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Computer Code Selection Criteria for Flow and Transport Code(s) to be Used in Undisturbed Vadose Zone Calculations for TWRS Environmental Analyses

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Abstract: Mandatory criteria and desirable features for computer codes used to model moisture flow and contaminant transport in relatively undisturbed Hanford Site soils for TWRS programs are identified.

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**Computer Code Selection Criteria
for Flow and Transport Code(s)
To be Used in Undisturbed Vadose Zone Calculations
for TWRS Environmental Analyses**

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**In support of
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December 31, 1998

Table of Contents

I. INTRODUCTION	1
II. MANDATORY ADMINISTRATIVE CRITERIA	3
A. Technical Documentation	3
B. Code Availability	3
C. Configuration Control	4
D. Input Flexibility	4
E. Real-Time Monitoring/Restart Capabilities	5
III. MANDATORY TECHNICAL CRITERIA	6
A. Moisture Flow	6
B. Contaminant Transport	6
C. Boundary Conditions	7
D. Source Term	7
E. Hydrologic Properties	7
F. Geochemical Model	8
G. Time-Dependent Hydraulic and Geochemical Values	8
H. Layering	8
I. Output	9
J. Interface Between Moisture Flow and Contaminant Transport	9
IV. DESIRABLE FEATURES	10
A. Ease of Use	10
B. Certification/Verification/Benchmarking	10
C. Reputation Among User Community	11
D. Additional Contaminant Transport Capabilities	11
E. Additional Moisture Flow Capabilities	12
F. Decay Products	12
G. User Support	13
H. Speed of Execution	13
I. Non-Proprietary Codes	13
J. Version	14
V. REFERENCES	16

List of Tables

1. Weight for Desirable Features	15
A-1. Comparison with other Documents	A-1

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

- tank contents leaking from tanks and associated facilities during the storage, retrieval, or closure periods and
- 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 tank contents or contaminants. This document presents the code selection criteria for those vadose zone analyses (a subset of the above analyses) where

- the hydraulic properties of the vadose zone are constant in time
- the geochemical behavior of the contaminant-soil interaction can be described by simple models, and
- the geologic or engineered structures are complicated enough to require a two- or three dimensional model.

Thus simple analyses would not need to use the fairly sophisticated codes which would meet the selection criteria in this document. Similarly, those analyses which involve complex chemical modeling (such as those analyses involving large tank leaks or those analyses involving the modeling of contaminant release from glass waste forms) are excluded. The analyses covered here are those where the movement of contaminants can be relatively simply calculated from the moisture flow.

These code selection criteria are 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. Appendix table A-1 provides a comparison between the criteria in these documents and those used here.

This document does not define the models (that is, the generalized input to the code that describes the process modeled by the code) that TWRS programs will create for their situations. Because of the different locations, facilities, inventories, and goals of the various TWRS programs, each program will define the models for their activities.

A decision board-like process will be used to select the code(s). The TWRS Decision Management Procedure (WHC 1996) will be followed.

The code selection criteria are listed in three chapters

- 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 features which the code should have, but the absence of which will not disqualify a code.

Each code selection criterion will not only be presented but it will also be justified.

II. MANDATORY ADMINISTRATIVE CRITERIA

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

A. Technical Documentation

1. **Criterion.** Documentation describing

- model theory, governing equations, and assumptions,
- computational techniques and algorithms,
- code verification,
- user input, and
- example applications

must be available.

2. **Requirements.** The proponent of the code shall submit the documentation that describes 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.

3. **Reason.** Environmental analyses performed on TWRS activities receive regulatory and public scrutiny. Therefore, it is important that the underlying principles of the codes be available to anyone interested. For some analyses, regulators or others may want to repeat calculations.

Codes are regularly improved. The TWRS programs do not want to penalize a code because required documentation (although available by the time of code use) is not published at the time of code selection.

B. Code Availability

1. **Criterion.** The executable version of the code shall be available (although possibly for a fee) for computers likely to be used by analysts performing TWRS environmental studies.

2. **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 4 processors) will not be considered.

3. **Reason.** TWRS does not want to select a computer code which requires expensive or exotic computer hardware or which is not available to interested parties. Such interested parties may wish to repeat calculations.

