

1.0 INTRODUCTION

TITLE: RHO-BW-CR-150 P - "PORFLO - A Continuum Model for Fluid Flow, Heat Transfer, and Mass Transport in Porous Media"

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DATE: September 1985

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DATE: February 28, 1986

SCOPE: General review of concepts presented in document and suitability of the concepts and code logic, assumptions, and operation to assess performance of the repository at the BWIP site. Reviewed within the context of probable hydrogeologic conceptual models of the BWIP site, as presented in this review.

KEYWORDS: 2-Dimensional, Porous Media, Fluid Flow, Heat Transfer, Mass Transport, Conceptual Models, Test Cases, Computer, Model, Porflo.

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2.0 SUMMARY OF DOCUMENT AND REVIEW CONCLUSIONS

2.1 SUMMARY OF DOCUMENT

The document received presents the PORFLO model theory, including equation development for each of three processes; fluid flow, heat transfer, and mass transport. The document provides the basis and assumptions of the governing equations and demonstrates the coupled and decoupled options of the model. The results of three test cases are discussed. This document is not a "user's" manual for the PORFLO program nor does it contain a listing of the code.

2.2 SUMMARY OF REVIEW COMMENTS

PORFLO is a two-dimensional (2D) finite difference continuum model that couples fluid/heat flow and radionuclide transport. The model incorporates mathematical assumptions which are common to other numerical models having similar capabilities (e.g. MAGNUM2D). Equations presented in the document and results of the test examples suggest that PORFLO, when properly used, is capable of adequately simulating the physics of two-dimensional continuum groundwater flow/transport problems with heat. If it can be demonstrated that a two-dimensional, equivalent porous medium approach is valid (or conservative) for assessing certain performance aspects of the BWIP site, it is Terra Therma's view that PORFLO can be a useful analytical tool for accomplishing the required analyses.

Several limitations of the PORFLO to model conditions at the BWIP site have been identified and are summarized below. In most cases, these limitations would apply not only to PORFLO, but to all 2-D continuum finite difference models.

1. The model is restricted to a two-dimensional geometry that would generally be applied to a horizontal plane or vertical section of the flow region. For the range of conceptual flow models currently being considered at the BWIP site, a 2-D approach may be valid or invalid, conservative or nonconservative, depending on the model selected. If models ultimately adopted for BWIP can be adequately (or conservatively) simulated in two dimensions, PORFLO will be a useful tool for quantifying these models. If, however, the adopted conceptual models require three dimensional simulations, PORFLO may have significant limitations.
2. The model uses an equivalent porous medium (continuum) approach to model fluid flow, heat transfer, and mass transport in a fractured media. This would generally require that mesh elements are sufficiently large to represent a representative elemental volume (REV) of the fractured medium. the size of REV's for various hydrostratigraphic units (HSU's) at the BWIP site have not been determined and may vary significantly within an HSU depending on the process under consideration (fluid flow, heat flow, radionuclide transport). Increasing the size (scale) of mesh elements increases the probability of satisfying REV requirements but reduces the capability of incorporating detail. Thus, it is anticipated that PORFLO,

if applicable, will be used for mid and far field simulations, but will not be appropriate for modeling groundwater flow/transport very close to the repository. It is also possible that dimensions of the HSU's (e.g. thickness of flow interiors) may be too small to allow definition of REV's at any grid scale.

3. It is not clear whether the model can simulate the effects of time-varying boundary conditions or parameter values by updating these effects "mid-run". This may be required, for example, if near-field repository models are used to define mid-field boundary conditions as input to PORFLO.
4. The sequential coupling of fluid flow, heat flow, and solute transport within a time-step, along the forward-time method of updating parameter values, may lead to instability or inaccuracy if time steps are too large or the mesh too coarse. Instability may also occur if greatly contrasting parameter values exist in adjacent elements. Defensible application of PORFLO may require parallel runs using different time steps and mesh sizes to insure that a stable and accurate solution has been achieved.
5. Although a minor limitation, the finite difference mesh geometry used in PORFLO may be inconvenient if the modeled region has very irregular shape or requires detail (i.e., smaller elements) in specific areas.

