
**EVALUATION OF COMPUTER
MODELS FOR PREDICTING
THE FATE AND TRANSPORT
OF SALT IN SOIL AND
GROUNDWATER**

PHASE I REPORT



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Phase I Report

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for

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Executive Summary

This report was prepared by MDH Engineered Solutions Corporation (MDH) for Alberta Environment (AE) to document Phase I of a two phase project to evaluate computer codes applied to predicting the fate and transport of salt in soil and groundwater.

A two-level ranking procedure was used to compare almost 250 (248) codes. The first stage of the process was based on review of readily available documentation, some discussion with model developers, and in-house expertise and experience of MDH personnel. This pre-screening stage eliminated over 200 (204) codes, leaving 43 for detailed analysis.

Stage II involved rating modeling codes based on 17 objective criteria. The rationale of the ranking scheme and the weighting of the 17 components are detailed in this report.

The top five codes from the ranking matrix were reviewed in detail for their strengths, weaknesses, and applicability to the AE salt release scenarios. Five of the top ten codes recommended for detailed analysis in Phase II are:

- 1) VS2DI (USGS);
- 2) SEVIEW (ESCI);
- 3) HYDRUS-1D or HYDRUS-2D (USSL-IGWMC);
- 4) UNSATCHEM (USSL); and
- 5) CHEMFLOW-2000 (OSU).

All the highly ranked codes have excellent documentation; good user interfaces, and provides numerous examples for validation and tutorial purposes.

Other codes in the top-ten ranking with similar functionality to some of those recommended include SWAP, LEACHM and SUTRA-2D.

MDH have attempted to recommend a “toolkit” of codes with different levels of sophistication. Together, these codes can be used to meet the varied levels of analysis that could be required at different stages of the site screening process.

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1.0 INTRODUCTION

This report was prepared to document Phase I of a project to evaluate computer codes for predicting the fate and transport of salt in soil and groundwater for Alberta Environment (AE). The project evaluates a wide range of existing computer models for their ability to predict the shallow movement of salts in the soil and groundwater. A two-level ranking procedure was used to compare the codes. This report describes the methodology used to perform the comparison and summarizes the strengths and weaknesses of a short list of codes ranked as most suitable for use in Alberta.

The objective of the project is to help AE choose software that is suitable for site-specific risk assessment or for the development of generic risk-based scenarios that can be used to guide remediation of soil and groundwater. Risk based corrective action (RBCA) strategies have been widely researched in the United States and Canada, and this project will draw on the accumulated experience in this area.

2.0 SCOPE

The scope of the project is to evaluate and recommend numerical computer codes that are suitable for site-specific risk assessment or for the development of generic risk-based scenarios that can be used to guide remediation of soil and groundwater. The project is divided into two phases:

- 1) Initial screening; and,
- 2) Code and model testing.

This report concerns the results of the initial screening portion (Phase I) of the project. The detailed scope of each phase is provided below:

2.1 *Phase I – Initial Screening*

The scope of Phase I of the project was to:

- 1) Conduct an initial screening evaluation of available non-proprietary modelling codes that can be used to predict the fate and transport of salts in soil and groundwater; and,
- 2) Provide an interim report to AE detailing the initial screening results.

In discussion with AE, the original scope was expanded to include proprietary codes when the licensing costs were considered to be modest (< \$750 US).

2.2 *Phase II – Model and Code Testing*

The scope of Phase II will be to:

- 1) Test the codes selected during the initial screening on three typical salt release scenarios in fine and coarse textured soils:
 - Localized subsurface sources from buried pipelines;
 - Short-term and long-term flare pits; and,
 - Short-term and long-term highway salt storage piles and,
- 2) Provide a report documenting the results of the test runs.

3.0 RBCA PROCEDURES

RBCA integrates EPA risk assessment practices with traditional site investigation and remedy selection activities in order to determine cost-effective measures for protection of human health and environmental resources. The ultimate endpoint of the RBCA planning process is the cleanup/closure of sites in an expedient, protective, and cost-effective manner. The purpose of this section is to place the model evaluation process in the RBCA context.

3.1 *RBCA Applied to Salt Release*

Under this integrated approach, salt release sites are characterized in terms of *sources, transport mechanisms, and receptors*. Remedial measures are then applied as needed to prevent environmental exposure to harmful levels of salt. Such risk-based corrective action can be achieved by addressing any step in the exposure process:

- a) Removing or treating the source;
- b) Interrupting contaminant transport mechanisms; and,
- c) Controlling levels at the point of exposure.

Under RBCA, risk management strategies are developed and implemented as a standardized procedure. Based upon available site information, a site classification step is first completed to characterize the relative magnitude and immediacy of site risks and prescribe immediate response actions. After any short-term hazards have been properly addressed, risk-based cleanup standards are developed to protect against potential environmental impacts associated with long-term exposure to low levels of contaminants.

To provide for economical use at both small and large facilities, the RBCA process is designed to match the planning effort to the relative risk or complexity of each site. For this purpose, a tiered approach is employed for calculation of risk-based cleanup levels, involving increasingly sophisticated levels of data collection and analysis. Upon completion of each tier, the user reviews the results and recommendations and decides if further analysis is required. To achieve the final risk management goals, the remedial action program may involve:

- 1) Source removal/treatment;
- 2) Containment measures;
- 3) Institutional controls; or,
- 4) Some combination of all three.

RBCA represents a risk management system that must be customized to fit the specific environmental concerns and legal/regulatory constraints of each provincial or federal regulatory program.

3.2 Model Evaluation for RBCA

Modelling is an integral part of the RBCA procedure. To facilitate efficient processing of site remediation/closure applications, clear guidance is required regarding pre-approved modeling and risk characterization protocols. A tiered approach is recommended. An overview of the recommended tiered approach is provided in Section 3.2.1 through Section 3.2.3.

3.2.1 Tier I Assessment

At this very preliminary level, only an estimate of maximum concentrations and total mass at the point of exposure (POE) and identification of receptors are required. A simple look-up table might be sufficient to decide whether the maximum concentration and/or total mass, or the site and/or the specific receptors, justify Tier 2 analysis.

3.2.2 Tier 2 Assessment

At this level, the affected porous media needs to be delineated together with determination of the site-specific transport processes and pathways from POE to receptor. Simple analytical models can be applied to screen site-specific cases. Simple analytical models form a basis for the decision whether or not to proceed to Tier 3 analysis.

3.2.3 Tier 3 Assessment

For a Tier 3 assessment, the affected porous media needs to be delineated further together with more thorough determination of site-specific transport processes and

transport pathways from POE to receptor. Numerical models can be applied at this level to investigate the extent of the problem and evaluate remediation alternatives.

3.3 Suitability of Models

The models recommended by this evaluation will be suitable for Tier 2 (analytical) and Tier 3 (numerical) analysis of salt contamination scenarios as detailed by AE. These scenarios include:

- 1) Localized subsurface sources from buried pipelines;
- 2) Short-term and long-term flare pits; and,
- 3) Short-term and long-term highway salt storage piles.