C. Configuration Control

1. **Criterion.** The selected code shall be maintained under a software quality management program that assures that modifications and updates are traceable, auditable, and documented. Audits by Lockheed Martin Hanford Company or its agents may occur.
2. **Requirement.** The proponent of the code must submit the software quality management program plan for the code.
3. **Reason.** Different versions of computer codes may give different results. It is crucial that the causes of any such differences are known. Configuration control of a software product is essential for traceability of results from analyses conducted over a multi-year period.

D. Input Flexibility

1. **Criterion.** The selected code shall allow the use of site- and facility-specific data/standard/guidelines as appropriate. For example, the ability to use site-specific vadose zone parameters is required rather than parameters from a generic soil type.
2. **Requirements.** The proponent of the code must show that the code can accept input that is site- and facility-specific.
3. **Reason.** TWRS has many different sites and facilities which must be analyzed. Generic values are not sufficient.

E. Real-Time Monitoring/Restart Capabilities

1. **Criterion.** The code must contain real-time monitoring capability during actual run-time. A restart option must be provided.
2. **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 timestamps written to a file.
3. **Reason.** Because of the complexity of the models, simulations may take many days. Therefore it is important that the analyst be able to determine progress and be able to restart the run if a problem is found to exist.

III. 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 (for example, conservation of mass, momentum, and energy) and well established engineering equations (for example, Darcy's law, Fick's law).

A. Moisture Flow

1. **Criterion.** The code shall be 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.
2. **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.
3. **Reason.** The technical basis is that contaminant transport modeling follows that for moisture flow. Because of the complexity of TWRS facilities, both two- and three-dimensionality are required. Under far-field vadose zone conditions, the fluid density is constant. Similarly, there should not be a significant temperature gradient in the situations where these codes will be employed. Because of man-caused disturbances of the vadose zone infiltration rate and because of facility degradation, transient calculations will be needed in many cases.

B. Contaminant Transport

1. **Criterion.** The code shall be capable of simulating contaminant fluxes in two- and three-dimensions as a function of driving hydrologic processes and mass transport phenomena, including advection, hydrodynamic dispersion, molecular diffusion, and adsorption.
2. **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 the listed mass transport processes. 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.

3. **Reason.** The ability to simulate contaminant transport driven by hydrologic processes is the main technical reason for the code. Because of the complexity of TWRS facilities, both two- and three-dimensionality is required. Previous Hanford studies have shown that the mass transport phenomena listed are the drivers for contaminant transport.

C. Boundary Conditions

1. **Criterion.** The code shall be capable of incorporating time-dependent upper boundary conditions (i.e., a variable infiltration rate). The code shall be 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. **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 satisfies the other boundary condition criteria.
3. **Reason.** Because of man-caused changes of surface conditions and of natural climatic changes, the amount of water entering the vadose zone may have to be modeled in a time-dependent manner. The other boundary condition criteria are needed to provide flexibility in modeling.

D. Source Term

1. **Criterion.** The code shall be able to 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. **Requirements.** The proponent of the code shall document the code can handle the source term criterion.
3. **Reason.** The source term will be time-dependent in many TWRS simulations (for example, small tank leaks and releases from waste forms). The source term will also differ between the TWRS programs.

E. Hydrologic Properties

1. **Criterion.** The code shall be able to use van Genuchten - Mualem relationships to represent moisture retention and unsaturated conductivity functions. Such values could be different in the various geohydrologic zones or structural zones of the simulation. The parameters need not be a function of environmental conditions.

2. **Requirements.** The proponent of the code shall document that the code has the capability to use these two functions in the simulation of moisture movement and that the code has the ability to have different values in each user chosen zone.
3. **Reason.** Most of the Hanford moisture/conductivity data have been fitted to van Genuchten - Mualem relationships. The hydraulic properties of the Hanford Site vadose zone are location dependent. The basis of this code selection is that the contaminant density does not affect moisture flow.

