID-6
10.	7.	5.	5.	7.	9.	8.	8.	ID-6
8.	8.	8.	8.	8.	7.	5.	5.	ID-6
4.	3.	4.	5.	4.	3.	3.	3.	ID-6
3.	4.	6.	9.	15.	30.	52.	52.	ID-6
52.	52.	52.	52.	52.	52.	52.	52.	ID-6
1	7.9448619685000E+06							
37	8.4379276017811E+06							
73	8.8569442681111E+06							
109	9.2788329948702E+06							
145	9.5757796310604E+06							
181	9.7672294811791E+06							
217	9.9585784380239E+06							
253	1.0092462671908E+07							
289	1.0188063995380E+07							
325	1.0254969911185E+07							
361	1.0302752282420E+07							
397	1.0350528346304E+07							
433	1.0417404239125E+07							
469	1.0503369363715E+07							
505	1.0579765650288E+07							
541	1.0656145788031E+07							
577	1.0732509776387E+07							
613	1.0808857614801E+07							
649	1.0885189302716E+07							
685	1.0961504839577E+07							
721	1.1028267684988E+07							
757	1.1075947860444E+07							
793	1.1114087457943E+07							
829	1.1142689506015E+07							
865	1.1180822036652E+07							
901	1.1228482021074E+07							
937	1.1266605465432E+07							
973	1.1295195398467E+07							
1009	1.1323783059839E+07							
1045	1.1352368449520E+07							
1081	1.1390478768633E+07							
1117	1.1447636674740E+07							
1153	1.1533356495160E+07							
1189	1.1676177423839E+07							
1225	1.1961648871888E+07							

1261 1.2455927729951E+07
1297 1.2949523721404E+07
1333 1.3442436693428E+07
1369 1.3934666493168E+07
1405 1.4426212967735E+07
1441 1.4917075964208E+07

SAMPLE OUTPRES FILE

2	2	1	1	1	1	0	0	IC-6-1
	5.	7936148.5		45.708		0.000		IC-6-2
3	3	1	1	1	1	0	0	IC-6-1
	5.	7934712.1		45.708		0.000		IC-6-2
4	4	1	1	1	1	0	0	IC-6-1
	5.	7933275.7		45.708		0.000		IC-6-2
5	5	1	1	1	1	0	0	IC-6-1
	5.	7932100.2		45.708		0.000		IC-6-2
6	6	1	1	1	1	0	0	IC-6-1
	5.	7931230.0		45.708		0.000		IC-6-2
7	7	1	1	1	1	0	0	IC-6-1
	5.	7930460.3		45.708		0.000		IC-6-2
8	8	1	1	1	1	0	0	IC-6-1
	5.	7929742.9		45.708		0.000		IC-6-2
9	9	1	1	1	1	0	0	IC-6-1
	5.	7929021.5		45.708		0.000		IC-6-2
10	10	1	1	1	1	0	0	IC-6-1
	5.	7928300.1		45.708		0.000		IC-6-2
11	11	1	1	1	1	0	0	IC-6-1
	5.	7927578.7		45.708		0.000		IC-6-2
12	12	1	1	1	1	0	0	IC-6-1
	5.	7926857.3		45.708		0.000		IC-6-2
13	13	1	1	1	1	0	0	IC-6-1
	5.	7926135.9		45.708		0.000		IC-6-2
14	14	1	1	1	1	0	0	IC-6-1
	5.	7925414.5		45.708		0.000		IC-6-2
15	15	1	1	1	1	0	0	IC-6-1
	5.	7924693.1		45.708		0.000		IC-6-2
16	16	1	1	1	1	0	0	IC-6-1
	5.	7923971.7		45.708		0.000		IC-6-2
17	17	1	1	1	1	0	0	IC-6-1
	5.	7923254.3		45.708		0.000		IC-6-2
18	18	1	1	1	1	0	0	IC-6-1
	5.	7922440.3		45.708		0.000		IC-6-2
19	19	1	1	1	1	0	0	IC-6-1
	5.	7921676.6		45.708		0.000		IC-6-2
20	20	1	1	1	1	0	0	IC-6-1
	5.	7921066.1		45.708		0.000		IC-6-2
21	21	1	1	1	1	0	0	IC-6-1
	5.	7920455.6		45.708		0.000		IC-6-2
22	22	1	1	1	1	0	0	IC-6-1
	5.	7919692.0		45.708		0.000		IC-6-2
23	23	1	1	1	1	0	0	IC-6-1
	5.	7918878.0		45.708		0.000		IC-6-2
24	24	1	1	1	1	0	0	IC-6-1
	5.	7918164.6		45.708		0.000		IC-6-2
25	25	1	1	1	1	0	0	IC-6-1
	5.	7917451.1		45.708		0.000		IC-6-2