The use of PORFLO to assess performance of the BWIP site is discussed within the context of six conceptual models presented in this review. Since conceptual models for the BWIP site are not within the scope of this review,

the proposed models are not fully developed and documented, but are presented for comparison purposes only. The models represent possible "generic" models of the BWIP system to serve as a basis for evaluating the PORFLO model.

3.0 SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM

It is generally expected that licensing of a HLW repository will depend, to a significant extent, upon performance assessments based on computer modeling. It is generally considered that at least some of this modeling will require analysis in zones where the effects elevated temperatures on fluid flow and solute transport must be considered. Programs with this capability, including PORFLO, will presumably be used for this task, and hence form a potentially important tool in licensing.

4.0 GENERAL COMMENTS ON REPORT

4.1 DESCRIPTION OF PORFLO

The PORFLO model is a coupled fluid, heat, and radionuclide transport simulator. The fluid flow component is similar in concept to a number of other published two-dimensional, finite difference groundwater flow simulation models, including Prickett-Lonnquist and McDonald-Harbaugh. Minor differences between the fluid flow aspects of PORFLO and other models include the treatment of buoyancy effects and density and viscosity variations.

Additional features of the model include components for simulating convective and conductive heat flow and radionuclide transport, which are coupled to the fluid flow component to simulate the dependence of these phenomena on fluid flow. Reciprocal effects of thermal energy and heat transfer on fluid flow are also modeled.

Three governing equations, one each for fluid flow, heat transfer, and radionuclide transport, are numerically solved in PORFLO. These equations are coupled sequentially, rather than solved simultaneously. At each time step, the fluid flow equation is first solved, resulting in a new pressure field throughout the model. Convective velocities are determined from these pressure values. The velocities are used as coefficients in the heat flow equation, which is next solved for temperature. The temperature field is used to update the coupling terms, i.e., the hydraulic conductives, through their dependence on fluid density and viscosity, buoyancy, and fluid expansion.

Pressure dependence of water density and viscosity is negligible as compared with temperature dependence, and has been ignored in PORFLO.

The adjusted hydraulic conductivity values will be used in the next subsequent time step. The concentration equation for radionuclide transport is solved last. There is only a one-way coupling between the flow (pressure) equation and the concentration; i.e., the pressure values generated in the flow equation affect the concentration equation, but concentration does not affect the flow equation. The pressure and concentrations are coupled through the convective velocities generated from the pressure field.

4.2 LIMITATIONS

PORFLO exhibits several limitations that are common in two-dimensional, finite difference models, including a "grid" geometry that is sometimes inconvenient if the region being modeled has an irregular shape, and may lead to an unstable solution under certain conditions. The grid geometric limitations can generally be overcome by varying grid sizes and selectively refining the mesh according to the geometry of the modeled region and the need for detail in specific areas. Numerical solution instabilities can be overcome by avoiding large disparities in grid sizes and selecting a time increment sequence that is compatible with the rate of change in heads throughout the region, under artificially imposed stresses as well as natural conditions.

However, there are two major limitations of the PORFLO model that may seriously limit its applicability for assessing repository performance at the

BWIP site: (1) the model's restriction to handling two-dimensional geometry and (2) its use of the "equivalent porous medium" approach in simulating flow of mass, heat, and radionuclides through a fractured medium. Specific ramifications of these two features, and other minor limitations are discussed in following paragraphs, relative to a series of conceptual models that have been considered for the BWIP site at Hanford.

From the existing documentation, it is not clear to what extent the PORFLO model incorporates the capability to simulate certain hydraulic boundary stresses that may be associated with "repository performance" including: (1) simulation of desaturation, including hysteresis effects and alteration of material properties; and resaturation, (2) time variant fluid or material properties or those that change in mid-run, (to simulate staged excavation and placement of waste, for example), (3) pressure-dependent permeability values, (4) repository geometry. Some of these complicated factors and processes can be adequately represented by simplified data sets or boundary conditions, so that the PORFLO model can provide an acceptable simulation. However each proposed application of this model should be judged individually, to determine whether the required complexity of the simulation and/or accuracy of the result exceeds the capability of the PORFLO model.

