OT.4 - 10

APR 19 1999

ENGINEERING DATA TRANSMITTAL

1. EDT 624998

2. To: (Receiving Organization) Immobilized Waste	3. From: (Originating Organization) Immobilized Waste	4. Related EDT No.:
5. Proj./Prog./Dept./Div.: Immobilized Waste	6. Design Authority/Design Agent/Cog. Engr.: J. A. Voogd	7. Purchase Order No.:
8. Originator Remarks: Selection of Numeric Code for 2001 ILAW PA for Vadose Zone Calculations		9. Equip./Component No.:
		10. System/Bldg./Facility:
		12. Major Assm. Dwg. No.:
11. Receiver Remarks:	11A. Design Baseline Document? ◯ Yes ◉ No	13. Permit/Permit Application No.:
		14. Required Response Date: April 15, 1999

15. DATA TRANSMITTED

(A) Item No.	(B) Document/Drawing No.	(C) Sheet No.	(D) Rev. No.	(E) Title or Description of Data Transmitted	(F) Approval Desig-nator	(G) Reason for Trans-mittal	(H) Origi-nator Dispo-sition	(I) Receiv-er Dispo-sition
1	EDT 624998 / HNF-4356		0	Recommendations for Computer Code Selection of A Flow and Transport Code to be Used in Undisturbed Vadose Zone Calculations for TWRS Immobilized Wastes Environmental Analyses	N/A	1		

16. KEY

Approval Designator (F)	Reason for Transmittal (G)	Disposition (H) & (I)
E, S, Q, D OR N/A (See WHC-CM-3-5, Sec. 12.7)	1. Approval 2. Release 3. Information 4. Review 5. Post-Review 6. Dist. (Receipt Acknow. Required)	1. Approved 2. Approved w/comment 3. Disapproved w/comment 4. Reviewed no/comment 5. Reviewed w/comment 6. Receipt acknowledged

17. SIGNATURE/DISTRIBUTION
(See Approval Designator for required signatures)

(G) Reason	(H) Disp.	(J) Name	(K) Signature	(L) Date	(M) MSIN	(G) Reason	(H) Disp.	(J) Name	(K) Signature	(L) Date	(M) MSIN
		Design Authority					1	R. W. Root			
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		Safety									
		Env.									

18.	19.	20.	21. DOE APPROVAL (if required)
J. A. Voogd (signature) 4-6-99	R. W. Root (signature) 4/1/99	See Above R. J. Murkowski	Ctrl No.
Signature of EDT Originator / Date	Authorized Representative for Receiving Organization / Date	Design Authority/ Cognizant Manager / Date	◯ Approved ◯ Approved w/comments ◯ Disapproved w/comments

BD-7400-172-2 (10/97)

BD-7400-172-1

Recommendations for Computer Code Selection of a Flow and Transport Code to be Used in Undisturbed Vadose Zone Calculations For TWRS Immobilized Wastes Environmental Analyses

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U.S. Department of Energy Contract DE-AC06-96RL13200

EDT/ECN: 624998 UC: 510
Org Code: 73400 Charge Code: 105864/AA30
B&R Code: EW3130010 Total Pages: 36

Key Words: TWRS, Code, Vadose Zone

Abstract: An analysis of three software proposals is performed to recommend a computer code for immobilized low activity waste flow and transport modeling. The document uses criteria established in HNF-1839, "Computer Code Selection Criteria for Flow and Transport Codes to be Used in Undisturbed Vadose Zone Calculation for TWRS Environmental Analyses" as the basis for this analysis.

4/19/99
Release Approval Date Release Stamp

Approved for Public Release

Recommendations for Computer Code Selection of a Flow and Transport Code to be Used in Undisturbed Vadose Zone Calculations for TWRS Immobilized Wastes Environmental Analyses

Combined Review Comments:

Recommendations for Computer Code Selection of a Flow and Transport Code to be used in Undisturbed Vadose Zone Calculations For TWRS Immobilized Wastes Environmental Analyses

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Fluor Daniel Northwest Company

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September 11, 1998

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I. INTRODUCTION

The Tank Waste Remediation System (TWRS) is responsible for the safe storage, retrieval, and disposal of waste currently being held in 177 underground tanks at the Hanford Site. In order to successfully carry out its mission, TWRS must perform environmental analyses describing the consequences of immobilized low-activity tank waste contaminants leaving disposal facilities.

Because of the large size of the facilities and the great depth of the dry zone (known as the vadose zone) underneath the facilities, sophisticated computer codes are needed to model the transport of the contaminants. Code selection criteria were established (Mann 1998) based on the information from the low-level waste programs of the U.S. Department of Energy [DOE] (Case 1988) and of the U.S. Nuclear Regulatory Commission (Kozak 1989a) as well as experience gained in the DOE Complex [Mann 1995, WSRC 1992] in applying these criteria.

This document analyzes each of the requirements and desirable features of the three codes that were submitted for consideration, PORFLOW (ACRi 1998, Runchal 1998a), STOMP (White 1996, Nichols 1997, White 1997, Freshley 1998), and VAM3D-CG (HG (1994), Puigh 1998). This version of the recommendation includes information received after April 30, 1998, from Runchal (1998b,c) and from Connelley (1998). This document follows the format of the code selection criteria document and judges how well each of these codes meet the criteria.

- Chapter II - Mandatory Administrative Criteria: those criteria dealing with how the code is created, maintained, and used;
- Chapter III - Mandatory Technical Criteria: the technical features which the code must have; and
- Chapter IV - Desirable Features: those feature which the code should have, but the absence of which will not disqualify a code.

The proposals from each of the code proponents was reviewed and evaluated against the criteria. The results of the review are organized by the code selection criteria (Mann 1998). Also attached are results from an independent review conducted by Bechtel, San Francisco, for the Groundwater/Vadose Zone Integration Project.

The TWRS Decision Management Procedure (LMHC 1998) was followed.

II. SUMMARY AND ANALYSIS

The code selection review process recommends that ILAW proceed with the use of VAM3D-CG as the basis for vadose zone modeling efforts leading to completion of the 2001 performance assessment. This recommendation evolves from the findings described in this document. While each code presented an impressive set of features for vadose zone modeling, each code represented a unique mix of features important to the ILAW disposal program.

In summary the key features that became discriminating factors for the recommendation included:

- Acceptance by the regulatory and technical community.
- The ability to utilize the investment in staff knowledge and working relationships.

A very knowledgeable and capable staff at PNNL supports the STOMP code. The staff supporting the geotechnical data collection for the performance assessment is closely tied to staff proposing use of the STOMP code. However, the ILAW program would be taking on a significant avoidable risk by using a code that has not been formally accepted by WDOE or EPA for use in an application like the TWRS Immobilized Low-Activity Waste Disposal effort. The proposal for the STOMP code indicated a path forward for resolving this issue but the ILAW Disposal Program would be taking on additional unnecessary risk.

The PORFLOW code is well accepted by both the technical and regulatory community. In fact, PORFLOW has been used by the ILAW Performance Assessment for vadose zone calculations. However, the previous modeler is not available due to illness. Analytical and Computational Research, Inc. has indicated a willingness to establish a local capability and work with the program on modeler assignment and training. However, the need to develop new working relationships and develop understandings of the project technical and programmatic issues was a risk the project would be taking on.

The VAM3D-CG code has been accepted by the regulatory community for applications similar to ILAW disposal. Fluor Daniel Northwest, Inc. and GeoHydraulic staff are knowledgeable and available to begin working on the performance assessment. There is a concern that the current version of the code does not adequately handle radioactive decay, however, this appears to be a risk that could be quantified (approximately $10,000) and controllable by the ILAW program.