4.0 INITIAL SCREENING

A two stage screening process was adopted. For the first stage, a comprehensive list of almost 250 codes (248) was assembled together with readily available documentation. The codes were reviewed for their applicability to the specified AE scenarios and their costs. At this stage, a large number of codes were eliminated based on generic pre-screening criteria as determined by MDH. The Stage I pre-screening is discussed in Section 4.1

The first stage screening reduced the number of codes to 43. These codes were then subjected to a detailed analysis using a ranking matrix in Stage II, with particular emphasis on their ability to meet AE criteria for modelling salt movement. The Stage II screening is discussed in Section 4.2.

4.1 Stage I – Pre-screening

Stage I of the investigation involved a preliminary assessment of available codes that appeared to be applicable to salt fate and transport modelling. The initial screening was based on review of readily available model documentation, some discussion with model developers, and the in-house expertise of the assembled MDH team who have utilized and previously compared many of the available software packages. At this stage the licensing costs of codes were determined. A number of generic criteria concerned with applicability were used to pre-screen the comprehensive list and eliminate many generic groups of codes. The total number of codes eliminated by pre-screening was over 200 (205).

The codes eliminated by pre-screening are listed in Appendix A. Codes are grouped based on the pre-screening criteria. Some of these codes, specifically those where cost (>\$750 US) or complexity (3-D models) was the pre-screening elimination criteria, would be suitable for analyzing the scenarios listed in section 2. However, because of the requirements of cost and simplicity set out in the contract, such codes were eliminated.

MDH would like to emphasize that elimination of codes should not be interpreted as an indication that those codes are in any way defective or inadequate. Codes were ranked

against specific criteria, judged to be important for application to a specific set of practical problems.

A large group of codes were eliminated (98 codes total) after preliminary examination and excluded from the ranking procedure because they were considered inappropriate for the intended application:

- 1) Models designed primarily for NAPLs and multiphase flow were eliminated (25 codes) because the project scope was to investigate the movement of salt;
- 2) Models with no solute transport capabilities (flow only) were eliminated (39 codes) as they are inappropriate for the intended application;
- 3) Surface water models were eliminated (5 codes) as they are inappropriate for the intended application;
- 4) Geochemical speciation models with limited or no flow simulation capabilities were eliminated (6 codes) as they are inappropriate for the intended application;
- 5) Codes that were primarily databases or pre-and post-processing interfaces were eliminated (20 codes); and,
- 6) Heat flow codes and codes concerned with evaporation only were eliminated as they are inappropriate to the application (3 codes).

Another group of codes were discounted (47 codes total) based on their lack of currency, availability, documentation or support:

- 1) Codes that could not be located after diligent searching were eliminated (20 codes);
- 2) Codes that had become obsolete or had been succeeded by later versions were eliminated (17 codes); and,
- 3) Codes with no North American distributor where documentation and/or support in the English language were a concern and were eliminated (10 codes).

A further group of codes were eliminated (50 codes total), because of technical limitations (but these codes were still subjected to stage II ranking to ensure a rigorous review):

- 1) 3-D codes were eliminated (11 codes) because the expected level of data availability for the AE scenarios cannot justify the use of the level of modelling complexity inherent in the 3-D codes; and,
- 2) Codes that only consider the saturated zone were eliminated (39 codes) as many of the AE salt release scenarios are largely in the unsaturated zone.

Finally, the codes with high cost were eliminated (but these codes were also subjected to stage II ranking to ensure a rigorous review):

- 1) Codes costing more than \$750 US to license were eliminated (10 codes) because the scope of the project specified low or modest costs could be considered.

4.2 Stage II - Ranking Matrix

Stage II of the investigation involved ranking of the modelling codes not eliminated during the pre-screening undertaken during the preliminary screening (Stage I). A ranking matrix with the following criteria was defined in the proposal submitted by MDH to AE:

- 1) Ability to model water balance for the range of soil and climate conditions found in Alberta;
- 2) Ability to model water and dissolved ion movement, including vertical (downward and upward) and lateral flow components;
- 3) Ability to model soil chemical processes including cation exchange, precipitation/dissolution and other chemical reactions;
- 4) Ability to model changes to soil physical conditions such as hydraulic conductivity resulting from changes in salinity;
- 5) Ability to model typical Alberta contamination scenarios such as highway maintenance yards, flare pits, and pipeline breaks;
- 6) Ability to handle both the saturated and unsaturated zones or ability to link with other codes;
- 7) Availability of the code and ease with which documentation can be found;

- 8) Approximate cost of licensing the code;
- 9) Ease of use;
- 10) Data requirements;
- 11) Simplicity and transparency;
- 12) Computational requirements (i.e. computational resources necessary to run the code);
- 13) Support availability and both level and quality of expected support;
- 14) Available code validation data sets and comparisons; and,
- 15) Code history (years in use, regulatory acceptance history).

This preliminary list was modified slightly as a result of difficulties encountered in the ranking process. Short titles corresponding to the headings used in the ranking matrix tables provided in Section 5.0 are used for this modified list. The final list of ranking criteria that was applied is as follows:

- 1) Water balance;
- 2) Subsurface flow model capability;
- 3) Transport mechanisms;
- 4) Chemical reactions;
- 5) Hydraulic conductivity (K) as a function of salinity;
- 6) Zones modelled;
- 7) Program availability;
- 8) Data requirements;
- 9) Simplicity and transparency;
- 10) Computational requirements;
- 11) Program installation;
- 12) Support availability;
- 13) Code validation;
- 14) Documentation quality;
- 15) Ease of use; and,
- 16) Ability to meet AE criteria.

All available codes (after pre-screening) were rated on a scale of 1 to 10 for each of the above 16 criteria. An objective weighting-factor for each of the criteria was applied based on their relative importance for the specific project.

4.2.1 Rationale for Rankings

This section deals with the criteria used to rank the individual codes. For preliminary screening, some information was unavailable or difficult to determine or the documentation was ambiguous. In such cases, MDH personnel used their experience to make a subjective judgment. These cases are highlighted in the tables (shaded).

While care was taken to characterize each code as accurately as possible, with such a large number of codes (almost 250) and numerous ranking criteria (78 reducing to 17), misinterpretation of documentation and errors are unlikely to have been eliminated entirely. Tables 4.1 through 4.16 provide the ranking rationale for each of the criteria.

TABLE 4.1 WATER BALANCE:

Ranking	Explanation
10	Computes flow and chemical mass balance.
8	Computes chemical mass balance but flow balance can be added.
6	Computes flow balance but chemical balance can be added.
4	Computes chemical mass balance only.
2	Computes flow balance only.
1	Does not compute flow or chemical mass balance.