F. Geochemical Model

1. **Criterion.** The code shall be able to represent geochemical retardation using the linear sorption isotherm or K_d model where the value for K_d depends only on the contaminant and on spatial position.
2. **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.
3. **Reason.** The basis for this code selection is that the role of geochemistry in the modeling is only geochemical retardation which can be modeled using the linear sorption isotherm (K_d) model. Geochemical retardation in the Hanford Site vadose zone can vary spatially, especially when engineering structures are present.

G. Time-Dependent Hydraulic and Geochemical Values

1. **Criterion.** The code shall be able to simulate engineered materials in the vadose zone which have hydrogeologic and geochemical properties which are time-dependent. Unless stated elsewhere, the code need not have the ability to model material property changes that are the function of the contaminants present.
2. **Requirements.** The proponent of the code shall document the ability of the code to simulate changes in material properties which are an explicit function of time.
3. **Reason.** Because of the long time periods under consideration, material properties of engineered structures will change. The simulations must be able to account for such changes.

H. Layering

1. **Criterion.** The code shall be capable of simulating engineered structures and various geologic features such as layering, heterogeneity, and anisotropy. The layering shall not be restricted to a horizontal representation.

2. **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.
3. **Reason.** The vadose zone under the Hanford Site exhibits layering and heterogeneities. The moisture flow is known to be anisotropic because of these properties.

I. Output

1. **Criterion.** The code shall 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. The code shall also 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. **Requirements.** The proponent of the code shall document that the code can provide the moisture flow and contaminant transport output as stated in the criterion.
3. **Reason.** Past experience with preparing environmental analyses has indicated that such capabilities are necessary to adequately portray the model runs.

J. Interface Between Moisture Flow and Contaminant Transport

1. **Criterion.** The code shall be 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. In the last case, redundant input will not be required.
2. **Requirements.** The proponent of the code shall document that the code performs the three classes of simulations. The proponent shall also document that redundant information is not needed for a combined moisture flow / contaminant transport simulation.
3. **Reason.** The three classes of simulations are needed for analyst flexibility. Often, the flow-field is established before the contaminant transport calculations are made. Multiple steady-state contaminant transport calculations can be made from one moisture flow calculation. Sometimes a single calculation is more appropriate.

IV. 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. Table 1 displays the weighting for each item.

A. Ease of Use

1. **Feature.** The code should interface with pre- and post-processing modules which allow the user to readily set up problems and to understand results. Graphical interfaces are preferred to text interfaces. Such pre- and post-processing modules could be an integral part 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.
2. **Proof.** 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.
3. **Reason.** The ability to obtain defensible results is directly related to ease of use. If the code's input is difficult to construct or its output is difficult to understand, then the probability that the analyst will misinterpret information greatly increases.

B. Certification/Verification/Benchmarking

1. **Feature.** The results of the code should be tested against experimental data from Hanford-relevant systems. The code should be verified and benchmarked against analytic solutions and other codes.
2. **Proof.** 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.

3. **Reason.** Although a code which predicts events thousands of years into the future is impossible to validate, it is important that the code be tested and evaluated against real conditions.

C. Reputation Among User Community

1. **Feature.** The code should be well regarded among the user and regulatory community. In particular, the code should be acceptable by the U.S. Environmental Protection Agency and the Washington State Department of Ecology for environmental analyses for the Hanford Site. The code should have been used in simulations of the Hanford Site vadose zone with the results published in externally reviewed documents.
2. **Proof.** 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 and the Washington State Department of 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.
3. **Reason.** The environmental analyses performed must gain acceptance by the regulatory agencies and by the public. A necessary condition is that the computer codes used have wide acceptance among the technical community and be accepted by the regulatory agencies. Such acceptance is more likely if the code has already been used to model the Hanford Site vadose zone with the results published in an externally reviewed paper or report.

D. Additional Contaminant Transport Capabilities

1. **Feature.** The code should be able to modify the chemical distribution coefficient (K_d value) of the linear sorption isotherm model based on moisture content. The code should also be able to modify the diffusion parameter based on moisture content. The code should be able to model sorption-enhanced dispersivity.
2. **Proof.** 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.

3. **Reason.** Research has shown that the chemical distribution coefficient (K_d value) of uranium depends on moisture content. Research has also shown that diffusion is also moisture dependent and that sorption-enhanced dispersion can be significant.