Each proposal was reviewed independently and evaluated against the specific criteria established in Mann 1998. The proposals were largely reviewed as written with some credit given based upon the experience and judgment of the reviewer. Criteria for the Mandatory Administrative features and Mandatory Technical features were evaluated on a met/not met basis. The Desirable Features were presented on a percentage basis. For two of the reviewers this percentage was based upon judgment, for the third reviewer the value represents the percentage of desirable feature attributes met by the code. Input from three independent reviewers was combined as shown in Table 1. The review data collection, analysis and final recommendation was performed by the ILAW Program Office.

Table 1.

SUMMARY OF RECOMMENDATIONS

Section	Description	PORFLOW	STOMP	VAM3D-CG
Administrative Criteria				
II-A	Technical Documentation	Met/Met/Met	Met/Met/Met	Met/Met/Met
II-B	Code Availability	Met/Met/Met	Met/Met/Met	Met/Met/Met
II-C	Configuration Control	Met/Met/Met	Met/Met/Met	Met/Met/Met
II-D	Input Flexibility	Met/Met/Met	Met/Met/Met	Met/Met/Met
II-E	Real-Time Monitoring/Restart capabilities	Met/Met/Met	Met/Met/Met	Met/Met/Met
Technical Criteria				
III-A	Moisture Flow	Met/Met/Met	Met/Met/Met	Met/Met/Met
III-B	Contaminant Transport	Met/Met/Met	Met/Met/Met	Met/Met/Met
III-C	Boundary Conditions	Met/Met/Met	Met/Met/Met	Met/Met/Met
III-D	Source Term	Met/Met/Met	Met/Met/Met	Met/Met/Met
III-E	Hydrologic Properties	Met/Met/Met	Met/Met/Met	Met/Met/Met
III-F	Geochemical Model	Met/Met/Met	Met/Met/Not	Met/Met/Met
III-G	Time-Dependent Hydraulic and Geochemical Values	Met/Met/Met	Met/Met/Not	Met/Met/Met
III-H	Layering	Met/Met/Met	Met/Met/Met	Met/Met/Met
III-I	Output	Met/Met/Met	Not/Not/Not	Met/Met/Met
III-J	Interface Between Moisture Flow and Contaminant Transport	Met/Met/Met	Met/Met/Met	Met/Met/Met
Desirable Features				
IV-A	Ease of use	40% 60% 100%	50% 30% 100%	50% 60% 00%
IV-B	Certification – Verification – Benchmarking	80% 80% 100%	100% 80% 100%	100% 100% 100%
IV-C	Reputation Among User Community	60% 90% 60%	25% 50% 60%	95% 90% 80%
IV-D	Additional Contaminant Transport Capabilities	80% 80% 100%	60% 60% 30%	75% 80% 30%
IV-E	Additional Moisture Flow Capabilities	35% 70% 66%	100% 70% 66%	100% 70% 66%
IV-F	Decay Products	90% 100% 100%	90% 100% 100%	40% 50% 0%
IV-G	User Support	50% 75% 100%	80% 75% 100%	90% 90% 100%
IV-H	Speed of Execution	N/A	N/A	N/A
IV-I	Proprietary Codes	50% 50% 100%	75% 75% 100%	50% 50% 100%
IV-J	Version	75% 75% 100%	90% 75% 100%	100% 90% 100%

The recommendation for the code was made after assuring that a code could meet all of the mandatory criteria then establishing a preferred code from comparison of the desirable features. All three codes were able to meet all of the Mandatory Administrative Criteria. The Mandatory Technical Criteria provided some discrimination between codes with one code failing to meet all of the Mandatory Technical Criteria. Discrimination between the codes became more apparent in the Desirable Features and the presentation of the proposals from each of the potential code suppliers.

Evaluation of the Mandatory Technical Criteria lead to the following:

1. PORFLOW was judged to meet all of the Mandatory Technical Criteria.

2. STOMP was judged unable to meet the Mandatory Technical Criteria for output. The specific technical criteria identified a need to provide mass balance and mass balance errors at each time step. The proposal states "The current released version of the STOMP simulator does not provide mass balance information after time step . . ." In addition, one reviewer judged that STOMP was unable to meet criteria for III-F Geochemical Models. A basis for this judgment was not provided by the reviewer and, therefore, was not a factor in the recommendation. STOMP was judged not to meet criteria III-G Time-Dependent Hydraulic and Geochemical Values by one reviewer. No basis for this judgment was provided by the reviewer, however, the STOMP submittal states "The current released version of the STOMP simulator can only accommodate time-dependent hydraulic and geochemical values through modification of rock/soil properties through the restart function."

3. VAM3D-CG was judged to meet all of the mandatory Technical Criteria.

The Desirable Features were evaluated on a comparative basis:

1. PORFLOW was distinguished by its ability provide Additional Contaminant Transport Capabilities and Decay Products. The factor that significantly affected the scoring for Ease of Use and User Support is lack of experienced PORFLOW users onsite that are also familiar with the ILAW disposal effort and the ILAW Performance Assessment in particular.

2. STOMP was distinguished by its ability to provide Decay Products and the absence of a fully proprietary Code. The factor that significantly affected scoring for Reputation among User Community was absence of regulatory acceptance and wide commercial use of the code.

3. VAM3D-CG was distinguished by its Certification-Verification-Benchmarking and Reputation among the User Community. VAM3D-CG scored poorly for its handling of decay products. The proposal indicated that this deficiency in VAM3D-CG could be remedied through several different methods for approximately $10,000.
Based upon the factors noted, VAM3D-CG is recommended for use leading to completion of the 2001 ILAW Performance Assessment.

III. MANDATORY ADMINISTRATIVE CRITERIA

These criteria deal with how the code is created, maintained, and used.

A. Technical Documentation

1. **Requirements.** The proponent of the code shall submit the documentation that describes
   - model theory, governing equations, and assumptions,
   - computational techniques and algorithms,
   - code verification,
   - user input, and
   - example applications

   The items listed above to the cognizant engineer along with a notation describing the location of each required item.

   It is recognized that the current version of the code may not have all the documentation at the time of code selection. If this is the case, the proponent shall supply documentation for the latest version of the code for which documentation exists along with a schedule of the expected availability of documentation for the current code version.

   General note: Verification documentation deals mainly with benchmarking tests (analytical and other codes) rather than code verification in computer science.

2. **PORFLOW.** Met/Met. Proposal (1998a) states that two documents exist, but do not reference them. However, ACRi 1998 does describe governing equations (Chapter 2), numerical basis (Chapter 4), and user input (Chapters 5, 6, and 7). Validation manual on web site could not be downloaded. Verification and benchmarking manual that was to be sent has not been received. Revised proposal (Runchal 1998b) references the documents, which were sent by E-mail.

   The online manual describes Version 3.5, while Version 4.0 is being proposed. There is no indication when documentation for Version 4.0 would be available. The revised proposal sent the Version 4.0 manual, which is substantially the same as the Version 3.5.

   An electronic copy of the Manual containing all the above items was sent as an attachment. In addition, a verification and benchmarking manual was mailed. (unable to open)

3. **STOMP.** Met/Met. Model theory, governing equations and assumptions, and computational techniques and algorithms are described in White 1996. User input is described in White (1997). Code verification and example applications are presented in Nichols (1997). Documents are cited by proponents, which is adequate since each document deals with specified component.

   Code is "continuously being upgraded and modified" (proponents' submittal for this requirement). Updated documentation is available on web site (which was checked) and will be incorporated in revisions.

   Pg. 2, A. The STOMP simulator is documented through three published guide manuals: application, theory, and users. Technical documentation descriptions of the code's governing equations, constitutive relations (secondary equations), primary assumptions, and numerical solutions techniques are provided in the STOMP Theory Guide (White and Oostrom 1996).

4. **VAM3D-CG.** Met/Met. Model theory, computational techniques and algorithms, code verification, user input, and example applications are given in HG (1994). The proponents described the location for each item. The version being proposed (3.1) is the one for which documentation was submitted.