26	26	1	1	1	1	0	0	IC-6-1
	5.	7916737.7		45.708		0.000		IC-6-2
27	27	1	1	1	1	0	0	IC-6-1
	5.	7916024.3		45.708		0.000		IC-6-2
28	28	1	1	1	1	0	0	IC-6-1
	5.	7915310.9		45.708		0.000		IC-6-2
29	29	1	1	1	1	0	0	IC-6-1
	5.	7914597.5		45.708		0.000		IC-6-2
30	30	1	1	1	1	0	0	IC-6-1
	5.	7913884.0		45.708		0.000		IC-6-2
31	31	1	1	1	1	0	0	IC-6-1
	5.	7913114.4		45.708		0.000		IC-6-2
32	32	1	1	1	1	0	0	IC-6-1
	5.	7912244.1		45.708		0.000		IC-6-2
33	33	1	1	1	1	0	0	IC-6-1
	5.	7911195.5		45.708		0.000		IC-6-2
34	34	1	1	1	1	0	0	IC-6-1
	5.	7909766.3		45.708		0.000		IC-6-2
35	35	1	1	1	1	0	0	IC-6-1
	5.	7908090.5		45.708		0.000		IC-6-2
2	2	1	1	41	41	0	0	IC-6-1
	6.14915437.7			75.000		0.000		IC-6-2
3	3	1	1	41	41	0	0	IC-6-1
	6.14914033.5			75.000		0.000		IC-6-2
4	4	1	1	41	41	0	0	IC-6-1
	6.14912629.4			75.000		0.000		IC-6-2
5	5	1	1	41	41	0	0	IC-6-1
	6.14911480.3			75.000		0.000		IC-6-2
6	6	1	1	41	41	0	0	IC-6-1
	6.14910629.6			75.000		0.000		IC-6-2
7	7	1	1	41	41	0	0	IC-6-1
	6.14909877.1			75.000		0.000		IC-6-2
8	8	1	1	41	41	0	0	IC-6-1
	6.14909175.8			75.000		0.000		IC-6-2
9	9	1	1	41	41	0	0	IC-6-1
	6.14908470.6			75.000		0.000		IC-6-2
10	10	1	1	41	41	0	0	IC-6-1
	6.14907765.4			75.000		0.000		IC-6-2
11	11	1	1	41	41	0	0	IC-6-1
	6.14907060.2			75.000		0.000		IC-6-2
12	12	1	1	41	41	0	0	IC-6-1
	6.14906355.0			75.000		0.000		IC-6-2
13	13	1	1	41	41	0	0	IC-6-1
	6.14905649.7			75.000		0.000		IC-6-2
14	14	1	1	41	41	0	0	IC-6-1
	6.14904944.5			75.000		0.000		IC-6-2
15	15	1	1	41	41	0	0	IC-6-1
	6.14904239.3			75.000		0.000		IC-6-2
16	16	1	1	41	41	0	0	IC-6-1
	6.14903534.1			75.000		0.000		IC-6-2