TABLE 4.2 FLOW MODEL CAPABILITIES:

Ranking	Explanation
10	Transient unsaturated and saturated vertical and lateral flow.
9	Steady state unsaturated and saturated vertical and lateral flow.
8	Transient unsaturated and saturated vertical flow.
7	Steady state unsaturated and saturated vertical flow.
6	Transient unsaturated vertical and lateral flow.
5	Steady state unsaturated vertical and lateral flow.
4	Transient unsaturated vertical flow.
3	Steady state unsaturated vertical flow.
2	Transient saturated vertical and lateral flow.
1	Steady state saturated vertical and lateral flow.

TABLE 4.3 TRANSPORT MECHANISMS:

Ranking	Explanation
10	Advection, dispersion, diffusion, density-dependent flow.
8	Advection, dispersion, diffusion.
6	Advection, dispersion, density-dependent flow.
4	Advection, dispersion.
3	Advection; density dependent flow.
1	Advection, particle tracking only.

TABLE 4.4 CHEMICAL REACTIONS:

Ranking	Explanation
10	Adsorption, cation exchange, precipitation/dissolution, decay.
9	Adsorption, cation exchange, decay.
8	Cation exchange, precipitation/dissolution, with or without decay.
7	Cation exchange with or without decay.
6	Adsorption, precipitation/dissolution, decay.
5	Adsorption, decay.
4	Adsorption.
3	Precipitation/dissolution, decay.
2	Precipitation/dissolution.
1	Decay.

TABLE 4.5 HYDRAULIC CONDUCTIVITY AS A FUNCTION OF SALINITY:

Ranking	Explanation
10	Built into the existing code.
8	Can be added easily to source code.
6	Can be added to source code with difficulty.
2	Possibility of adding; source code available.
0	No possibility of adding; or source code not available.

TABLE 4.6 ZONES MODELLED:

Ranking	Explanation
10	Root /vadose/saturated zone.
9	Root /vadose/saturated zone; must be linked to flow model.
8	Vadose/saturated zone.
7	Vadose/saturated zone; must be linked to flow model.
6	Vadose zone.
4	Vadose zone; must be linked to flow model.
2	Saturated zone.
1	Saturated zone; must be linked to flow model.

TABLE 4.7 CODE AVAILABILITY:

Ranking	Explanation
10	Readily available from free website, automatic installation.
9	Readily available from free website, requires manual installation.
8	Readily available from commercial website, automatic installation.
7	Readily available from commercial website, manual installation.
6	Available after email request.
5	Commercially available via email and/or order form processing.
4	Available but difficult to install (needs compilation and editing).
3	Available but obsolete or too old to readily install.
2	Hard to locate and install.
1	MDH could not locate installable version.

TABLE 4.8 DATA REQUIREMENTS:

Ranking	Explanation
10	Provides soil, chemical, climatic data; little input to run.
9	Provides soil/chemical or soil/climatic data; little input to run.
8	Provides soil data, little input to run.
7	Provides some data, little input to run.
6	Provides no data, little input to run.
5	Provides soil, chemical, climatic data; major input to run.
4	Provides soil/chemical or soil/climatic data; major input to run.
3	Provides soil data, major input to run.
2	Provides some data, major input to run.
1	Provides no data, major input to run.

TABLE 4.9 SIMPLICITY AND TRANSPARENCY:

Ranking	Explanation
10	Simple EXCEL spreadsheet macro.
9	Pre-made problem-specific mesh.
8	1-D homogeneous; source code included.
7	1-D heterogeneous; source code included.
6	2-D homogeneous; source code included.
5	2-D heterogeneous; source code included.
4	1-D; well documented; source code not included.
3	2-D; well documented; source code not included.
2	1-D; poorly documented; source code not included.
1	2-D; poorly documented; source code not included.

TABLE 4.10 COMPUTATIONAL REQUIREMENTS:

Ranking	Explanation
10	Standard CPU, Windows GUI.
9	Standard CPU, Windows GUI, EXCEL.
8	Standard CPU, Windows GUI, C/Fortran compilers.
7	Standard CPU, Windows GUI, added memory.
6	Standard CPU, Windows GUI, added memory, C/Fortran compilers.
5	Fast CPU, Windows GUI.
4	Fast CPU, Windows GUI, added memory.
3	Fast CPU, Windows GUI, added memory, C/Fortran compilers.
2	Standard CPU, DOS/Unix OS and/or DOS/Unix graphics.
1	Obsolete OS.

TABLE 4.11 PROGRAM INSTALLATION:

Ranking	Explanation
10	Code downloaded and installed successfully.
8	Code downloaded and compiled successfully.
7	Program downloaded, not compiled, no problems expected.
6	Demo version downloaded and installed successfully.
5	Program downloaded, not installed, may be difficult to install.
4	Code downloaded and compiled with many changes.
3	Code/demo version downloaded, will not install or compile.
2	Code or demo requested by email, not received.
1	Code or demo not available, or no download available.

TABLE 4.12 SUPPORT AVAILABILITY:

Ranking	Explanation
10	Professional commercial support and maintenance by authors.
8	Commercial support through distributors.
7	Commercial support at cost.
6	Government agency support.
4	Email author support.
3	Government agency maintenance.
2	Author maintenance, limited support.
1	No support

TABLE 4.13 CODE VALIDATION:

Ranking	Explanation
10	Established widely used code.
9	New version of established code.
8	Extensively tested code.
6	New program validated against more established codes.
4	Regulatory program intended for screening purposes.
3	Older, obsolete or little used code.
2	Educational and/or development code.
1	No information found concerning validation.

TABLE 4.14 DOCUMENTATION QUALITY:

Ranking	Explanation
10	Good up-to-date manual, many sample data sets, available online.
8	Good manual, some sample data sets, available online.
6	Adequate manual, many sample data sets, available online.
5	Manual not available online, but well documented.
4	Adequate manual, some sample data sets.
3	Poor manual, some sample data sets, available online.
2	Poor documentation and availability.
1	Documentation unavailable or in language other than English.

TABLE 4.15 EASE OF USE:

Ranking	Explanation
10	Good Integrated Windows GUI.
9	Adequate Integrated Windows GUI.
8	Difficult Integrated GUI.
7.5	No demo, assumed to be adequate Windows GUI.
7	Good CLI and post-processing tools.
6	Adequate/Difficult CLI and post-processing tools.
5	Adequate/Difficult CLI and no post-processing tools.
4.5	No demo, assumed to be adequate CLI
4	Good batch processor and post-processing tools.
3	Adequate/Difficult batch processor and post-processing tools.
2	Good batch processor and no post-processing tools.
1	Adequate/Difficult batch processor and no post-processing tools.