   Technical documentation is included in Appendix A (Documentation and User's Guide):

   - Model theory, governing equations and assumptions: pg. 2-1 through 2-26
   - Computational techniques and algorithms: pg. 3-1 through 3-30
   - Code verification: pg. 4-1 through 4-67
   - User input: pg. 8-1 through 8-49
   - Example applications: pg. 4-1 through 4-67

B. Code Availability

1. **Requirements.** The proponent of the code shall document the availability of the executable version of the code and list those computers (and operating systems) on which it will run.

   Satisfactory computer hardware are Intel-compatible processors using the Windows or NT operating system or Sun/SGI/HP computers using the UNIX operating system. Large parallel systems (having more than four processors) will not be considered.

2. **PORFLOW.** Met/Met. Claim installations on UNIX and Intel PCS under Windows.

   PORFLOW Simulation Tool is available for practically any computer and operating systems; the installations have included:

1. Intel x-86 and Pentium processors
2. IBM RISC
3. Sun
4. HP
5. SGI

6-9. Others

Among the current installations are those on:

1. Windows 95
2. Windows NT
4. UNIX (including variations from IBM, HP, SUM, SGI, DEC)

3. **STOMP.** Met/Met. Code has been compiled on a number of UNIX computers without warning messages. However, code proponents do not state on which the code has been shown to run. A subsequent E-mail indicates that the code runs on various UNIX machines and INTEL PCS.

   Pg. 3, B, The U.S. Department of Energy has granted copyright for the software to Battelle Memorial Institute (Battelle), with the stipulation that the simulator be made available to Federal and State agencies through the Energy and Science Technology Software Center or alternate route without royalties to Battelle. . . . The code has previously been compiled on NIX base operating systems around the world and currently compiles free of warning messages.

4. **VAM3D-CG.** Met/Met. Code is available on SGI UNIX and Intel PC computers.

   The executable version of VAM3D-CG Version 3.1 is available for use by on site on the Silicon Graphics, Inc. workstation operating under the UNIX system. Appendices B & C provide the verification and benchmarking information for VAM3D-CG installed on the SGI workstation.

   VAM3D-CG version is also available for use by FDNW on an INTEL PC operating under Windows NT4.0. The code has been verified and benchmarked for the INTEL platform for use in the 200 Areas low-level solid waste performance assessment maintenance activities.

C. Configuration Control

1. **Requirement.** The proponent of the code must submit the software quality management program plan for the code.

2. **PORFLOW.** Met/Met. Original proposal (Runchal 1998a) stated that code is designed to meet "ASME Software QA criteria," but no reference given. Revised proposal (Runchal 1998b) provides a QA procedure which is acceptable.

3. **STOMP.** Met/Met. Submitted acceptable configuration management plan based on IEEE standards.

Pg. 4, C. The STOMP Configuration Management Plan is a version of the IEEE Std. 828-1990, "Software Configuration management Plans." . . . In brief, version control for the STOMP simulator was initiated on June 19, 1997, using the Revision Control System (RCS) utility on the "muse" cluster of IBM RISC 6000s at the PNNL. RCS is a conventional UNIX utility, which is designed to keep track of multiple file revisions.

4. **VAM3D-CG.** Met/Met. Plans are consistent with Fluor Daniel Hanford requirements, to which Lockheed Martin Hanford Corporation is a subcontractor.

Configuration control for VAM3D-CG Version 3.1 is maintained per . . . FDNW practice 134.200.0960, "Control of Engineering Software," . . . and assures that the control is consistent with Fluor Daniel Hanford "Configuration Management Plan," HNF-MP-013, Rev. 0, and "Quality Assurance Plan," HNF-MP-014, Rev.1.

D. Input Flexibility

1. **Requirements.** The proponent of the code must show that the code can accept input that is site- and facility-specific.

2. **PORFLOW.** Met/Met. Proposal not responsive. However, online manual (ACRi 1998) indicates that input is site- and facility-specific (MATE card in Chapter 7 of ACRi 1998).

"PORFLOW provides the most comprehensive set of input options and flexibility of any such code currently available. Among these are:

1. Over 20 options for soil-moisture and conductivity's

2. Built-in functions (space, time, or phase variable) for:

- Boundary conditions
- Initial conditions
- Field conditions
- Sources
- Properties (fluid density, fluid viscosity, storativity, diffusivity, specific heat).

3. **STOMP.** Met/Met. Input manual (White 1996) indicates that all parameters can be submitted. An example is cited where each grid cell had different parameter set. Pg. 4, D, A primary assumption associated with this numerical scheme is that all physical properties within each grid cell are represented by their values at the cell centroid. In respect, each grid cell is identified with a rock/soil type, which relates geohydrologic properties to the grid cell. Table 1, pg. 5 lists the User Defined Rock/Soil properties.

3. **VAM3D-CG.** Met/Met. Input manual (Section 8 Input Data Preparation of HG 1944) indicates that all parameters can be submitted. Examples are provided where site- and facility-specific data are used.

4. VAM3D-CG does not use any generic data as input for either the site or the facility. The code can use Hanford site-specific data and vadose zone parameters.

E. Real-Time Monitoring/Restart Capabilities

1. **Requirements.** The proponent of the code shall document the real-time diagnostic and restart capability of the code. The monitoring activity can be satisfied by time stamps written to a file.

2. **PORFLOW.** Met. See ACRi 1998, particularly Section 6.4.

   PORFLOW provides extensive real-time monitoring and restart capabilities. Among its monitoring capabilities are:

   1. Step number and time
   2. Any of the phase variables
   3. The change in any variable
   4. The residual of any of the equations
   5. The flux balance for any of the equations.

   Any combination of any of these can be monitored at any given time or with any given equency.

   PORFLOW provides two types of files, which can be used, for restarting.

3. **STOMP.** Met/Met. Real-time monitoring performed by writing a user-chosen subset of cells to special files (documented in Section 7.2 of White 1977). Restart files are created in every run and can be generated at user selected times (documented in Section 7.5 of White 1997). Restart runs are denoted on Solution Control Card (Appendix A.2).

   Pg. 6, E, For real-time monitoring the user can specify particular grid cells within the computational domain as reference nodes. Reference node output is written to standard output (e.g., typically the screen) and an output file called "output." Every STOMP simulation concludes with the creation of a restart file . . . For example, the restart file entitled "restart.342" would have been created at the conclusion of time step number 342.

4. **VAM3D-CG.** Met/Met. Capabilities involve use of special history files (Section 8.4 Special History Files). Restart capabilities are stated in Section 6.5, "Restart Procedures."

   The real-time monitoring capability is controlled via input data preparation and is described in pg. 8-44 and 8-45 (Appendix A). A restart option is provided in the code for continuation of solution to time-dependent problems.

IV. MANDATORY TECHNICAL CRITERIA

These criteria are the technical features, which the code must have. In general, the theoretical framework of the code shall be based on appropriate scientific principles (e.g., conservation of mass, momentum, and energy) and well established engineering equations (e.g., Darcy's law, lick's law).

A. Moisture Flow

1. **Requirements.** The proponent of the code shall document that the code can perform two- and three-dimensional modeling of unsaturated, constant density moisture flow in an isothermal setting, both under steady state and transient conditions. The code proponent shall supply the authors, titles, and document identifiers of some published papers or reports that document use of the code to model moisture flow.

2. **PORFLOW.** Met/Met. See online manual, particularly Chapter 1. A partial list of publication reports was sent with proposal, including Hanford Site applications. PORFLOW has been used widely to perform simulation under conditions of:

   - 2D & 3D Geometry
   - Steady and transient flow
   - Unsaturated and saturated flow
   - Constant and varying density
   - Isothermal and non-isothermal conditions.
   - A partial list of publications is included (por_pub.doc).