Of significant concern to this review is that the case studies presented in the available documentation of PORFLO do not address the question of whether PORFLO can successfully simulate hydrogeologic conditions potentially existing at the BWIP site. The documentation contained several case studies, some of which show that the PORFLO model can reproduce certain idealized solutions.

Other case studies compare PORFLO results to the results of another model (MAGNUM 2D). None of the case studies attempted to match model results with an extensive set of field measurements, particularly for a site with as complex a set of hydrologic conditions as the BWIP site. It is recognized that data for history-matching may be scarce, and will probably be available for flow only. Prior to applying this model in a "production" mode, however, at least one, but preferably several test cases should be run, to test model results against field hydrologic measurements at the BWIP site. This might include simulation and comparison of the stresses imposed by LHS testing.

4.3 POTENTIAL CONCEPTUAL MODELS

4.3.1 Introduction

Evaluation of site performance at BWIP will require quantification of a site conceptual model (or series of conceptual models). A groundwater conceptual model for the site must provide the minimum features of the hydrogeologic system which are needed to quantitatively determine the relevant behavior of the flow system. This includes a description of:

1. subsurface materials including stratigraphy, lateral variability, and relative values of hydraulic properties for each material type.
2. flow system boundary conditions including physical boundaries and recharge/discharge relationships.

3. transient and steady-state potential gradients driving groundwater flow.

For performance assessment, it is not generally necessary that the conceptual model include all aspects of the real flow system. However, if simplifying assumptions are applied, it must be demonstrated that these modifications will have a negligible influence or lead to conservative results when the conceptual model is quantified (e.g., provide underestimates of radionuclide travel times). It is Terra Therma's view that site conceptual models and (associated numerical models) should be raised only to the level of sophistication required to conservatively evaluate groundwater flow/transport mechanisms and to answer the relevant questions regarding site performance.

Development of conceptual models for the BWIP site is an ongoing activity to be coordinated with information obtained from the hydrologic and geologic testing program. To date, there is insufficient information to allow delineation of a single flow/transport conceptual model for the site. Thus, a series of potential models have been formulated based on available data. As new data are obtained (e.g., from LHS testing), it is anticipated that the individual models can be refined and/or eliminated.

4.3.2 Conceptual Models Currently Considered

Currently, a high degree of uncertainty exists regarding groundwater flow and transport at the BWIP site. As such, potential conceptual models to be considered at this stage of site characterization cover a wide range of

possible hydrogeologic conditions. Conceptual models consistent with current information and uncertainty are summarized below.

1. Continuously layered; both interflows and flow interiors are relatively homogeneous with assigned bulk parameter values.
2. Continuously layered; interflows are highly heterogeneous with a wide range of parameter values; flow interiors are relatively homogeneous with assigned bulk parameter values.
3. Continuously layered; interflows are relatively homogeneous with assigned parameter values; flow interiors are heterogeneous with isolated high permeability features.
4. Continuously layered; interflows are heterogeneous with a wide range of parameter values; flow interiors are heterogeneous with isolated high permeability structures.
5. High permeability discontinuities within the flow system combined with either 1, 2, 3, or 4.
6. Low permeability discontinuities within the flow system combined with either 1, 2, 3, or 4.

These conceptual models for performance assessment are illustrated in Figures 1 through 6, respectively. As new data become available for the BWIP site, it is anticipated that certain aspects of the above models will be refined, combined, or eliminated from consideration.

4.4 APPLICATION OF PORFLO FOR QUANTIFYING CONCEPTUAL MODELS

4.4.1 Geometric Limitations.

The following discussion of appropriate applications of the PORFLO model applies to all three transport modes simulated: mass, heat, and radionuclides. Geometric limitations of the model determine its adequacy for depicting pertinent characteristics of the host medium, which in turn affect all three modes of transport. Though minor variations may exist as to the effect of PORFLO's geometric limitations on the simulation of each mode of transport, the overall effects on all three modes are anticipated to be quite similar. Therefore the present discussion does not differentiate among them, except where exceptions to the generalization are specifically discussed.