17	17	1	1	41	41	0	0	IC-6-1
	6.14902832.8			75.000		0.000		IC-6-2
18	18	1	1	41	41	0	0	IC-6-1
	6.14902037.1			75.000		0.000		IC-6-2
19	19	1	1	41	41	0	0	IC-6-1
	6.14901290.5			75.000		0.000		IC-6-2
20	20	1	1	41	41	0	0	IC-6-1
	6.14900693.7			75.000		0.000		IC-6-2
21	21	1	1	41	41	0	0	IC-6-1
	6.14900096.9			75.000		0.000		IC-6-2
22	22	1	1	41	41	0	0	IC-6-1
	6.14899350.4			75.000		0.000		IC-6-2
23	23	1	1	41	41	0	0	IC-6-1
	6.14898554.7			75.000		0.000		IC-6-2
24	24	1	1	41	41	0	0	IC-6-1
	6.14897857.2			75.000		0.000		IC-6-2
25	25	1	1	41	41	0	0	IC-6-1
	6.14897159.8			75.000		0.000		IC-6-2
26	26	1	1	41	41	0	0	IC-6-1
	6.14896462.4			75.000		0.000		IC-6-2
27	27	1	1	41	41	0	0	IC-6-1
	6.14895765.0			75.000		0.000		IC-6-2
28	28	1	1	41	41	0	0	IC-6-1
	6.14895067.6			75.000		0.000		IC-6-2
29	29	1	1	41	41	0	0	IC-6-1
	6.14894370.2			75.000		0.000		IC-6-2
30	30	1	1	41	41	0	0	IC-6-1
	6.14893672.8			75.000		0.000		IC-6-2
31	31	1	1	41	41	0	0	IC-6-1
	6.14892920.3			75.000		0.000		IC-6-2
32	32	1	1	41	41	0	0	IC-6-1
	6.14892069.6			75.000		0.000		IC-6-2
33	33	1	1	41	41	0	0	IC-6-1
	6.14891044.6			75.000		0.000		IC-6-2
34	34	1	1	41	41	0	0	IC-6-1
	6.14889647.4			75.000		0.000		IC-6-2
35	35	1	1	41	41	0	0	IC-6-1
	6.14888009.2			75.000		0.000		IC-6-2
1	1	1	1	1	1	0	0	IC-6-1
	1. 7937824.3			45.708		0.000		IC-6-2
1	1	1	1	2	2	0	0	IC-6-1
	1. 8431354.3			47.607		0.000		IC-6-2
1	1	1	1	3	3	0	0	IC-6-1
	1. 8850798.7			49.360		0.000		IC-6-2
1	1	1	1	4	4	0	0	IC-6-1
	1. 9273052.5			50.860		0.000		IC-6-2
1	1	1	1	5	5	0	0	IC-6-1
	1. 9570247.0			51.880		0.000		IC-6-2
1	1	1	1	6	6	0	0	IC-6-1
	1. 9761891.1			52.680		0.000		IC-6-2

1	1	1	1	7	7	0	0	IC-6-1
	1.	9953404.9		53.360		0.000		IC-6-2
1	1	1	1	8	8	0	0	IC-6-1
	1.	10087405.5		53.840		0.000		IC-6-2
1	1	1	1	9	9	0	0	IC-6-1
	1.	10183089.1		54.180		0.000		IC-6-2
1	1	1	1	10	10	0	0	IC-6-1
	1.	10250053.2		54.420		0.000		IC-6-2
1	1	1	1	11	11	0	0	IC-6-1
	1.	10297884.0		54.620		0.000		IC-6-2
1	1	1	1	12	12	0	0	IC-6-1
	1.	10345718.1		54.860		0.000		IC-6-2
1	1	1	1	13	13	0	0	IC-6-1
	1.	10412671.5		55.180		0.000		IC-6-2
1	1	1	1	14	14	0	0	IC-6-1
	1.	10498718.8		55.520		0.000		IC-6-2
1	1	1	1	15	15	0	0	IC-6-1
	1.	10575192.5		55.840		0.000		IC-6-2
1	1	1	1	16	16	0	0	IC-6-1
	1.	10651649.9		56.160		0.000		IC-6-2
1	1	1	1	17	17	0	0	IC-6-1
	1.	10728091.2		56.480		0.000		IC-6-2
1	1	1	1	18	18	0	0	IC-6-1
	1.	10804516.3		56.800		0.000		IC-6-2
1	1	1	1	19	19	0	0	IC-6-1
	1.	10880925.3		57.120		0.000		IC-6-2
1	1	1	1	20	20	0	0	IC-6-1
	1.	10957313.2		57.420		0.000		IC-6-2
1	1	1	1	21	21	0	0	IC-6-1
	1.	11024133.9		57.660		0.000		IC-6-2
1	1	1	1	22	22	0	0	IC-6-1
	1.	11071857.4		57.840		0.000		IC-6-2
1	1	1	1	23	23	0	0	IC-6-1
	1.	11110030.8		57.980		0.000		IC-6-2
1	1	1	1	24	24	0	0	IC-6-1
	1.	11138666.6		58.120		0.000		IC-6-2
1	1	1	1	25	25	0	0	IC-6-1
	1.	11176842.5		58.300		0.000		IC-6-2
1	1	1	1	26	26	0	0	IC-6-1
	1.	11224545.8		58.480		0.000		IC-6-2
1	1	1	1	27	27	0	0	IC-6-1
	1.	11262703.0		58.620		0.000		IC-6-2
1	1	1	1	28	28	0	0	IC-6-1
	1.	11291321.8		58.740		0.000		IC-6-2
1	1	1	1	29	29	0	0	IC-6-1
	1.	11319938.4		58.860		0.000		IC-6-2
1	1	1	1	30	30	0	0	IC-6-1
	1.	11348557.5		59.000		0.000		IC-6-2
1	1	1	1	31	31	0	0	IC-6-1
	1.	11386715.9		59.200		0.000		IC-6-2