3. **STOMP.** Met/Met. The code can model moisture flow (see White 1996). Two/three dimensional is determined by grid card (A3 of White 1997). All calculations are transient, thus making steady-state calculations a special case.

   Examples are provided.

   Pg. 7, A, . . . the STOMP simulator operates on Cartesian and vertically oriented cylindrical grid domains of either one, two, or three dimensions. The STOMP simulator has robust capabilities for modeling multiple-, pseudo multiple- and single-phase fluid flow through subsurface environments. All STOMP simulations are technically transient where the time step is controlled by user specified limitations or by the nonlineartities of the particular problem. Steady-state solutions are obtained by simulating from an initial condition through a transient solution until steady conditions are achieved.

   References Las Cruces Trench Site - Rockhold, Yucca Mountain - Eslinger, Edwards AFB - White and Gilmore, SX-109 - Ward, water through vadose zone of low-level radioactive waste disposal sites - Meyer.

4. **VAM3D-CG.** Met/Met. From Section 8 of HG (1994) (Input Data Preparation) and from examples of HG (1994) (Example Verification and Application Problems). Hanford Site applications show capability.

   VAM3D-CG is capable of simulating two- and three-dimensional unsaturated flow of water of a constant density in an isothermal setting under both steady state and transient flow-field conditions, particularly under conditions expected at the Hanford Site. . . . The ability to model moisture flow under both steady state and transient flowfield conditions at the Hanford Site is documented in 200E Burial Grounds PA (Wood, et al. 1996), 200W Burial Grounds PA (Wood, et al. 1995b), ERDF PA (Wood, et al. 1995a) and TWRS EIS (DOE 1996).

B. Contaminant Transport

1. **Requirements.** The proponent of the code shall document that the code can simulate contaminant transport in two- and three-dimensions as a function of hydrologic conditions established by the moisture flow subsystem and by advection, hydrodynamic dispersion, molecular diffusion, or adsorption. The code proponent shall supply the authors, titles, and document numbers of some published papers or reports that document use of the code to model contaminant transport.

2. **PORFLOW.** Met/Met. See online manual, particularly Chapter 1. A partial list of publication reports was sent with proposal, including Hanford Site applications. "PORFLOW provides for a very comprehensive set of options for transport of contaminants." List provided.

3. **STOMP.** Met/Met. The code can model contaminant transport (see White 1996). Two/three dimensional is determined by grid card (A3 of White 1997).

   Two-dimensional examples are provided.

   - Per the STOMP Application, Theory, and User's Guides, the STOMP simulator solves the governing equation for solute transport over multiple phases. Solutes are assumed to be transported via advection, hydrodynamic dispersion, and molecular diffusion.

   - Las Cruces Trench Site, those of strontium transport at the 100-N Area, Hanford Site, and the investigations of soluted-transport solution scheme are three pertinent examples of STOP generate solution to two dimensional solute transport problems.

   (Note 3D not discussed).

4. **VAM3D-CG.** Met/Met. From Section 8 of HG (1994) (Input Data Preparation) and from examples of HG (1994) (Example Verification and Application Problems). Hanford Site applications show capability.

VAM3D-CG is capable of simulating two-/three-dimensional contaminant transport (including advection, hydrodynamic dispersion, molecular diffusion, decay, and adsorption). The ability to model contaminant transport at the Hanford Site is documented in 200E Burial Grounds PA (Wood, et al. 1996), 200W Burial Grounds PA (Wood, et. al 1995b), ERDF PA (Wood, et al. 1995a) and TWRS EIS (DOE 1996).

C. Boundary Conditions

1. **Requirements.** The proponent of the code shall document the code's ability to simulate moisture flow for an infiltration rate which varies with time. The proponent shall also document that the code is capable of simulating homogeneous and non-homogeneous Dirichlet and Neumann boundary conditions. It shall be possible to configure the boundary conditions to simulate either upward or downward migration and fate of contaminants.

2. **PORFLOW.** Met/Met. See discussion of BOUN card in Chapter 7 of ACRi 1998.

Dirichlet type, Neumann, Mixed Radiation, Open boundary, and switching between the Dirilicht & Neumann.

Boundary conditions can vary as arbitrary functions of time, space phase variables, user defined variables. Boundary conditions can be imposed in any manner and combination, such as:

- element by element
- material type
- block elements
- whole boundary directed by direction cosines.

3. **STOMP.** Met/Met. Boundary conditions are defined on Boundary Conditions card (Section A.20 of White 1997).

Pg 8, C. 1) All surfaces on the exterior boundaries of the computational domain require boundary conditions; 4) Boundary conditions variables can be defined as time dependent or constant . . . Beyond these basic rules, the user is free to specify boundary conditions as needed.

. . . if a user created a one-dimensional simulation and attempted to declare inward flow boundaries (Neumann-type boundary conditions) on both ends of the domain, STOMP would attempt to find an aqueous pressure solution to the problem. . . . The 'Initial Condition' type boundary condition is a special form of the Dirichlet boundary condition, where the value of the boundary surface variable is set equal to the initial value of the field variable at the node adjacent to the boundary surface.

4. **VAM3D-CG.** Met/Met. From Section 8 of HG (1994) (Input Data Preparation) and from examples of HG (1994) (Example Verification and Application Problems). Hanford Site applications show capability.

   A time-dependent boundary condition is handled via Group 17 input data (pg. 8-2, 8-32, 8-33, Appendix A), "Transient flux boundary condition." Other boundary conditions including Dirichlet and Neumann, boundary conditions, are handled via Groups 15 and 16 (pg. 8-2, 8-29, through 8-31; Appendix A) input data.

D. Source Term

1. **Requirements.** The proponent of the code shall document the code can accept a specified time-dependent release rate from one or more volume sources and from disconnected surface sources and then simulate the release until the inventory is depleted.

2. **PORFLOW.** Met/Met. The original proposal (Runchal 1998a) was not responsive. The capabilities are probably contained in SOUR card (Chapter 7 of ACRi 1998), but proposal provides only generalities. The revised proposal (Runchal 1998b) confirmed that the SOUR card does contain information.

   "The SOURce command with TABLe and TIME modifier meets the requirements as stated. In fact, any functional relationship can be specified by the SOURce command or in combination with ALLOCate, SET, and SOURce commands."

3. **STOMP.** Met/Met. Source terms conditions are defined on Source Conditions card (Section A.21 of White 1997). Disconnected surface sources must be modeled at the boundary between active and inactive cells. User inputs explicit time history.

   "As documented in the STOMP User's Guide, source can be specified as time dependent with unique start and stop times. Unlike boundary conditions, multiple sources can be specified for a single grid cell and most source types offer two specification options, volume dependent, and independent."

4. **VAM3D-CG.** Met/Met. From Section 8 of HG (1994) (Input Data Preparation) and from examples of HG (1994) (Example Verification and Application Problems). User inputs explicit source history.

   VAM3D-CG is capable of simulating specified time-dependent release rates from one or more volume sources and from disconnected surface sources. Such capability is handled via Group 18I input data input data and prescribing variables

NDCSRC (number of sources to be considered) and TLDCS contaminant release time duration (pg. 8-33; Appendix A).

E. Hydrologic Properties

1. **Requirements.** The proponent of the code shall document that the code has the capability to use the van Genutchen - Mualem relationships to represent moisture retention and unsaturated conductivity functions in the simulation of moisture movement and that the code has the ability to have different values in each user chosen zone.

2. **PORFLOW.** Met/Met. The original proposal (Runchal 1998a) indicates that PORFLOW has van Genutchen/Mualem relationships and past Hanford Site applications have used this feature. Chapter 3.3 and 3.5 of ACRi 1998 indicate that van Genuchten and Mualem relationships, respectively, are supported by the code. However, the proposal does not indicate where in the manual nor is it obvious which input card contains information. The revised proposed (Runchal 1998b) Providees that the option is available with the MULTphase command using the VAN and MUALem modifiers.