Geometric Options Available

The geometry of the BWIP site is in fact three-dimensional, while the PORFLO model is capable of simulating variations in only two dimensions. The model can be applied either to a planar, cartesian system (no variation in the third dimension), or to a radially symmetrical, cylindrical system (no variation around the axis of symmetry). In general, the regional geometry is more compatible with the cartesian system; faults, fractures, and axes of synclines and anticlines are more or less linear and fairly straight. However, there may be limited applications in localized areas where use of the axisymmetric model geometry will be appropriate.

Cartesian Geometry

A two-dimensional, horizontal model geometry could be applied to simulation of regional flows under Concepts 1 or 2, where both diffuse and discrete vertical transport through the flow interiors can be neglected or applied uniformly without large error. (A possible exception is that flow interiors with low hydraulic conductivity may have significant thermal conductivities that should not be neglected or "blanketed" in the model). Assuming that thermal conductivity of the flow interior is, along with the other transport characteristics of the flow interior, relatively low, the two-dimensional, cartesian model could be applied to a horizontal section of a single flow or interflow, in which either homogeneous or heterogeneous aquifer characteristics can be simulated. It is recommended for this type of application that only a single interflow be modeled, in preference to modeling an entire flow or sequence of flows.

The two-dimensional model could be applied to a vertical section under Concepts 1 and 2 if the model can be aligned parallel to the regional direction of horizontal flow, if interflow heterogeneities do not appreciably alter local horizontal flow directions, and if interflow heterogeneities can be incorporated into the model using bulk parameter values. In this case, flow interiors, as well as interflows, would be modeled as "active cells".

For Concepts 3 and 4, a horizontal, cartesian geometry may be appropriate, if the isolated, high-permeability flow interior features either do not exist in the modeled area, or can be defined adequately using source/sink terms. It

is doubtful that the model could be applied in vertical section because interflows would have some degree of radial (non-two-dimensional) flow towards the isolated high permeability features.

For Concepts 5 and 6, the applicability of a two-dimensional model in horizontal plane would be very limited because flows of mass, heat and radionuclides may be dominated by three-dimensional geometry. Applications would probably be limited either to relatively small regions, where major structural discontinuities are not present, to very large regions, where the scale of the model is much larger than the effective spacing of major structural discontinuities or to areas for which the discontinuities can be treated as boundary conditions or line source/sinks. The two-dimensional model could be applied in vertical section if the modeled area is aligned parallel to the regional flow direction and roughly perpendicular to the discontinuities (to minimize non-uniformity in the third dimension not modeled).

Axisymmetric Geometry

An axisymmetric geometry, with its assumption of angular uniformity, implies uniform characteristics in concentric rings around some single axis. The layered nature of basalt flows does not allow this symmetry to exist around a horizontal axis. A model with axisymmetric geometry in vertical section may be useful in depicting conditions in a localized situation, where flow is dominated by movement toward or away from a center, such as a dewatered repository zone. The axisymmetric geometry around a vertical axis would be

applicable to Concept 1 and may possibly be applied to Concept 2 if interflow heterogeneities (1) can be incorporated using bulk parameter values and (2) do not result in appreciable variations from radial flow to/from the axis of symmetry. It is doubtful that an axisymmetric simulation could be applied to Concepts 3 and 4 since isolated high permeability features would be of limited lateral extent. Axisymmetric geometry would also not apply to Concepts 5 and 6 because tectonic structures tend to be linear.

4.4.2 Equivalent Porous Media Limitations

Transport Phenomena In Fractured Media

It is generally recognized that the medium at the BWIP site is fractured, that the major flow of groundwater occurs through flow tops, (particularly for Concepts 1 and 2) and also through structural discontinuities (Concepts 5 and 6). Changes in fluid pressure may affect the permeability; pressure decreases can result in a reduction in fracture aperture. Under certain conditions, fracture flows may not be laminar, and permeabilities can change significantly over a moderate change in Reynolds number. The basalt flow interiors occupy a majority of the rock volume, yet typically exhibit low permeabilities relative to the flow tops. These flow interiors can however contain localized features that are highly permeable, including fractures, joints, spiracles, and brecciated zones.

Fracture Flow and Transport Models

There are very few models that realistically simulate flow through fractured media; even though the logic exists, there is seldom sufficient data to accurately describe the fracture system: location, size, direction, frequency, etc. To compensate for the lack of available data (and the fact that it is prohibitively expensive and impractical to collect), most fracture flow models incorporate a stochastic algorithm to describe the flow system. In most applications, equivalent porous medium models are much more practical to use than fracture flow models, and provide a level of detail consistent with existing data.