1	1	1	1	32	32	0	0	IC-6-1
	1.11443946.0			59.500		0.000		IC-6-2
1	1	1	1	33	33	0	0	IC-6-1
	1.11529781.3			59.980		0.000		IC-6-2
1	1	1	1	34	34	0	0	IC-6-1
	1.11672818.6			60.880		0.000		IC-6-2
1	1	1	1	35	35	0	0	IC-6-1
	1.11958683.5			62.520		0.000		IC-6-2
1	1	1	1	36	36	0	0	IC-6-1
	1.12453460.0			64.600		0.000		IC-6-2
1	1	1	1	37	37	0	0	IC-6-1
	1.12947552.3			66.680		0.000		IC-6-2
1	1	1	1	38	38	0	0	IC-6-1
	1.13440960.2			68.760		0.000		IC-6-2
1	1	1	1	39	39	0	0	IC-6-1
	1.13933683.5			70.840		0.000		IC-6-2
1	1	1	1	40	40	0	0	IC-6-1
	1.14425722.2			72.920		0.000		IC-6-2
1	1	1	1	41	41	0	0	IC-6-1
	1.14917076.0			75.000		0.000		IC-6-2
36	36	1	1	1	1	0	0	IC-6-1
	2. 7906366.8			45.708		0.000		IC-6-2
36	36	1	1	2	2	0	0	IC-6-1
	2. 8399942.5			47.607		0.000		IC-6-2
36	36	1	1	3	3	0	0	IC-6-1
	2. 8819429.2			49.360		0.000		IC-6-2
36	36	1	1	4	4	0	0	IC-6-1
	2. 9241719.1			50.860		0.000		IC-6-2
36	36	1	1	5	5	0	0	IC-6-1
	2. 9538938.1			51.880		0.000		IC-6-2
36	36	1	1	6	6	0	0	IC-6-1
	2. 9730601.5			52.680		0.000		IC-6-2
36	36	1	1	7	7	0	0	IC-6-1
	2. 9922131.7			53.360		0.000		IC-6-2
36	36	1	1	8	8	0	0	IC-6-1
	2.10056143.9			53.840		0.000		IC-6-2
36	36	1	1	9	9	0	0	IC-6-1
	2.10151835.7			54.180		0.000		IC-6-2
36	36	1	1	10	10	0	0	IC-6-1
	2.10218805.5			54.420		0.000		IC-6-2
36	36	1	1	11	11	0	0	IC-6-1
	2.10266641.1			54.620		0.000		IC-6-2
36	36	1	1	12	12	0	0	IC-6-1
	2.10314481.1			54.860		0.000		IC-6-2
36	36	1	1	13	13	0	0	IC-6-1
	2.10381442.1			55.180		0.000		IC-6-2
36	36	1	1	14	14	0	0	IC-6-1
	2.10467497.7			55.520		0.000		IC-6-2
36	36	1	1	15	15	0	0	IC-6-1
	2.10543979.0			55.840		0.000		IC-6-2