   "The MULTiphase command with VAN and MUALem modifiers meets the requirements as stated."

3. **STOMP.** Met/Met. Van-Genutchen/Mualem representations can be specified by proper choices on Saturation Function Card (Section 1.9 of White 1997) and on Aqueous Relative Permeability Card (Section A.10). Each grid could have a different property.

   Hydrologic properties are specified for rock/soil types, which in turn are specified across domains of grid cells. Table 3 identifies Saturation-Capillary Pressure (s-P) function options. Table 4 identifies Aqueous Relative permeability-Saturation (k-s) function options.

4. **VAM3D-CG.** Met/Met. From Section 8 of HG (1994) (Input Data Preparation). Hanford Site applications show capability.

   VAM3D-CG can use either table lookup or van Genuchten-Mualem relationships to represent moisture retention and unsaturated hydraulic conductivity functions. VAM3D-CG has the capability to assign van Genuchten-Mualem parameters by different material types.

F. Geochemical Model

1. **Requirements.** The proponent of the code shall document that the code can simulate geochemical retardation using the linear sorption isotherm model where K_d only depends on the contaminant and the spatial position.

2. **PORFLOW.** Met/Met. The original proposal (Runchal 1998a) indicates that PORFLOW can use the linear sorption isotherm model and past Hanford Site applications have used this feature. However, the proposal does not indicate where in the manual nor is it obvious which input card contains information. The revised proposal (Runchal 1998b) states that ability is present using TRANsport, PROPerty, DISTribution, and RETArdation commands.

   "The linear sorption isotherm model is invoked by an appropriate selection of TRANsport (constant kd or Rd for each material type), PROPerty (to interpret input as kd or Rd), ISTribution (kd as a function), RETArdation (Rd as function) commands. In addition, non-linear isotherm can be specified by a combination of DISTribution, RETArdation, and REACtion commands."

3. **STOMP.** Met/Met. Kd values can be specified on Solute/Porous Media Interaction Card (Section A.18 of White 1997) for each rock type.
   As referenced in the STOMP User's and Theory Guide, the STOMP simulator transports solutes as a function of the solute and rock/soil type according to a linear adsorption isotherm model. . . . additionally allow solute transport via the Freundlich and Langmuir adsorption models.

4. **VAM3D-CG.** Met/Met. From Section 8 of HG (1994) (Input Data Preparation). Hanford Site applications show capability. Note RPROG(I,2) specifies Kd.

   "VAM3D-CG can simulate geochemical retardation using the linear sorption isotherm or Kd model where the value of Kd depends on the contaminant and on the spatial location. Such a capability is handled via Group 11 input data and prescribing data for PROP(J,4) for each contaminant species being modeled (pg. 8-18; Appendix A). VAM3D-CG has the capability to assign Kds by material types."

G. Time-Dependent Hydraulic and Geochemical Values

1. **Requirements.** The proponent of the code shall document the ability of the code to simulate changes in hydrogeologic and geochemical properties which are an explicit function of time.

2. **PORFLOW.** Met/Met. The original proposal (Runchal 1998a) indicates that PORFLOW can use time-dependent variables. Past Hanford Site applications have used the restart feature instead. However, proposal does not indicate place in manual nor is it obvious which input card contains information. The revised proposal (Runchal 1998b) states that ability is present using STORativity, DISTribution, RETArdation, and VISCOsity commands.

   See assessment above. "In addition, RESTart feature and MATEreal type designation can be used to assign step-wise changes in properties with time."

3. **STOMP.** Met/Met. Uses restart capability.

"The current released version of the STOMP simulator can only accommodate time-dependent hydraulic and geochemical values through modification of rock/soil properties through the restart function. . . . requires the user to use the restart function . . . Drastic changes in rock/soil properties could result in convergence problems upon restart . . ."

"An alternative would be to modify the simulator to accept time-dependent input for the rock/soil properties. . . . This modification would eliminate the need to halt and restart the simulation as all the rock/soil property transitions could be specified within the input file. A modification of this nature would require approximately one to two man-weeks to implement . . ."

4. **VAM3D-CG.** Met/Met. Uses restart capability.

"VAM3D-CG can simulate time-dependence of hydraulic and geochemical parameters for the engineered facility. Such a capability is accomplished by controlling Group 6 "Temporal discretization data" (pg. 8-12; Appendix A) and invoking the restart option."

H. Layering

1. **Requirements.** The proponent of the code shall document that the code can readily simulate:

   - geologic or engineered layering (including structures),
   - heterogenous features, and
   - anisotropic conditions that would affect moisture flow or contaminant transport.

   The layering shall not be restricted to a horizontal representation.

2. **PORFLOW.** Met/Met. No reference was given in the original proposal (Runchal 1998a) to check that capabilities presence. The revised proposal (Runchal 1998b) documents such capabilities.

   Each material type is assigned with a MATEreal command. Each type may be arbitrarily located and may be contiguous or non-contiguous in any geometric shapes. Multiple commands with the same material type may be used to handle spatial non-uniformity.

   Properties can be assigned to each material type in a heterogenoeus manner.

   For each material type anisotropic properties can be assigned with HYDRaulic, THERmal, and TRANsport commands.

   Additional complexity can also be accommodated with STOR, DIST, RETA, and VISC commands.

3. **STOMP.** Met/Met. Uses orthogonal grid systems to define geometry. Nonuniform spacing allowed (Section 4.5.3 of White 1997). Heterogeneous features can be specified as each cell can have different properties. Anisotropic moisture conditions specified by hydraulic properties card (Section A.7 of White 1997).

   All geologic features and engineered structures below the ground surface can be incorporated into a geohydrologic conceptual model for the STOMP simulator with the restriction that the shape of such structures are approximated by grid cells defined by the computational grid.

4. **VAM3D-CG.** Met/Met. From Section 8 of HG (1994) (Input Data Preparation). Savannah River Site application shows layering capability.

   VAM3D-CG uses curvilinear grid and transition elements to represent inclined geologic formations and complex geometries such as the engineered system. Unlike finite-difference and integrated finite difference models (e.g., PORFLO), use of finite-element discretization and curvilinear grids in VAM3D-CG avoids "stair-stepping" to represent inclined boundaries.

   The use of curvilinear grid and transition elements is invoked via Group 3 ICURVL input parameter and Group curvilinear mesh data.

   The heterogeneities in geologic formations are modeled in VAM3D-CG via variable NMAT. The anisotropic behavior in saturated media flow and transport properties is modeled in VAM3D-CG via Group 9 input data for the principal components of saturated hydrualic conductivity tensor and Group 11 transport parameters.

I. Output

1. **Requirements.** The proponent of the code shall document that the code can provide moisture content throughout model domain and contaminant concentration and flux at user chosen points, internal surfaces, and/or along boundary segments; all as functions of time as well as be able to calculate flow lines for user chosen source points. The code shall be able to report mass balance and mass balance errors at each time step.

2. **PORFLOW.** Met/Met. No reference was given in the original proposal (Runchal 1998a) to check that capabilities presence. No indication in proposal mass balance is outputted, but past Hanford applications indicate that this is done. The revised proposal (Runchal 1998b) does document capabilities.

3. **STOMP.** Potentially not met/Not. Most output options allowed (see exceptions below). Mass balance errors are a user-specified value (however, where value is specified could not be found). Flowlines would have to be calculated using external software, but is discouraged.

   Two principal output mechanisms for the simulator are reference nodes and plot files. Reference nodes allow the user to specify that a collection of variables are printed or displayed for a number of grid cells after an interval of converged time step.