TABLE 4.16 MEETS ALBERTA ENVIRONMENT CRITERIA:

Ranking	Explanation
10	Can simulate 100% of scenarios with density dependent flow.
9	Can simulate 100% of scenarios without density dependent flow.
7	Can Simulate ~70% of scenarios with density dependent flow.
6	Can simulate ~70 % of scenarios without density dependent flow.
4	Can simulate 100 % of scenarios when coupled with another model.
2	Can simulate ~70% of scenarios when coupled with another model.
1	Designed for a specific application other than salt transport.

4.2.2 Rationale for Weighting Factors

MDH personnel selected the objective weighting factors applied to each of the ranking criteria. The weighting factors were determined by MDH based on preliminary discussions held between MDH and AE personnel on 24 September 2002. The weighting factors applied to the ranking matrix are provided in Table 4.17.

TABLE 4.17 WEIGHTING FACTORS

Criterion	Weight	Rationale
Meets Alberta Environment Criteria	4	The code must be capable of application to the specific problem(s) outlined by Alberta Environment.
Ease of Use	3	If many consultants and regulators with different levels of modelling experience are to use the code, ease of use is considered a high priority.
Chemical Reactions	3	Chemical reactions such as cation exchange and adsorption are important for modelling salt fate and transport. At the request of Alberta Environment, high weighting was given to this category.
Support Availability	2	If many consultants and regulators with different levels of modelling experience are to use the code, support availability is considered a high priority.
Documentation Quality	2	Documentation quality is key to simplicity transparency and ease of use and can substitute for support availability.
Code Validation	2	The results must be acceptable to the regulatory agencies and have the confidence of the professional community.

All other factors, generally concerned with the technical capabilities of the code, were weighted 1.

5.0 RESULTS OF INITIAL SCREENING

The results of the initial screening are summarized in Table 4.18. The full ranking matrix (excluding all models eliminated during the pre-screening process) is provided in Appendix B.

5.1 Retained Codes

A final group of 43 codes were retained for more detailed review. These codes are provided in Table 4.18. The mean weighted rankings (out of 10) range from 8.8 to 2.9.

Of these 43 retained codes, 11 codes can be eliminated because of their zero ranking for the primary criterion (AE salt release scenarios), leaving a short list of 32 codes. All 15 codes with mean weighted rankings above 6.0 are credible candidates for analysis of the salt release problems identified by AE. Small changes in the ranking criteria or the relative weighting of components could change the ranking order, but it is unlikely that codes with rankings below 6.0 could rise to the top of the list.

The top ten codes in the ranking were VS2DI, SEVIEW, WHI UNSAT SUITE, HYDRUS-2D, UNSATCHEM, HYDRUS-1D, CHEMFLO-2000, SWAP, SUTRA-2D, LEACHM. These are all first class codes, however, only the five highest rated codes will be further analyzed.

Two of the top ten codes are proprietary interfaces for multiple codes available in the public domain: SEVIEW and WHI UNSAT SUITE. Five of the remaining eight codes were 1D codes including SEVIEW, WHI UNSAT SUITE, UNSATCHEM, HYDRUS-1D, CHEMFLO-2000, SWAP and LEACHM. Three of the top ten codes were 2D models: VS2DI, HYDRUS-2D and SUTRA-2D.

Five codes will be further analyzed, and the rationale for the final elimination is duplication of functionality. The eliminated models are as follows:

- (1) WHI UNSAT SUITE: Both WHI UNSAT SUITE and SEVIEW include the lumped-parameter SESOIL model together with additional codes. SEVIEW automatically transfers data from the unsaturated zone model SESOIL to the

analytical saturated zone model AT123D and also includes the simple spreadsheet application BIOSCREEN. The commercial interface WHI UNSAT SUITE includes HELP, PESTAN, VLEACH and VS2DI. It was eliminated because it is primarily targeted towards landfill and pesticide applications. The public domain version of VS2DI, available from USGS, is ranked first overall as a standalone program. Nevertheless WHI UNSAT SUITE is recommended as an alternative interface combining SESOIL with VS2DI.

- (2) SWAP: The 1-D codes SWAP and LEACHM ranked lower than UNSATCHEM, HYDRUS-1D and CHEMFLO-2000. The SWAP program is eliminated only because it ranks behind other codes with similar functionality.
- (3) LEACHM: LEACHM was eliminated for the same reason as SWAP. One concern with LEACHM was the documentation of version upgrades. The version of LEACHM downloaded from the website may be upgraded at any time without notice to users. If LEACHM is used, it is advised that Alberta Environment obtain permission to distribute a “static” version of the program that they have verified.
- (4) SUTRA-2D: The 2D codes HYDRUS-2D and SUTRA-2D ranked below VS2DI. SUTRA-2D is eliminated because it provides no additional functionality over the more highly ranked codes.

HYDRUS-2D could have been eliminated for the same reason as SUTRA-2D, however, because HYDRUS-1D was retained and HYDRUS-2D can be obtained for the same cost with additional 2D functionality, either of the HYDRUS codes is recommended. UNSATCHEM and HYDRUS-1D are very closely related and could be treated as alternatives rather than independent choices so UNSATCHEM also duplicates much of the functionality of HYDRUS-1D.

An overview of the selected codes is provided in Sections 5.1.1 through 5.1.5. A more thorough description is provided in Section 6.0.