Assumptions of EPM Models

PORFLO is a deterministic, rather than a stochastic model, that simulates mass flow by replacing the discrete fracture flow system with a porous medium that is intended to produce the same rate of diffuse flux as the fracture system would produce under similar imposed stresses such as hydraulic or thermal gradients. The use of this "equivalent porous medium" representation carries with it the assumption that each grid cell is a homogeneous (though possibly anisotropic) porous medium, with fluid and solid matrix properties considered uniform. The solid matrix is treated as a equivalent porous medium, and fluid flow through this matrix is assumed everywhere laminar. Permeability is considered independent of fluid pressures, velocities, and gradients.

In general, the difficulty with using PORFLO and other EPM models to simulate transport through fractured media is that the "equivalent porous medium" can be forced to mimic the behavior of the real fracture system only under a relatively narrow range of stresses. This is because the hydraulic properties of the equivalent medium are not pressure or Reynolds number-dependent. Additionally, the three modes of transport PORFLO simulates (mass, heat, and radionuclides) do not necessarily share a single relationship with pressure, velocity, and other variables (e.g. thermal conductivity may exhibit a much weaker dependence on Reynolds number than hydraulic conductivity). Furthermore, it is possible for the EPM assumption to be acceptable for groundwater and heat flow, but totally inappropriate (and nonconservative) with regard to radionuclide transport.

Consideration For Effective Application of PORFLO At The BWIP Site

It would, at first, appear that PORFLO is not at all applicable to the BWIP site due to the major limitation of simulating a fractured medium as a equivalent porous medium. However, the key to using the PORFLO model effectively is to apply the model cautiously and conservatively; i.e.: (1) apply the model only in those regions where the geometric or EPM limitations are not grossly exceeded, using a geometry that aligns as closely as possible with the dominant features of the site in terms of hydrology, heat and contaminant transport; (2) to compensate for the lack of a stochastic algorithm, conduct sensitivity runs, using reasonable ranges of all major parameter values, rather than just one estimated or average value; (3) make

appropriate parameter adjustments, where appropriate, to compensate for the EPM simplification (e.g. recognize that the EPM hydraulic conductivity may accurately predict mass flux, but not actual flow velocity; the contaminant transport diffusion coefficients should be coupled to the fracture, rather than to the EPM hydraulic conductivity.); (4) interpret model results conservatively, examining the assumptions and limitations of each run to ensure that possible "worst-case" conditions have not been neglected.

The following paragraphs discuss specific concerns of applying PORFLO at the BWIP site, relative to the purpose and required accuracy of any proposed application, selection of an appropriate model scale, and considerations for simulating heat and radionuclide transport in addition to mass flux. It is anticipated that these considerations will be equally important regardless of what overall conceptual model of the geohydrologic system is adopted. Therefore, the following discussion does not differentiate according to conceptual models as described above.

Proposed Applications

Since none of the case studies presented in the model documentation indicates whether PORFLO is capable of simulating flow and transport behavior at the hydrologically complex BWIP site, it is recommended that test runs be made to attempt to match available data on site. However, it will not be possible to "history match" repository performance conditions, which have not yet taken place. Therefore, the safest course to ensure reasonable and valid results is

to set up modeling scenarios that depart to the minimum possible extent from existing or previously observed conditions.

For example, it is known that "repository performance" will include significant thermal loading conditions that have not previously been observed at the BWIP site. If possible, the simulation of this "anticipated" thermal effect should be superimposed on "previously observed" hydrologic conditions. If instead, an attempt is made to simultaneously model "anticipated" thermal loading and a previously unobserved hydrologic regime, the simulation could exceed the capability of the model, and it would be difficult to judge whether the results are reasonable, given so many unknowns in the input dataset. This recommendation follows conventional modeler's wisdom to "vary only one parameter at a time"; in the case of the possible application of PORFLO at the BWIP site, the value of this practice is emphasized, given the many yet-undiscovered site characteristics, and the open question of applicability of this particular model.