E. Additional Moisture Flow Capabilities

1. **Feature.** The code should have the ability to use different representations (including table lookup) for hydraulic conductivity and moisture retention as a function of moisture content. The code should be able to model saturation-dependent anisotropy for dry moisture regimes. The code should have the ability to distinguish between wetting and drying conditions and include these effects in the flow calculation.
2. **Proof.** 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 anisotropy. The proponent shall document how the code treats moisture hysteresis. The code proponent may submit additional capabilities that may be advantageous to TWRS.
3. **Reason.** Because many of the analyses will involve dry conditions, various functional representations of a single experimental data set may provide different calculational results. The ability to determine the sensitivity of calculational results to functional representation is important. Saturation-dependent anisotropy and moisture hysteresis effects may affect calculational results.

F. Decay Products

1. **Feature.** The code should be able to treat the effects of complex decay chains (for example, the decay of uranium).
2. **Proof.** 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.
3. **Reason.** The transport of the actinide radionuclides and their daughters are important to TWRS environmental analyses. However, the contaminant transport of various radioelements may differ, principally because of the differences in geochemical interaction.

G. User Support

1. **Feature.** The better the user support by the code developer, the better the code for TWRS analyses.
2. **Proof.** The proponent of the code shall document available user support (including applicable costs). The code proponent shall also document relevant instances of user support.
3. **Reason.** Much of the cost of using a code is the time that it takes an analyst to understand and apply the code. The better the user support, the better the answer will be and the more efficient the code will be to use. However, the benefit of technical support must be weighed against its cost.

H. Speed of Execution

1. **Feature.** The faster the code simulation for a given degree of accuracy, the better. Such speed could come from the superiority of algorithms, the better implementation of methods, and/or the greater use of hardware features.
2. **Proof.** The proponent of the code shall provide evidence of the relative speed of the code.
3. **Reason.** Many of the problems run for TWRS analysts might take days to complete. Thus, speed of execution is an important consideration.

I. Non-Proprietary Codes

1. **Feature.** Proprietary codes should be used only if they provide a distinct advantage over public domain codes and only if the author(s)/custodian(s) allow inspection and verification of the source code. If a proprietary code is used, the source code must be made available by lease or purchase to Richland Operations Office of the Department of Energy and its contractors (including Lockheed Martin Hanford Company and its agents for verification) and to any oversight agencies.
2. **Proof.** 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 necessary conditions above can be satisfied. The proponent shall also supply the licensing cost (and any other mandatory fees for the use of the code).
3. **Reason.** TWRS has a responsibility to ensure that the code behaves as claimed. It is desirable that others can confirm the investigation made by TWRS. The cost of the code should not be a major fraction of the cost of analyst. If it is, the code may not be acceptable.

J. Version

1. **Feature.** The version of the code should be a recent version, preferably the last one that has been fully tested, of a family of codes. For codes that are well established, the use of a well-tested version may outweigh the use of the newest, but less tested version.
2. **Proof.** The proponent of the code shall document the history of code versions and shall indicate where the particular version submitted falls in this history.
3. **Reason.** Computer codes have errors. Also, developers of codes learn how to better implement features of their codes. Thus, the latest version of a code usually is preferable to an earlier version.

Table 1.
Weight for Desirable Features *

Section	Description	Weight ⁺
A.	Ease of Use	
B.	Certification/Verification/Benchmarking	
C.	Reputation Among User Community	
D.	Additional Contaminant Transport Capabilities	
E.	Additional Moisture Flow Capabilities	
F.	Decay Products	
G.	User Support	
H.	Speed of Execution	
I.	Proprietary Codes	
J.	Version	

* If the costs of obtaining and using a code are excessive, the code may be disqualified.

+ The weighting fractions have been determined, but they will be kept in confidence by the decision makers.