TABLE 4.18 LONG LIST OF RETAINED CODES FOR ALBERTA ENVIRONMENT

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Chemical Reactions	K as a Function of Salinity	Zones Modelled	Program Availability	Data Requirements	Simplicity and Transparency	Computational Requirements	Program Installation	Support Availability	Code Validation	Documentation Quality	Ease of Use	Alberta Env Scenario Criteria	Model Type	Developer/Distributor
WEIGHTING FACTOR		1	1	1	1	1	1	1	1	1	1	1	2	2	2	3	4		
VS2DI	8.8	10	10	8	9	2	8	10	8	5	10	10	7	10	10	10	9	U/S	USGS
SEVIEW	8.6	10	10	8	9	1	10	8	10	7	10	6	10	10	5	10	9	U/S	ESCI
WHI UNSAT SUITE	8.4	10	10	8	9	2	8	8	8	5	10	6	10	10	5	10	9	USAT	WHI
HYDRUS-2D	8.2	10	10	8	9	2	10	8	3	5	10	6	7	6	10	10	9	U/S	USSL
UNSATCHEM	8.2	10	10	8	8	10	10	10	8	7	10	10	6	6	10	9	6	U/S	USDA-ARS
HYDRUS-1D	8.1	10	10	8	9	6	10	8	8	7	10	6	7	6	10	10	6	U/S	USSL
CHEMFLO2000	7.8	10	4	8	5	2	6	10	8	4	10	10	10	10	10	10	6	USAT	OSU
SWAP	7.6	10	8	8	5	2	10	10	8	7	10	10	6	10	10	7.5	6	U/S	DLO & WAU
SUTRA-2D	7.4	10	10	10	5	2	8	10	1	5	10	10	7	10	6	6	10	U/S	USGS
LEACHM	7.1	10	4	8	10	2	6	10	9	7	10	10	4	9	8	5	6	USAT	FUSA
SESOIL	7.0	10	4	8	9	2	6	5	10	7	10	10	8	10	5	5	6	USAT	ORNL
BIOSCREEN	6.8	10	2	6	5	2	2	10	6	10	9	10	7	10	4	9	6	SAT	GSI
SWMS_2D	6.5	10	10	8	5	6	10	4	2	5	8	8	4	9	10	2	9	U/S	USDA-ARS
UNSATCHEM2D	6.5	10	10	8	8	2	10	4	2	5	8	8	4	6	10	2	9	U/S	USDA-ARS
HYDRUS6	6.4	10	4	8	9	6	10	4	8	7	8	8	4	6	10	2	6	REP	USDA-ARS
CONTAM	5.7	10	4	8	4	2	6	10	6	10	9	10	1	2	1	9	6	USAT	Soil Vision
PESTAN	5.6	10	4	8	5	2	6	10	8	8	2	5	7	10	4	2	6	USAT	EPA
PRZM3	5.6	10	4	8	5	2	6	9	6	8	8	10	3	10	4	2	6	USAT	EPA -CEAM,ORD
MPNE1D	5.6	10	4	8	5	6	6	4	6	8	8	8	4	2	6	5	6	USAT	USSL
VLEACH v2.2	5.6	10	4	8	4	2	6	10	9	8	2	5	7	10	4	2	6	USAT	EPA
EMSOFT	5.5	10	4	8	5	2	6	10	6	8	10	10	2	6	4	8	1	USAT	NCEA
FATMIC 2D	5.4	10	10	10	5	2	8	4	3	5	8	8	3	3	4	1	10	U/S	EPA
CHAIN2D	5.4	10	10	8	5	2	10	4	2	5	8	7	1	3	6	1	10	U/S	USDA
AT123D	5.3	10	2	8	5	2	2	5	9	5	10	10	7	10	4	5	1	SAT	ORNL
BLT	5.3	10	10	10	5	2	7	3	3	5	8	1	1	10	1	1	10	U/S	ORNL
CHEMFLO	5.2	10	4	8	5	2	6	10	6	2	2	10	3	10	4	2	6	USAT	OSU
FOCUS PRZM	5.2	10	4	8	5	2	6	9	7	2	10	6	3	6	4	8	1	USAT	FOCUS
SUMMERS	5.2	10	4	4	4	6	6	8	6	8	2	1	7	8	1	4.5	6	USAT	IGWMC
CANVAS	5.1	10	10	4	4	1	8	8	2	1	10	1	7	1	1	7.5	6	U/S	EPA
SAM	4.8	10	3	4	5	2	6	2	9	6	8	1	2	10	6	1	6	USAT	TRRP
SWAGMAN	4.8	10	4	8	10	1	6	6	6	2	10	1	2	8	1	5	1	USAT	CSIRO
BIO1D	4.8	10	4	4	5	1	8	8	6	2	8	1	7	2	1	4.5	6	U/S	GeoTrans Inc.
PATRIOT	4.8	10	4	8	5	2	6	4	6	2	2	10	3	10	1	2	6	USAT	EPA-CEAM, ORD, AERL
MULTIMED	4.4	10	8	8	5	2	8	9	6	8	2	3	3	10	1	2	1	U/S	EPA-CEAM, ORD
VIRTUS	4.4	10	4	4	5	2	6	7	6	7	2	1	7	8	1	4.5	1	USAT	UOC & USDA
CMLS94	4.3	10	4	4	5	2	6	9	6	2	10	10	2	2	4	4.5	1	USAT	OSU
GETOUT	4.1	10	4	8	5	2	4	5	6	7	2	1	1	1	1	4.5	6	USAT	ORNL
PAGAN	4.1	10	4	8	5	2	4	5	6	7	2	1	1	1	1	4.5	6	USAT	ORNL
ICE-1	3.9	10	4	8	1	2	6	8	6	7	10	1	7	1	1	4.5	1	USAT	IGWMC and BPNL
BIOTRACKER	3.7	10	6	1	1	1	6	8	7	2	10	1	8	6	1	3	1	USAT	ENSSI
FATE5	3.7	10	8	4	1	1	8	8	7	2	9	1	1	1	1	7.5	1	U/S	GSI
VIRALT	3.6	10	10	4	4	1	8	7	1	1	2	1	7	1	1	4.5	1	U/S	EPA
DIFMOD	2.9	10	4	8	1	1	4	5	6	7	2	1	1	1	1	4.5	1	USAT	ORNL

5.1.1 VS2DI

The highest ranked code (8.8) is VS2DI from the USGS. This is a public-domain 2-D unsaturated/saturated numerical flow and transport code with a Windows GUI. Full source code is provided. This is an excellent code for Tier 3 RBCA analysis.

5.1.2 SEVIEW

The second ranked code (8.6) is SEVIEW. SEVIEW is a commercial Windows GUI for a group of simple public domain codes (SESOIL, AT123 and BIOSCREEN). SEVIEW also provides databases for generic material parameters. The SEVIEW package is widely used in a regulatory context at the Tier 2 level. Although the components of SEVIEW are available as public-domain codes, the SEVIEW interface has a license fee of \$750 to \$795 US. The vendors for SEVIEW have agreed to make source code available to MDH for validation and review purposes.

5.1.3 HYDRUS1-D or HYDRUS-2D

The fourth ranked code (8.2) is HYDRUS-2D from the Soil Salinity Laboratories of USDA. HYDRUS-2D provides all the functionality of HYDRUS-1D for the same cost (currently \$600 US). The disadvantage is that on 1-D problems, input is a little more complex and execution times are slowed by a factor of about five.

The sixth ranked code (8.1) is HYDRUS-1D is derived from the same original code as UNSATCHEM. The “engine” is a public domain 1-D unsaturated/saturated numerical flow and transport code for multiple solutes (freely available as HYDRUS6)

There is a license fee of \$600 U.S. for either the HYDRUS-1D or HYDRUS-2D Windows GUI. Both HYDRUS-1D and HYDRUS-2D are recommended for Tier 3 RBCA analysis.

5.1.4 UNSATCHEM

The fifth ranked code (8.2) is UNSATCHEM from the Soil Salinity Laboratories of USDA. It is a public domain 1-D unsaturated/saturated numerical flow and transport code for multiple solutes with a Windows GUI. Full source code is provided. It is an excellent 1-D code for Tier 3 RBCA analysis and has the added advantage of a 2-D version, UNSATCHEM-2D, being available if required.

5.1.5 CHEMFLO-2000

The seventh ranked code (7.8) is CHEMFLO-2000 from Oklahoma State University. It is a public domain 1-D unsaturated/saturated numerical flow and transport code with a Java-based GUI. Full source code is provided. CHEMFLO-2000 is another excellent code for Tier 3 RBCA analysis but it also duplicates much of the functionality of HYDRUS-1D and UNSATCHEM. CHEMFLO-2000 can be modified to deal with solutions of high ionic strength.