   The current released version of the STOMP simulator does not provide mass balance information after each time step and does not provide flow-line calculations from selected points.

4. **VAM3D-CG.** Met/Met. From Section 8 of HG (1994) (Input Data Preparation). Output at user chosen points, internal surfaces, and/or along boundary segments is handled by VAM3D-CG. TECPLOT (document not supplied) creates flowlines as demonstrated in Hanford Site application. Mass balance input defined in Section 8.

   VAM3D-CG outputs on moisture contents through model domain, contaminant concentrations, and fluxes at user-chosen points (specified nodes), internal surfaces and/or along boundary segments, all as functions of time, are controlled via Group 5 input variables . . . .

   Via TECPLOT, the code is able to draw flow lines for user chosen source points. TECPLOT is a commercial graphical package . . . VAM3D-CG is able to report mass balance errors at each time step for both flow and transport; the option is invoked by setting IMBAL=1 on Group 5 input data.

J. Interface Between Moisture Flow and Contaminant Transport

1. **Requirements.** The proponent of the code shall document that the code is able to perform a moisture flow simulation only, a steady-state contaminant transport simulation based on a previously run moisture flow calculation, and a combined moisture flow/contaminant transport simulation performs. The proponent shall also document that redundant information is not needed for a combined moisture flow/contaminant transport simulation.

2. **PORFLOW.** Met/Met. The original proposal (Runchal 1998a) indicates that requirement met and past Hanford Site applications also indicate that requirement is met. The revised proposal (Runchal 1998b) documents use of SOLVE, SAVE, and RESTART commands.

3. **STOMP.** Met/Met. Solution Control Card (Section A.2 of White 1997). As referenced in the STOMP User's Guide, the STOMP simulator has options for executing a flow only simulation, a transport only simulation, or a combined flow and transport simulation. . . . Sequencing the solute transport equation solutions allow for first order chemical reactions and radioactive chain decay, but does not allow for complex chemical systems to be resolved. . . .Converting between the three different simulation types only requires single word modification to the input file; no duplication of input file variables is required.

4. **VAM3D-CG.** Met/Met. From Section 8 of HG (1994) (Input Data Preparation). VAM3D-CG can perform a moisture flow simulation only, a steady-state contaminant transport simulation based on a previously run moisture flow simulation and a combined moisture flow/contaminant transport simulation. Note that for a combined VAM3D-CG moisture flow/contaminant transport simulation, only one set of input file is required; no redundant input files is required.

V. DESIRABLE FEATURES

These items are features which the code should have, but the absence of which will not disqualify a code. However, code selection will depend on the applicability of these desired features. Notably poor performance on a desired feature (such as excessive cost) can be reason for code disqualification. The following sections are listed in order of priority.

A. Ease of Use

1. **Criteria.** The proponent of the code shall document the pre- and post-processing modules that aid user's use of the code and the user's understanding of the output of the code. In particular, the capability to graphically display the numerical grid discretization along with zone identifiers, the contaminant, and moisture fluxes across selected boundaries and/or regions in the modeling domain and contours, spatial cross sections, and time histories of contaminant concentrations is highly desired. The pre- and post-processing systems can be commercial or public domain products not developed by those responsible for the vadose zone code.

   (General note: responses poorly documented ease of use.)

2. **PORFLOW.** 40%/60%. A GUI (undescribed and undocumented) is available for Windows 95 and NT operating systems and is under development for UNIX. A post-processor is available, but is not described or documented. Because of output format, third party software can be used. The validation documentation could not be downloaded from the website. Because of illness, there is no experienced user of PORFLOW in the Hanford Site community and the proposal was submitted by the code developer. Based on proposal's lack of responsiveness, the difficulty of interface with nonlocal users and lack of providing helpful information, ranking is downrated.

   PORFLOW provides on-line manual for problem setup and an acrSHELL work environment. The acr PLOT post processor provides for XY, Vector, Contour, Raster, 3D Surface, and Profile plots. In addition, PORFLOW provides an open file format which has been integrated with powerful post-processing packages such as TECPLOT, SURFER, PLOT3D, etc.

   The code developer has indicated a willingness to establish a local office and provide a senior knowledgeable staff should PORFLOW be chosen.

3. **STOMP.** 50%/60%. Input format is flexible and is checked by code. A graphical interface is available for Macintosh (which is not hardware under consideration). A link between GIS and input is under development. Several undocumented post-processing utilities are available. However, calculation of flowlines (a mandatory requirement) is difficult and is discouraged. Property changes require restarting

the run rather than a smooth transition during a run. Downrated because of lack of specificity and comparison to other codes.

The simulator contains a considerable amount of error check utilities and will provide the user with information about the type of error that was discovered.

This utility (GEOSTOMP) will provide an interface between geologic data contained in GIS or Earth vision, geohydrologic descriptions of the rock/soil types . . . .

Several undocumented post process utilities have been written for the STOMP simulator, that are primarily used to convert output in the "output" and "plot" files to formats required for plotting or visualizing.

PNNL has a local staff knowledgeable of the program, however, code is the least developed of the alternatives.

4. **VAM3D-CG.** 50%/70%. Undocumented pre- and post-processors are available. The use of curvilinear coordinates is a significant feature given that structural components and geologic layers will not be parallel to surface or to each other. However, property changes require restarting the run rather than a smooth transition during a run. Downrated because of lack of specificity and comparison to other codes.

   RETC is a code that provides best fit curve to measured data on soil hydraulic properties . . . . VAMGEN is a customized pre-processor which generates a geometry of the numerical grid discretization along with zone identifiers. VAM2TEC is a post-processor that reads the output files . . . and formats the data for use with the graphical package TECPLOT to display . . . .In addition, at HGL, VAM3D-CG is fully integrated with ARGUS MESH MAKER . . . to generate finite-element mesh with GIS interface.

   Some local staff is available through FDNW and teaming with Hydro Geologic, Inc.

B. Certification/Verification/Benchmarking

1. **Criteria.** The proponent of the code shall supply documentation of such testing. The experimental data need not be from the Hanford Site, but should reflect similar environmental conditions (dryness, geochemistry). The proponent shall also supply any information concerning verification/benchmarking simulations against other codes which are relevant for Hanford Site vadose zone-like conditions.

2. **PORFLOW.** 80%/80%. Validation document could not be downloaded from web site. Alternate website could not be contacted. The proposal states a large number of users of the code, but provides no references to documents providing certification, verification, and benchmarking data in this section. List of publications does provide some (including Hanford Site) references. Because of

its use in 98 ILAW PA, PORFLOW is known to have a well documented testing base. Downrated because of poorness of response. Even revised proposal (Runchal 1998c) does not provide references.

3. **STOMP.** 100%/80%. The proposal referenced and supplied good documentation on benchmarking. Documents are cited for Hanford Site-relevant conditions including the relevant simulation of the Sisson-Lu experiment.

   Although the verification process has been formally documented in the STOMP Application Guide, the simulator continues to be compared against analytic solutions, numerical solutions, and experimental data.

   With respect to benchmarking against field experiments at the Hanford Site, the simulator was applied against the injection experiment of Sisson and Lu. There is implied benchmarking against Las Cruces Trench Site.

4. **VAM3D-CG.** 100%/100%. The proposal referenced and supplied good document action on benchmarking. Documents are cited for Hanford Site-relevant conditions including the relevant simulation of the Sisson-Lu experiment.

   Detailed information on VAM3D-CG certification, verification, and benchmarking for the Hanford Site is provided in Appendices B and C. Additional testing of VAM3D-CG using data from a field experiment (Sisson and Lu 1984) in 200 East Area is described by Lu and Khaleel (1993). Additional benchmarking and testing identified . . . .