Model Scale Selection

The first consideration in selecting a model scale is that it is compatible with the required detail of the site geometry, available data, and also with the required level of detail of results. In order to achieve a stable solution, it is best to limit the variation in grid size to one or at most two orders of magnitude in either of the two dimensions in a cartesian system. For a standard application of an axisymmetric system, where the activity "driving" the model is located at or near the axis of symmetry, more than an

order of magnitude of radial grid dimension can be tolerated, because the large, outer grid cells are relatively inactive.

Beyond these considerations, adverse effects of the EPM assumption can best be minimized by selecting a model scale large enough to encompass a representative number and size of the ubiquitous fractures present in the basalt flows, yet small enough to allow individual model grid cells to be used to simulate the effects of major structural discontinuities. Without a more detailed definition of the location of a proposed model application, it is not known whether the model scale can be sized to avoid intersecting a major structural discontinuity. These structural discontinuities may be relatively small in cross-section, so that a model grid may have to be sized substantially smaller than surrounding grids to provide a geometrically similar configuration to the real system. If this presents a stability problem for grid sizing, the size of the grid can be increased so that its size is compatible with the rest of the model, and the numerical values describing its transport properties can be adjusted downward to compensate for the larger size (i.e. the "EPM" concept is applied to the discontinuity, just as it is to the rest of the material in the modeled area.)

Mass, Heat, and Radionuclide Transport

The PORFLO model may be used most safely in predicting mass flows; the relationship between hydraulic conductivity and both thermal conductivity and dispersion of radionuclides suggests that contaminant transport, in particular should be coupled to the maximum fracture hydraulic conductivity, rather than

to the EPM "average" conductivity. The relationship between hydraulic and thermal conductivity is even more tenuous; analyses of BWIP data by some investigators has indicated that the thermal conductivity may be relatively independent of the hydraulic conductivity; thermal effects may actually "drive" the hydraulics.

5.0 RECOMMENDATIONS

The underlying concern in reviewing the PORFLO model document is the lack of stress testing data from the BWIP site with which this model, or any model, can be evaluated. At this stage in the site characterization and performance assessment, models are being compared to other models, rather than existing site data. Although we recognize that model to model comparison can provide verification of the model's ability to solve physics and chemistry problems, it does not demonstrate that the model can simulate real conditions at the BWIP site. We also recognize the lead time required in developing relatively complex models, but would caution against proceeding so far ahead of the actual data collection process, that one loses sight of the constant feedback required between modeling efforts and data needs. Data which has been collected to date will permit analytical analyses to test various conceptual models, but a full-scale stress test is required to provide a sufficient database for model verification. Comparing models to models will not provide the necessary confidence to assess repository performance.

Several detailed recommendations concerning the use of PORFLO, given its limitations within the context of probable conceptual models, are listed:

1. Since none of the case studies presented in the model documentation indicates whether PORFLO is capable of simulating flow and transport behavior at the BWIP site, it is recommended that test runs be made to attempt to match available data on site. The PORFLO model may also be set

up in the expectation that LHS test data may be available in the near future.

2. Adverse effects of the EPM assumption can best be minimized by selecting a model scale large enough to encompass a representative number and size of the ubiquitous fractures present in the basalt flows, yet small enough to allow individual model grid cells to be used to simulate the effects of heterogeneity and the presence of major structural discontinuities.
3. The key to using the PORFLO model effectively is to apply the model cautiously and conservatively; i.e.: (1) apply the model only in those regions where the geometric or EPM limitations are not grossly exceeded, using a geometry that aligns as closely as possible with the dominant features of the site in terms of hydrology, heat and contaminant transport; (2) to compensate for the lack of a stochastic algorithm, conduct sensitivity runs, using reasonable ranges of all major parameter values, rather than just one estimated or average value; (3) make appropriate parameter adjustments, where appropriate, to compensate for the EPM simplification (e.g. recognize that the EPM hydraulic conductivity may accurately predict mass flux, but not actual flow velocity; the contaminant transport diffusion coefficients should be coupled to the fracture, rather than to the EPM hydraulic conductivity.); (4) interpret model results conservatively, examining the assumptions and limitations of each run to ensure that possible "worst-case" conditions have not been neglected.