6.0 RECOMMENDATIONS

The following list summarizes the recommended codes on which to complete the more detailed analysis and testing in Phase II of the work plan:

- 1) The SEVIEW commercial package incorporating SESOIL, AT123D and BIOSCREEN is recommended for Tier 2 analysis of salt contaminated sites in Alberta. The interface and associated packaged codes can be licensed for \$750 to \$795 US.
- 2) For more sophisticated Tier 3 numerical analysis, the public domain codes UNSATCHEM (1-D), CHEMFLO-2000 (1-D) and VS2DI (2-D) with free Windows GUIs are recommended.
- 3) At the present stage, it is not clear that analysis involving reactive transport is a major requirement and it is unclear whether HYDRUS-1D or HYDRUS-2D (with a proprietary licensed Windows GUI) has significant advantages over the public-domain code UNSATCHEM (with a public-domain Windows GUI). It is recommended that HYDRUS-1D or HYDRUS-2D be retained for further evaluation in Phase II.

All the recommended codes have excellent documentation with many examples and tutorials for new users. All have good intuitive user interfaces with graphical post-processing and report generation capabilities.

Both HYDRUS and UNSATCHEM are excellent codes, derived from a common source, for 1-D reactive transport in variably saturated media. It is possible that the multi-component reactive transport capabilities of UNSATCHEM or HYDRUS may not be justified by the data available for analysis of salt contamination. However, if simulation of cation-exchange type reactions are considered a high priority, these codes should be retained.

6.1 Discussion of Recommended Codes

6.1.1 VS2DI

The VS2DI package contains all the tools that a user needs to create, run, and view results for a simulation of flow and transport through variably saturated porous media. The package seamlessly integrates a graphical user interface (within which the user can draw the simulated domain and enter or modify model parameters) with existing USGS models of flow and solute transport (VS2DT) and flow and energy transport (VS2DH), and a postprocessor that displays simulation results.

VS2DI is an interface based on the original VS2D code by Healy (1987). VS2DT and VS2DH have been extensively used by scientists at the USGS, and at various universities and consulting companies. VS2DI Version 1.0 was released in 1999. Version 1.1 released in 2000 was extended to work with the heat flow code VS2DH and has added post-processing capabilities. This release contains revised versions 3.0 of VS2DT and VS2DH which allow run time selection of hydraulic function and adsorption type.

The model can analyze problems in one or two dimensions using either cartesian or radial coordinate systems. Relations between pressure head, moisture content, and relative hydraulic conductivity may be represented by functions developed by van Genuchten, Brooks and Corey, Haverkamp and others, or by data points. Initial hydraulic condition can be specified as static equilibrium, specified pressure head, or specified moisture content. Boundary conditions include specified pressure or total head, specified flux, infiltration with ponding, evaporation, plant transpiration, and seepage faces. Solute transport processes include advection, dispersion, first-order decay, adsorption, and ion exchange.

6.1.2 SEVIEW

SEVIEW is a commercial interface for the public-domain codes SESOIL, AT123D and BIOSCREEN. It has been modified and improved over an extended period of time.

SESOIL is a one-dimensional vertical transport screening-level model for the unsaturated (vadose) zone that simulates remediation by natural attenuation (RNA) based on diffusion, adsorption, volatilization, biodegradation, cation exchange and hydrolysis. SESOIL is an acronym for the Seasonal Soil compartment model. It contains three submodels that simultaneously simulate contaminant transport, soil water movement and soil erosion. It is the vadose zone model by which all other vadose zone models are judged. What sets SESOIL apart is its ability to simulate seasonal climatic variations and varying soil properties with depth.

SESOIL was developed for US Environmental Protection Agency in 1981 by Bonazountas and Wagner (at Arthur D. Little Inc.). SESOIL has been updated several times. In 1984 Bonazountas and Wagner added a fourth soil. SESOIL was modified extensively by Hetrick et al., at Oak Ridge National Laboratory to enhance its capabilities. The enhanced version of SESOIL included with SEVIEW was modified in 1997 by M. J. Barden (then of the Wisconsin Department of Natural Resources) to correct for a mass balance error which was discovered using the SEVIEW mass balance report. In 1997, Mr. Robert Schneiker (of ESCI) modified SESOIL to run to 999 years. SESOIL now includes the water diffusion coefficient for use in AT123D.

SESOIL can be used to simulate the fate of residual contaminant levels in soil to establish site-specific cleanup objectives. It can also simulate time-dependent releases from underground storage tanks, landfills and agricultural practices. The public domain version of SESOIL was enhanced to simulate up to 999 years of contaminant transport. SEVIEW links the time-dependent contaminant load to groundwater from SESOIL to the AT123D and BIOSCREEN groundwater models.

AT123D was developed by G.T. Yeh (1981), at Oak Ridge National Laboratory (ORNL). Significant modifications to the version of the code included with SEVIEW, were made by John Seymor (1982), Darryl Holman (1984), and Howard Trussell (1986), of the University of Wisconsin-Madison. An enhanced version of AT123D that can simulate up to 400 years was created by R. A. Schneiker (1997) at ESCI. Version 6.0 of AT123D includes a correction to the steady-state calculation by Mr. Schneiker in 2002.

AT123D is a generalized three-dimensional groundwater transport and fate model. It can be used to simulate contaminant transport under one-dimensional groundwater flow. Transport and fate processes simulated include advection, dispersion, adsorption and biological decay.

AT123D can model the time-dependent contaminant releases from the SESOIL vadose zone model in the saturated zone through the SEVIEW interface. AT123D was enhanced to simulate up to 400 years of contaminant migration. Results can be used to estimate how far a contaminant plume will migrate and can be compared to groundwater standards to evaluate risk at specific locations and times. AT123D is a simple analytical model.

BIOSCREEN was developed under contract from the US Air Force by Ground Water Services Inc. BIOSCREEN version 1.3 was released in 1996, followed in 1997 by version 1.4. The latest version contains an estimated mass flux of contamination entering surface water bodies. No modification to the original code is made to the version of BIOSCREEN included with SEVIEW.

When used with SEVIEW, BIOSCREEN can use the time-dependent contaminant load to groundwater from SESOIL. Results can be used to estimate how far a contaminant plume will migrate and can be compared to groundwater standards to evaluate risk at specific locations and times.

6.1.3 HYDRUS-1D or HYDRUS-2D

The HYDRUS codes (produced by USSL) are designed to simulate one- and two-dimensional water flow, heat transport, and multi-component solute transport in variably saturated media.