C. Reputation Among User Community

1. **Criteria.** The proponent of the code shall document examples of use of the code beyond the developing organization. The proponent shall document whether the code has been accepted by the U.S. Environmental Protection Agency (EPA) and the Washington State Department of Ecology (Ecology) for environmental analyses for the Hanford Site. If the code has not been accepted, then the proponent shall indicate plans for achieving such acceptance. The code proponent shall supply the authors, title, and document identifiers of some of the reports which have used the code to model moisture flow and contaminant transport in the Hanford Site vadose zone. The proponent shall indicate for each report cited the type of external review that was conducted. Such external reviews shall be provided if requested.

2. **PORFLOW.** 60%/100%. The proposal notes that PORFLOW has been used by a wide variety of users. Although unstated by the proposal, but of significant importance, is the use of PORFLOW in the 98 ILAW PA (Mann 1998) as well as performance assessments at other DOE sites. The proposal makes no acknowledgment of acceptance of the code by the EPA or Ecology for use at the Hanford Site, although a earlier version has been accepted for Hanford Site use by the two agencies. The proposal does not "indicate for each report cited the type of external review that was conducted." Even though PORFLOW has an extremely

high reputation among the user community, the proposal was downrated because of lack of responsiveness.

The proposal included a long list of users and references including the U.S. Nuclear Regulatory Commission (NRC) and numerous DOE contractors.

3. **STOMP.** 25/50%. As noted by the proposal, because of the newness of the code, STOMP has not yet developed a large user reputation. However, it was used by the Hanford Site Environmental Remediation Contractor (although not for 200E Area analyses) and by a member of the NRC staff. Significant concerns are that the output files contain the disclaimer "Results from this version of STOMP should not be used for license related applications." The analyses to be performed, if not "license related applications," are at the same level as they will be reviewed as part of a regulatory decision making process by the DOE, the NRC, and Ecology. The proposal notes discussion has been held with EPA concerning the use of STOMP on Hanford Site analyses, but makes no indication whether conversations have been held with Ecology (the lead agency for most of our activities). Downrated because of lack of acceptance in user community, "license-related" remark, and because of lack of discussions with Ecology.

The simulator has gained recognition among the Hanford Site community through the application by M. Connelley at CH2M Hill Incorporated.

Extensive academic usage: Oklahoma Christian University has used the simulator as part of the curriculum for an engineering design class. Ed Hill at the University of North Carolina used the simulator to investigate the behavior of DNAPL pools during enhanced remediation by surfactant and co-solvent flushing.

Stomp has yet to be formally accepted by EPA or Ecology.

4. **VAM3D-CG.** 95%/90%. The proposal notes that EPA and Ecology have accepted VAM for Hanford Site uses in 1990; however, this was for earlier version of code. The proposal notes that code has been used in Hanford Site performance assessments approved by DOE. The proposal also notes approval of analyses by NRC using code. Proposal slightly downrated because of much earlier version approved by EPA and Ecology not recent version, but this probably reflects more on agencies than on code.

Under TPA milestone M-29-01 "Description of Codes and Models to be Used in Risk Assessment," a committee was established in 1990 comprised of personnel from RL, contractors, and regulators. The committee recommended that VAM2D, a predecessor of VAM3D-CG, be selected as one of the vadose zone codes at Hanford. A series of peer-reviewed articles (Huyakorn, et al. 1986, 1985, 1984; McCord, et al. 1991) on VAM3D-CG and its predecessors have appeared in Water Resource Research, a journal that is ranked number one in impact factor in the water resource category by the ISI Journal Citation Reports.

Use by other DOE, U.S. Department of Defense (DOD), Superfund, Resource Conservation and Recovery Act of 1976 (RCRA), and commercial sites.

NRC funding of HG to develop VAM3D-CG.

D. Additional Contaminant Transport Capabilities

1. **Criteria.** The proponent of the code shall document whether the code has the ability to modify the K_d value and/or the diffusion parameter based on moisture content and whether the code can model sorption-enhanced dispersivity. The code proponent may submit additional capabilities that may be advantageous to TWRS.

2. **PORFLOW.** 80%/80%. The proposal claims that criteria are satisfied, but does not provide references to the user's manual and it is not obvious where in user's manual such capabilities are described. Note has been made of proposed added capabilities. The revised proposal (Runchal 1998c) repeats the claims, but does not provide significantly more information.

   In response to Mandatory Criteria G above: Time-Dependent Hydraulic and Geochemical Values; distribution and retardation co-efficients are stated to be arbitrary functions of time, space, phase variables, and user defined variables.

3. **STOMP.** 60%/60%. The proposal claims that the first two criteria are satisfied, but does not provide references to the user's manual. A modification of code to allow sorption-enhanced dispersion and to allow a single run of time dependent Kd would be easy.

   "The simulator also offers two models for the effective diffusion co-efficient as a function of aqueous saturation. The conventional model reduces the molecular diffusion co-efficient by the tortuosity and aqueous saturation . . . The current released version of the STOMP simulator does not address sorption-enhanced dispersivity."

4. **VAM3D-CG.** 75%/80%. The code handles moisture-dependent diffusion co-efficients and sorption-enhanced dispersivities and provides references to their collection in the user's manual. It does not handle moisture-dependent Kds but the capacity can be added. Note has been made of proposed added capabilities.

   VAM3D-CG does not accept Kd as a function of saturation, however, in computing the retardation factor, the variability in saturation is included. The code can be modified to account for variation in Kd due to saturation.

Additional capabilities that may be advantageous:

- molecular diffusion co-efficient
- sorption-enhanced dispersivity
- upstream weighting and uncertainty analysis
- flow and transport predictions with quantified uncertainty.

E. **Additional Moisture Flow Capabilities**

1. **Criteria.** The proponent of the code shall document the functional representations available in the code to represent hydraulic conductivity and moisture retention as well as the ability to treat saturation-dependent anistropy. The proponent shall document how the code treats moisture hysteresis. The code proponent may submit additional capabilities that may be advantageous to TWRS.

2. **PORFLOW.** 35%/70%. The proposal states a number of representations are available in the code, but does not point to reference in user's manual. No mention is made of hysteresis. Moisture-dependent anistrophy is available in an earlier version and could be easily added to current version. The revised proposal (Runchal 1998c) again makes claims, but does not add significantly more information.

   Options include Van Genuchten with Mualem and Burdine, Brooks and Corey with Mualem and Burdine, Exponential Characteristic, 4th Order Polynomial Characteristic, Logarithmic Characteristic, Power (and Inverse) Law Characteristic, Arbitrary Tabulated Values.

   In PORFLOW the user flexibility is further increased by the fact that the characteristic for saturation characteristic can be different than that for relative conductivity.

3. **STOMP.** 100%/70%. Criteria are in code and adequately presented in proposal. Added capabilities were noted.

   "Constitutive functions for relative permeability, saturation, and capillary pressure currently recognized by the STOMP simulator are shown in Tables 3 and 4. The hysteretic k-s-p model applied in the STOMP simulator for the Water Operational Mode follows the theory of Kaluarachchi and Parker . . ."

4. **VAM3D-CG.** 100%/70%. Criteria are in code and adequately presented in proposal. Added capabilities were noted.

   VAM3D-CG can use Brooks-Carey relationships for representing soil moisture characteristics data. Saturation-dependent anistropy option is invoked by . . . . This is a significant field-scale phenomenon for the dry, heterogenous sediments such as those expected beneath the ILAW disposal facility. VAM3D-CG can include soil moisture retention data for both main drainage and main wetting curves and can model hysteresis phenomena in flow calculations. Additional

VAM3D-CG capabilities of interest include mass lumping and Newton-Raphson technique and upstream weighting.

F. **Decay Products**

1. **Criteria.** The proponent of the code shall document those features of the code which allow different contaminant transport properties to be assigned automatically to progeny by the code based on position in the radioactive decay chain.