V. REFERENCES

- Case 1988, M.J. Case and M.D. Otis, *Guidelines for Radiological Assessment of DOE Low-Level Radioactive Waste Sites*, DOE/LLW-62T (Section 4.5.2.5), U.S. Department of Energy, Idaho Operations Office, Idaho Falls, Idaho, July 1988.
- Kozak 1989a, M.W. Kozak, M.S.Y. Chu, C.P. Harlan, and P.A. Mattingly, *Background Information for the Development of a Low-Level Waste Performance Assessment Methodology: Identification and Recommendation of Computer Codes*, NUREG/CR-5453 [SAND89-2509], Volume 4 (Section 2.0), U.S. Nuclear Regulatory Commission, Washington, D.C., December 1989.
- Kozak 1989b, M.W. Kozak, C.P. Harlan, M.S.Y. Chu, B.L. O'Neal, C.D. Updegraff, and P.A. Mattingly, *Background Information for the Development of a Low-Level Waste Performance Assessment Methodology: Selection and Integration of Models*, NUREG/CR-5453 [SAND89-2509], Volume 3, U.S. Nuclear Regulatory Commission, Washington, D.C., December 1989.
- Mann 1995, F.M. Mann, *Computer Code Selection Criteria and Considerations of the Hanford Low-Level Waste Interim Performance Assessment*, WHC-SD-WM-CSWD-073, Westinghouse Hanford Company, Richland, Washington, March 1995.
- WHC 1995, "Decision Management", *TWRS Systems Engineering Manual*, WHC-IP-1231, Section 7.0, Rev. 0, Westinghouse Hanford Company, Richland, Washington, May 1996.
- WSRC 1992, *Radiological Performance Assessment for the Z-Area Saltstone Disposal Facility*, WSRC-RP-92-1360 (Appendices B.1), Westinghouse Savannah River Company, South Carolina, April 1992.

HNF-1839
Rev. 0

Table A-1.
Comparison with other Documents

DOE Guidance (Case 1988)	
Description	This Document
Model important transport and exposure processes	III.A, III.B
Address problem scenarios of concern	III.A, III.B
Function properly for the particular climate and geographical region	II.D
State of the art in a given modeling area	IV.I, general
Spatial and temporal simulation capabilities	III.A, III.B
Ability to accept site-specific characterization data	II.D
Flexibility to eliminate irrelevant processes	handled by scope of the project
Existence of adequate documentation	II.A

HNF-1839
Rev. 0

Description	This Document
Implement models of NUREG/CR-5453, Vol. 3 (Kozak 1989b)	II.A, III.B
Have sufficient and adequate documentation	II.B
Been extensively used or accepted by user community	IV.C
A public code is preferred to a proprietary code unless the proprietary code has some outstanding or unique feature	IV.J
Most recent version of a family of codes is preferred	IV.I
Complexity of the code should be commensurate with the amount of information available about the physical setting	III.A, III.B
Codes that can be run on existing NRC machines or personal computers are preferred.	II.B
Groundwater codes that can simulate both saturated and unsaturated zones are preferred.	Groundwater flow not in scope
Codes that simulate both flow and transport are preferred.	III.J, made mandatory
Handle time-dependent source injection rate	III.C
Capability to account for radioactive decay chains are preferred	IV.D

HNF-1839
Rev. 0

IPA Code Selection (Mann 1995)		
Identification	Description	This Document
2.1.1	Code shall be based on appropriate scientific principles and well established engineering equations	III.
2.1.2	Code shall be documented	II.A
2.1.3	Code shall be maintained under a software quality management program	II.C
2.1.4	Code shall allow the use of site- and facility-specific data/standards/guidelines	II.D
2.1.5	Code shall have diagnostic monitoring capability during run-time	II.E
2.2.1	Documentation of actual version shall be available when code is run	Not applicable, will be a program requirement
2.2.2	Verification of actual version shall be published	Not applicable, will be a program requirement
2.3.1	Code should be certified	IV.B
2.3.2	Degree of complexity shall be consistent with the quantity and quality of data and the objectives of the computation	Complexity not directly addressed as only one class of codes being considered
2.3.3	Computer hardware requirements should be consistent with available platforms and be affordable.	Made mandatory, restricted to Intel, UNIX computers having only a few processors.
2.3.4	Proprietary codes should be used only if they provide a distinct advantage and only if the code is available for inspection	IV.J
2.3.5	Ease of interfacing code input/output with other codes is desirable	IV.A