HYDRUS-1D numerically solves the Richards' equation for variably-saturated water flow and convection-dispersion type equations for heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The solute transport equations consider convective-dispersive transport in the liquid phase, as well as diffusion in the gas phase. The transport equations also include provisions for

nonlinear non-equilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero order production, and two first order degradation reactions. In addition, physical non-equilibrium solute transport can be accounted for by assuming a two region, dual porosity type formulation that partitions the liquid-phase into mobile and immobile regions.

HYDRUS-2D is a 2D extension of HYDRUS-1D and can be used to analyze water and solute movement in unsaturated, partially saturated, or fully saturated porous media. The flow region may be composed of non-uniform soils. Flow and transport can occur in the vertical, horizontal, or a generally inclined direction. The water flow part of the model can deal with prescribed head and flux boundaries, boundaries controlled by atmospheric conditions, as well as free drainage boundary conditions. A proprietary, graphics-based user interface is provided for both data preparation and graphical post-processing in Windows for both HYDRUS-1D and HYDRUS-2D.

6.1.4 UNSATCHEM

Version 2.0 of UNSATCHEM (produced by the U. S. Salinity Laboratory of the USDA) is a code for simulating one-dimensional water flow, heat transport, carbon dioxide transport and solute transport with major ion equilibrium and kinetic chemistry in variably saturated media.

UNSATCHEM numerically solves the Richards' equation for variably-saturated water flow and convection-dispersion type equations for heat, carbon dioxide and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The heat transport equation considers transport due to conduction and convection with flowing water. Diffusion in both liquid and gas phases and convection in the liquid phase are considered as CO_2 transport mechanisms. The major variables of the chemical system are Ca, Mg, Na, K, SO_4 , Cl, NO_3 , H_4SiO_4 , alkalinity, and CO_2 . The model accounts for equilibrium chemical reactions between these components such as complexation, cation exchange and precipitation-dissolution.

UNSATCHEM may be used to analyze water and solute movement in unsaturated, partially saturated, or fully saturated porous media. The flow region may be composed of

non-uniform soils. Flow and transport can occur in the vertical, horizontal, or a generally inclined direction. The water flow part of the model can deal with prescribed head and flux boundaries, boundaries controlled by atmospheric conditions, as well as free drainage boundary conditions. UNSATCHEM differs from other water flow and solute transport models in that it considers the effects of chemical composition on hydraulic conductivity.

6.1.5 CHEMFLO-2000

CHEMFLO was originally developed as a 1-D code for water and chemical at Oklahoma Agricultural Experiment Station, Oklahoma State University (Nofziger et al, 1989). Since that time, the code has been used extensively and a graphical user-interface has been added.

CHEMFLO was written to enhance understanding of flow and transport processes. It is highly interactive and graphics oriented. CHEMFLO enables users to define water and chemical movement systems. The software then solves mathematical models of these systems and displays the results graphically. The software is designed to be used by students, regulators, consultants, scientists and persons involved in managing water and chemicals in soil.

CHEMFLO supports simulation of layered soils. The software supports flow in soil systems where the initial water content, matric potential, and/or concentration are not uniform throughout. There is also support for boundary conditions that change with time. Soil properties can be defined using conductivity equations given by Brooks and Corey (1964), Gardner (1958), and van Genuchten (1980). Water characteristic curves can be described using equations of Brooks and Corey (1964), Simmons et al. (1979), or van Genuchten (1980).

For transport processes, CHEMFLO models diffusion, dispersion, decay and linear sorption processes. Partitioning and movement of the chemical in the vapour phase is ignored in this model.

CHEMFLO provides a very convenient method of assessing parameter sensitivity graphically. The user simply defines and simulates results for one system of interest. The lines representing these results are retained on the screen. The user is then free to change any part of the system to a new value and simulate flow for that system.

6.2 Strengths and Weaknesses of Recommended Codes

All the five short listed codes are high quality programs with excellent interfaces, documentation, and broad functionality. The ranking matrix gave these codes ranks between 8.8 and 7.8 out of ten for their applicability to the salt-release problems identified by AE. The recommended programs were selected to work together as a toolkit and to some extent provide cover for their respective weaknesses.

SEVIEW is the simplest model (or group of models) suitable for Tier 2 RBCA applications. It's strength is it's simplicity and transparency and it's greatest weakness is it's inability to model "real world" complexities. Although SESOIL, AT123D and BISCREEEN can be obtained as public-domain codes at no cost, MDH strongly recommends the SEVIEW interface for its ability to simplify and speed the site screening process.

The remaining four numerical codes are: CHEMFLO-2000, VS2DI, UNSATCHEM and HYDRUS. These models require site-specific data and would fit into the RBCA process at the Tier 3 level.

CHEMFLO-2000 is the least sophisticated code. Its major strengths are its ease of use and simplicity. It is a single-species transport model. It cannot model cation exchange or changes in hydraulic conductivity as a function of chemistry (salinity). CHEMFLO is restricted to the vadoze zone and can only model uptake of water and chemicals by plants at the surface. The standard version of CHEMFLO does not model solutes with high ionic strength but MDH understands that the authors will provide a version with this added functionality.

UNSATCHEM is the only recommended code that can handle reactive transport of multiple species and changes in hydraulic conductivity with chemistry. Its strengths are

its ability to model complex soil/water/plant interactions. Its principal weakness is that the limited data available from site investigations may be insufficient for UNSATCHEM to be successfully applied. UNSATCHEM is limited to modelling a specific set of major ions. It can model precipitation/dissolution reactions (including gypsum), but is limited in its ability to model sorption/desorption and decay processes.

HYDRUS is a more general solute transport code that includes nonlinear adsorption and degradation. Unlike UNSATCHEM, it is not limited to a specific set of major ions. It cannot handle general cation exchange. Although less sophisticated than UNSATCHEM in terms of some chemical transport functions, HYDRUS is more complex than CHEMFLO-2000. HYDRUS has an advantage over CHEMFLO-2000 in its ability to simulate both unsaturated and saturated flow and vapour phase reactions.

VS2DI is the most highly recommended 2-D code and its major strength relative to the other recommended codes is this 2D functionality. It is a saturated/unsaturated flow and transport code without reactive transport capabilities (other than ion exchange). It is less sophisticated than UNSATCHEM in terms of its chemical transport functions but can also be used as a 1-D model. Retention of HYDRUS-2D may provide an alternative to VS2DI.

MDH have attempted to recommend a “toolkit” with codes at different levels of sophistication to meet the varied levels of analysis that might be justified at different stages in the site screening process. SEVIEW is the first-level screening tool with CHEMFLO as a follow-up for 1-D analysis of geologically heterogeneous profiles. VS2DI and HYDRUS-2D tools for more complex flow regimes, HYDRUS-1D and UNSATCHEM are tools for shallow soil/water/plant chemical interactions and each has specific capabilities of interest in modelling salt releases.

7.0 DISCLAIMER

MDH gathered the data for this report from web and literature sources between September and November 2002.