2. **PORFLOW.** 90%/100%. Proposal claims ability. Documented in ACRi 1998 using DECA line. Downrated because location not provided. The revised proposal (Runchal 1998c) again makes claim, but does not provide information.

3. **STOMP.** 90%/100%. Proposal claims ability, although how implemented could not be found in user's manual in a quick search. Proposal provides method of solution, a bonus.

   "As referenced in the STOMP User's Guide, the simulator can address multiple solutes with radioactive decay and complex decay chains."

4. **VAM3D-CG.** 40%/50%. Capability not available in submitted version, but could be added based on capability of alternate version.

   To model decay chain, VAM3D-CG uses RESTART option. VAM2D and VAM3DF model the chanted decay transport with much more ease. Benchmarking and certification of VAM3DF decay chain option $10K.

G. **User Support**

1. **Criteria.** The proponent of the code shall document available user support (including applicable costs). The code proponent shall also document relevant instances of user support.

2. **PORFLOW.** 50%/75%. Schedule of 1998 charges supplied. Proposal does not contain relevant instances of user support. Analytic and Computational Research, Inc. is a well established and well thought of company. However, based on responsiveness of proposal, user support may not be adequate.

   Telephone conversation indicates that ACRi would set up office in the Tri-Cities, if necessary, to support ILAW. The issue is dedicated knowledgeable staff tied to ILAW and it's needs. There would be several months learning for ACRi and devotion of project staff to support learning estimate $20 – $30K.

3. **STOMP.** 80%/75%. Applicable costs not supplied. However, proposal does provide instance of Hanford Site support. Major concern is that the code is still considered by developers as a scientific tool rather than as a tool used for license-type applications.

"For private clients, government agencies, and government contractors, the policy has been to provide user support through a cost recovery basis. Because the original development team continues to apply and modify the simulator, the laboratory can offer full user support for STOMP, including application consulting, code modifications, and output interpretation. An example of user support for the stomp simulator being extended to a Hanford Site contractor is the investigative project of 90-Sr migration by M. Connelley at CH2M Hill."

4. **VAM3D-CG.** 90%/90%. Applicable costs not supplied. However, proposal does contain instances of Hanford Site support. More significantly, proposal contains teaming letter with commercial firm which developed VAM. A phone call from Connelley (1998) indicated that as of July 1, 1998, HydroGeologic, Inc. has opened a Northwest Office in Richland. However, rating was not changed.

Five knowledgeable VAM3D-CG users are with Fluor Daniel Northwest, Inc. (FDNW) and its consultants. In addition to the code developer, a total of 25 VAM3D-CG modelers are with HydroGeologic, Inc. A teaming arrangement has been worked out with the code developer for ILAW modeling support.

H. Speed of Execution

1. **Criteria.** The proponent of the code shall provide evidence of the relative speed of the code.

General Note: No comparison figures were provided.

2. **PORFLOW.** Not rated because of lack of information. However, code does provide a number of solvers. Past experience indicates that execution speed of PORFLOW is not a basis for elimination. The revised proposal (Runchal 1998c) is silent.

To handle a variety of applications, it provides for a number of efficient matrix solvers. In addition, an interface is provided so that any external matrix solver can be used without any code modification.

Typical execution time for a vadose flow problem on an Intel Pentium II 400MHz system is on the order of 0.02 millisecond per element per step per equation. This means that a flow and transport problem with 10,000 elements and 1,000 time steps can be completed in less than seven minutes.

3. **STOMP.** Not rated because of lack of information. However, according to the proposal, the predecessor to STOMP was slower than other codes because of use of multiple-phase calculations. As this application will be mainly single-phase application, STOMP is expected to be slower than other codes, but not to a significant extent.

   "The current release version of the STOMP simulator has not been subjected to a formal comparison for execution speed against comparable software. (The predecessor MSTS) - MSTS was executed against the multi-phase and single-phase codes for two isothermal, unsaturated flow problems. With respect to execution speed, MSTS was comparable to the other multi-phase simulators, but slower than the dedicated single-phase simulators. The STOMP simulator currently offers a variety of options to decrease execution time ..."

4. **VAM3D-CG.** Not rated because of lack of information. Past experience indicates that execution speed of VAM3D-CG is not a basis for elimination.

   A comparison of PORFLO and VAM3D-CG run times for a PA production run shows the processing times for the two codes are comparable and runs can be completed overnight.

I. Non-Proprietary Codes

1. **Criteria.** The proponent of the code shall document whether the code is proprietary. If the code is proprietary, then the code proponent must document that the source code will be made available by lease or purchase to the U.S. Department of Energy, Richland Operations Office (RL) and its contractors (including LMHC and its agents. The proponent shall also supply the licensing cost (and any other mandatory fees for the use of the code).

2. **PORFLOW.** 50%/50%. PORFLOW is a proprietary code. The source code is available by lease. License cost was provided. Downrated because code is proprietary.

   "We have reason to believe that PORFLOW can handle all current and future needs of the Hanford Site with minimal, if any, additional development costs." Any cost savings of a public domain code will be more than offset by the future development costs."

3. **STOMP.** 75%/75%. STOMP is a mixture of proprietary code and code developed under DOE support. The source code is available and there is no license cost. The parts that are proprietary will probably not be used by TWRS. Downrated because the code is not fully in public domain.

   Battelle maintains copyright on all versions, revisions, and operational modes of STOMP simulator as granted by the DOE with stipulation that Versions 1.x of the STOMP simulator be made available to Federal and State agencies. RL and its contractors under Battelle's copyright stipulations will be provided a royalty-free copy of the STOMP software source coding for use on the TWRS environmental analysis program.

4. **VAM3D-CG.** 50%/50%. VAM3D is a proprietary code. The source code is at FDNW and is available from the code developer for inspection by other parties. License costs have already been paid by FDNW. Downrated because code is proprietary.

   Although proprietary, VAM3D-CG, Version 3.1, including the source code, is already available for FDNW use. The required licensing fees have been paid and no other mandatory fees are required. If needed, the source code for VAM3D-CG can be made available, via HGL, to a third party without additional fees for inspection and verification.

J. Version

1. **Criteria.** The proponent of the code shall document the history of code versions and shall indicate where the particular version submitted falls in this history.

2. **PORFLOW.** 75%/75%. PORFLOW, Version 4.0 is the latest version in a long line. However, no mention of the previous history is given in the proposal.

   PORFLOW, Version 4.0 is fully tested. The release of each version of PORFLOW is tested against a suite of 42 test problems. A beta version was released in mid-1997. The current version was released in December 1997. As such, it has already been in use by our clients for a few months.

3. **STOMP.** 90%/75%. The current version in Version 1, Revision 1. The proposal does not give indication of sub-versions (e.g., revision is 12). Information is obtainable from configuration management file.

   "The current release version of the simulator is Version 1, with various revision numbers depending on the particular library file. . . . currently carries the revision number 12 . . . . The RCS revision log which documents the modifications made to this file is shown in Figure 1."

4. **VAM3D-CG.** 100%/90%. History of versions provided.

   A timeline for different versions of VAM3D-CG is provided below:

   1988 - VAM2D
   1991 - VAM2D v 5.0
   1993 - VAM3D v 2.4b
   1994 - VAM3D v 3.1
   1995 - VAM3DF

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DISTRIBUTION SHEET

To	From	Page 1 of 1
R. W. Root	R. J. Murkowski	Date 4-14-99
Project Title/Work Order		EDT No. 624998
Recommendations for Computer Code Selection of a Flow and Transport Code to be Used in Undisturbed Vadose Zone Calculations for TWRS Immobilized Wastes Environmental Analyses, HNF-4356, Rev. 0		ECN No.

Name	MSIN	Text With All Attach.	Text Only	Attach./ Appendix Only	EDT/ECN Only
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