HNF-1839

Rev. 0

IPA Code Selection (Mann 1995)		
Identification	Description	This Document
2.3.6	Familiarity with the code is desirable	Code familiarity not addressed because we do not know code users. Implication captured in IV.A
2.3.7	Code should be generally known and accepted by user community	IV.C
2.3.8	Code should be recent version	IV.I
3.1.1	Flow code shall be capable of simulating steady-state and transient flow fields	III.A
3.1.2	Flow code shall be capable of simulating two-dimensional flow of water of a constant density in an isothermal setting	III.A
3.1.3	Flow code shall be capable of simulating unsaturated flow under dry soil conditions using standard unsaturated hydraulic conductivity and water retention functions	III.F
3.1.4	Flow code shall be capable of simulating saturated groundwater flow	Groundwater flow is not part of scope
3.2.1	Flow code should be capable of simulating two-dimensional analysis in groundwater zone	Groundwater flow is not part of scope
3.2.2	Flow code should be capable of incorporating time-dependent boundary conditions	Only upper surface boundary condition is time dependent, but this is mandatory condition
3.2.3	Flow code should be capable of simulating various geohydrologic features	III.H; Made mandatory
3.2.4	Flow code should be able to handle both tabular and closed form expressions	III.F, IV.F; Van Genuchten/Mualem made mandatory

HNF-1839
Rev. 0

IPA Code Selection (Mann 1995)		
Identification	Description	This Document
4.1.1	Transport code shall be capable of calculating waste inventory as a function of time and computing contaminant fluxes at designated locations	III.B, III.D
4.1.2	Transport code shall be two- or two-/three-dimensional	III.B, III.K
4.1.3	Transport code shall consider transport mechanisms	III.B
4.1.4	Transport code shall accept a specified waste form release rate and simulate the release until the inventory is depleted.	III.D
4.1.5	Transport code shall be capable of simulating homogenous and non-homogeneous, time-dependent Dirichlet and Neumann boundary conditions	III.C; Time-dependent boundary conditions are not required
4.2.1	Transport code should be capable of simulating waste inventory daughter products as a function of time	IV.D
4.2.2	Transport code should simulate both flow and transport	III.K; Made mandatory
4.2.3	Transport code should simulate both saturated and unsaturated zones	Groundwater flow is not part of scope
4.2.4	Output of the code should be ready for a post-processor	III.I, IV.A; Some made mandatory
4.2.5	Transport code should be capable of simulating a mixed boundary condition	Cauchy boundary conditions were not addressed

HNF-1839
Rev. 0

Savannah River Performance Assessments (WSRC 1992)		
Identification	Description	This Document
1R	Code shall be based on appropriate scientific principles and well established engineering equations	III
2R	Code shall be verified	II.A
3R	Code shall be documented	II.A
4R	Code shall be maintained under a software QA and management program	II.C
1S	Code should allow site- and facility-specific application	II.D; Make mandatory
2S	Transport code should be capable of tracking waste inventory over time and computing fluxes at designated locations	III.B, IV.D; Some items made mandatory
3S	Code should be validated	IV.B
4S	Degree of complexity should be consistent with the quantity and quality of data and the objectives of the computation	Covered by scope of activity
5S	Hardware requirements should not be exotic	II.B; Made mandatory
6S	Proprietary codes should be used only if they provide a distinct advantage and only if the code is available for inspection	IV.J
7S	Ease of interfacing code output with other codes is desired	IV.A
8S	Familiarity with the code is desirable	Code familiarity not addressed because we do not know code users. Implication captured in IV.A

DISTRIBUTION SHEET

To J. A. Voogd	From F. M. Mann	Page 1 of 1
		Date 1-14-198
Project Title/Work Order Computer Code Selection Criteria for Flow and Transport Code(s) To be Used in Undisturbed Vadose Zone Calculations for TWRS Environmental Analyses.		EDT No. 622994
		ECN No.

Name	MSIN	Text With All Attach.	Text Only	Attach./ Appendix Only	EDT/ECN Only
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E. A. Fredenburg	H6-21	X			
F. M. Mann	B4-43	X			
D. A. Myers	G3-21	X			
J. A. Voogd	H6-37	X (3)			
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