36	36	1	1	16	16	0	0	IC-6-1
	2.10620444.2			56.160		0.000		IC-6-2
36	36	1	1	17	17	0	0	IC-6-1
	2.10696893.2			56.480		0.000		IC-6-2
36	36	1	1	18	18	0	0	IC-6-1
	2.10773326.0			56.800		0.000		IC-6-2
36	36	1	1	19	19	0	0	IC-6-1
	2.10849742.7			57.120		0.000		IC-6-2
36	36	1	1	20	20	0	0	IC-6-1
	2.10926137.8			57.420		0.000		IC-6-2
36	36	1	1	21	21	0	0	IC-6-1
	2.10992964.3			57.660		0.000		IC-6-2
36	36	1	1	22	22	0	0	IC-6-1
	2.11040692.2			57.840		0.000		IC-6-2
36	36	1	1	23	23	0	0	IC-6-1
	2.11078868.9			57.980		0.000		IC-6-2
36	36	1	1	24	24	0	0	IC-6-1
	2.11107508.1			58.120		0.000		IC-6-2
36	36	1	1	25	25	0	0	IC-6-1
	2.11145688.3			58.300		0.000		IC-6-2
36	36	1	1	26	26	0	0	IC-6-1
	2.11193396.0			58.480		0.000		IC-6-2
36	36	1	1	27	27	0	0	IC-6-1
	2.11231556.5			58.620		0.000		IC-6-2
36	36	1	1	28	28	0	0	IC-6-1
	2.11260178.2			58.740		0.000		IC-6-2
36	36	1	1	29	29	0	0	IC-6-1
	2.11288797.7			58.860		0.000		IC-6-2
36	36	1	1	30	30	0	0	IC-6-1
	2.11317420.2			59.000		0.000		IC-6-2
36	36	1	1	31	31	0	0	IC-6-1
	2.11355583.4			59.200		0.000		IC-6-2
36	36	1	1	32	32	0	0	IC-6-1
	2.11412820.8			59.500		0.000		IC-6-2
36	36	1	1	33	33	0	0	IC-6-1
	2.11498667.6			59.980		0.000		IC-6-2
36	36	1	1	34	34	0	0	IC-6-1
	2.11641726.6			60.880		0.000		IC-6-2
36	36	1	1	35	35	0	0	IC-6-1
	2.11927631.0			62.520		0.000		IC-6-2
36	36	1	1	36	36	0	0	IC-6-1
	2.12422457.6			64.600		0.000		IC-6-2
36	36	1	1	37	37	0	0	IC-6-1
	2.12916600.0			66.680		0.000		IC-6-2
36	36	1	1	38	38	0	0	IC-6-1
	2.13410058.0			68.760		0.000		IC-6-2
36	36	1	1	39	39	0	0	IC-6-1
	2.13902831.5			70.840		0.000		IC-6-2
36	36	1	1	40	40	0	0	IC-6-1
	2.14394920.2			72.920		0.000		IC-6-2

36	36	1	1	41	41	0	0
	2.14886324.2			75.000		0.000	

IC-6-1
IC-6-2

PROGRAM PRESRC

```
PROGRAM PRESRC(INPRES,OUTPRES,TAPE5=INPRES,TAPE6=OUTPRES)
DIMENSION DX(100),DZ(100),Z(101),X(101),P(101,101),T(101)
HZBASE      = 0.0
HZGRAD      = 0.0
HXGRAO      = 0.0
C**
C**      READ PROB SIZE, GRADIENTS, AND GRID SPACINGS
C**
      READ(5,1000) IX,KZ,HXGRAO,HZBASE,HZGRAD
1000  FORMAT(2I5,3F10.0)
      READ(5,1001) (DX(I),I=1,IX)
1001  FORMAT(7F10.0)
      READ(5,1001) (DZ(K),K=1,KZ)
C**
C**      INITIALIZE PROBLEM DEPENDENT VARIABLES
C**
      TO      = 75.
      TRF     = 26.85
      TGRAD   = -.04
      XO      = -200.
      HZ      = 0.0
      RHOZ    = 997.
      CT      = -0.00075
      CW      = 4.4E-10
      ZO      = -817.05
      IXM     = IX-1
      X(1)    = XO+0.5*DX(1)
      Z(1)    = ZO-0.5*DZ(1)
      KZ1     = KZ+1
      IX1     = IX+1
C**
C**      SET UP COORDINATE SYSTEM
C**
      DO 10 I = 2,IX
10    X(I)    = X(I-1)+(DX(I)+DX(I-1))*0.5
      DO 20 K = 2,KZ
20    Z(K)    = Z(K-1)-0.5*(DZ(K)+DZ(K-1))
      N1      = 1
      N2      = 1
25  CONTINUE
C**
C**      READ INITIAL PRESSURE DISTRIBUTION
C**
      DO 30 K = 1,KZ
      READ(5,1002) ID,(P(I,K),I=N1,N2)
1002  FORMAT(I5,F20.0)
30    CONTINUE
      PREF    = P(1,KZ)
```

```

35 CONTINUE
C**
C** DO FOR I = 1
C**
      I      = 1
      DO 58 K = 1,KZ
      ZK      = Z(K)
      HZ      = HZBASE+HZGRAD*(ZK+1575.)
      T(K)    = TO+TGRAD*(ZK+1575.)
      RHO     = RHOZ*(1.+CT*(T(K)-TRF)+CW*(P(I,K)+RHOZ*9.81*HZ-PREF))
      XX      = X(I)-X(1)
      HX      = HXGRAD*XX
      P(I,K)  = P(I,K)+RHO*9.81*(HZ+HX)
CDEBUG WRITE(6,1005) I,K,X(I),Z(K),ZK,HZ,HX,T(K),RHO,P(I,K)
58 CONTINUE
C**
C** DO FOR I = IX
C**
      I      = IX
      DO 59 K = 1,KZ
      ZK      = Z(K)
      HZ      = HZBASE+HZGRAD*(ZK+1575.)
      T(K)    = TO+TGRAD*(ZK+1575.)
      RHO     = RHOZ*(1.+CT*(T(K)-TRF)+CW*(P(I,K)+RHOZ*9.81*HZ-PREF))
      XX      = X(I)-X(1)
      HX      = HXGRAD*XX
      P(I,K)  = P(I,K)+RHO*9.81*HX
CDEBUG WRITE(6,1005) I,K,X(I),Z(K),ZK,HZ,HX,T(K),RHO,P(I,K)
59 CONTINUE
      K      = 1
      ZK      = Z(K)
      HZ      = HZBASE+HZGRAD*(ZK+1575.)
      T(K)    = TO+TGRAD*(ZK+1575.)
      DO 40 I = 2,IXM
      RHO     = RHOZ*(1.+CT*(T(K)-TRF)+CW*(P(I,K)+RHOZ*9.81*HZ-PREF))
      XX      = X(I)-X(1)
      HX      = HXGRAD*XX
      P(I,K)  = P(I,K)+RHO*9.81*HX
CDEBUG WRITE(6,1005) I,K,X(I),Z(K),ZK,HZ,HX,T(K),RHO,P(I,K)
40 CONTINUE
      K      = KZ
      ZK      = Z(K)
      HZ      = HZBASE+HZGRAD*(ZK+1575.)
      T(K)    = TO+TGRAD*(ZK+1575.)
      DO 61 I = 2,IXM
      RHO     = RHOZ*(1.+CT*(T(K)-TRF)+CW*(P(I,K)+RHOZ*9.81*HZ-PREF))
      XX      = X(I)-X(1)
      HX      = HXGRAD*XX
      P(I,K)  = P(I,K)+RHO*9.81*HX
CDEBUG WRITE(6,1005) I,K,X(I),Z(K),ZK,HZ,HX,T(K),RHO,P(I,K)

```

```

1005 FORMAT(2I3,1P7E12.5,OPF10.1)
61 CONTINUE
C**
C**      INITIAL AIF
C**
      K      = 1
      IONE   = 1
      IZERO  = 0
      ZERO   = 0.
C**
C**      WRITE PRESSURE BC CARDS IN SWENT FORMAT
C**
C**      TOP PLANE
      PLAN   = 5.
      DO 55 I = 2,IXM
      WRITE(6,1003) I,I,IONE,IONE,K,K,IZERO,IZERO
1003 FORMAT(8I5,T73,"IC-6-1")
      TK     = TD+TGRAD*(Z(K)+1575.)
      WRITE(6,1004) PLAN,P(I,K),TK,ZERO
1004 FORMAT(F10.0,F10.1,2F10.3,T73,"IC-6-2")
      55 CONTINUE
C**
C**      BOTTOM PLANE
C**
      K      = KZ
      PLAN   = 6.
      DO 65 I = 2,IXM
      WRITE(6,1003) I,I,IONE,IONE,K,K,IZERO,IZERO
      TK     = TO+TGRAD*(Z(K)+1575.)
      WRITE(6,1004) PLAN,P(I,K),TK,ZERO
      65 CONTINUE
C**
C**      LEFT PLANE
C**
      I      = 1
      PLAN   = 1.
      DO 75 K = 1,KZ
      WRITE(6,1003) I,I,IONE,IONE,K,K,IZERO,IZERO
      WRITE(6,1004) PLAN,P(1,K),T(K),ZERO
      75 CONTINUE
C**
C**      RIGHT PLANE
C**
      I      = IX
      PLAN   = 2.
      DO 85 K = 1,KZ
      WRITE(6,1003) I,I,IONE,IONE,K,K,IZERO,IZERO
      WRITE(6,1004) PLAN,P(IX,K),T(K),ZERO
      85 CONTINUE
      CALL EXIT
      END

```


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