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8.0 CLOSURE

We trust that this report meets all your present requirements. Should you have any questions or comments please contact us. We look forward to discussing this report further with you in the near future.

Respectfully submitted,

MDH Engineered Solutions
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APPENDIX A

LIST OF ELIMINATED MODELS

List of Models that Cost over \$750 U.S.

CHEMFLUX2D
CTRAN/W
FEFLOW
FRACTRAN
HYDROGEOCHEM2
MIGRATEv9
POLLUTEv6
PORFLOW
TARGET
VAM2D

List of 3D Models

3DADE
3DFEMFAT
CHEMFLUX3D
FATMIC 3D
FEMWATER
FRAC3DVS
N3DADE
SOLUTRANS
STAFF3D
SWMS_3D
VADSAT

List of Models that Simulate the Saturated Zone Only

1D Step Injection
AGU-10
ANALGWST
AQUA3D v4
ASMWIN
BEAVERSOFT
BIOCHLOR

BIOMOC
CHAINT
DPCT
DSTRAM
DUST-BNL
EPA-VHS
FLONET/TRANS
FLOWPATH II
FTWORK
HPS
HST3D
MAP
MOC
MOC3D
MOCDENSE
MS-VMS
MT3D
ONED
PARSSIM
PLUME
PLUME2D
PRINCE
RAND3D
RANDOM WALK
RWH
SOLUTE
SWICHA
SWIFT-98
TRAFRAP-WT
USGS-SOL
VERTPAK-1
WINTRAN

List of Models Designed Primarily for NAPL Simulations

AIRFLOW/SVE
ARMOS
BIOF&T -2D
BIOF&T -3D
BIOPLUME III
BioSVE
BIOTRANS
BIOVENTING
HSSM
HYPERVENTILATE
MAGNAS
MARS
MOFAT
NAPL SIMULATOR
RITZ
ROAM
RT3D
SEAM3D
SPILLCAD
SWANFLOW
TMVOC
TOUGH2
UTCHEM
VENT2D
VENT3D

List of Models with No Solute Transport Capabilities (Flow Only)

ABCFEM
CAPZONE
FEMWATER 2D
FLAC
FLOWTHRU
FRAC2D

GFLOW
GWDIVIDE
GWFLOW
HELP v3.0
HOTWTR
INFIL
JOB2D-3D
MODFLOW
MOD-HMS
MODPATH
MODRET
NETFLO
PAT
PATH3D
PLASM
QUICKFLOW
RADFLOW
SEEP/W
SEEP2D
SEEP3D
SHARP
SOILCOVER
SVFLUX2D
SVFLUX3D
TETRA
THWELLS
TWODAN
VADOSE/W
WATERMOD2
WhAEM2000
WHPA
WINFLOW
wtPROFILE

List of Surface Water Models

AGNPS
BREACH
DISPERS
FLDWAV
HYDRA

List of Geochemical Speciation Models with Limited or No Flow Simulation

Capabilities

HydroChem
MINTEQA2
NETPATH
PHREEQC
PHREEQE
PHRQPITZ

List of Codes that were Primarily Databases

BORDEN DATA SET
ENVES&T
LIMS
PEST2000
RETC
ROSETTA
SOIL VISION
STF
VISUAL PEST

List of Codes that were Primarily Pre-and Post-Processing Interfaces

ARGUS ONE
EIS-GWM
GMS
GROUNDWATER VISTAS
MFI
MODIME

SEQUENCE
SHOWFLOW 2
SUTRA-GUI
VISUAL MODFLOW
VS2DI

List of Heat flow Codes and Codes Concerned with Evaporation Only

HT
UNSAT-H
VS2DH

List of Codes that could not be Located After Diligent Searching

2PAR_DEGRADE
ADE 3D
ANALYT
AQUIFEM-N
CADIL_AGTEHM
FRACFLO
FRACFLOW
FRACNET
GEOFLOW
MOTIF
NEFTRAN II
PERCPLAN
POLUT2D
SANGRE
SEEPS2D
SPLIT
SWIFT II
TBC
VaMP
VSAFT2

List of Codes with No North American Distributor or Where Documentation and/or Support in the English Language was a Concern

2D_V_HYDRO_S
BEAVER
FEHM
FLOW2D
GGU-SS FLOW3D
MACRO
MARTHE
MSEEP
SEFTRANS
SIMULAT

List of Codes that had Become Obsolete or had Been Succeeded by Later Versions

ASM
BALANCE
BIOPLUMEII
FEMWASTE
FEMW-FEMA
MOTRANS
PRZM
PRZM2
SATURN
SOILCO2

List of That No Longer Appear to be Sold

EXPRES
FEMSEEP
FTRAN
KYSPILL
MULAT
TDPLUME
UNSAT2

APPENDIX B

DETAILED RANKING TABLES

APPENDIX C

LIST OF ACROYNMS

ACRONYM	COMPANY NAME
ABCI	Adrian Brown Consultants Inc
ACRI	Analytic & Computational Research, Inc.
Argus	Argus Holdings Limited
BPNL	Battelle Pacific Northwest Laboratory
cee-odu	Civil/Environmental Model , Old Dominion University
CFFM	Compendium of Fractured Flow Models
CSIRO	Commonwealth Scientific and Industrial Research Organization in Australia
CSU	California State University
CH2M	CH2M Engineers in Seattle
DLO & WAU	DLO Winand Staring Center and Wageningen Agricultural University.
DRI	Desert Research Institute
DUT	Delft Univerisity of Technology
ENSSI	Environmental Software Solutions
EPA	United States Environmental Protection Agency
EPA CEAM	Center for Exposure Assessment Modeling
EPA CSMoS	Center for Subsurface Modeling Support
ERT	Environment Resource Trust Inc.
ES&T	Environmental Systems & Technologies - A division of GES (Groundwater & Environmental Services Inc.)
ESCI	Environmental Software Consultants Incorporated
ESI	Environmental Simulations International
ESTSC	U.S. Department of Energy Energy Science and Technology Center
ETA	Engineering Technologies Associates
ETH	Eidgenossische Technische Hochschule Zurich (SFIT).
Fitts	Fitts Geosolutions

ACRONYM	COMPANY NAME
FOCUS	FORum for the Co-ordination of pesticide fate models and their Use
FUSA	Flinders University of South Australia - School of Chemistry, Physics and Earth Sciences
GAEA	GAEA Technologies Limited
GEOSLOPE	GEO-SLOPE INTERNATIONAL
GeoTrans Inc	GeoTrans Inc.
Golder Associates	Golder Associates
GGSS	Geotechnical and Geoenvironmental Software Directory
Greenhat Software	Greenhat Software
GSI	Groundwater Services, Inc.
HIS	Haitjema Software, Inc.
HYDROGeologic	HYDROGeologic Inc.
Hydrology Group	Hydrology Group at Pacific Northwest National Laboratory (PNNL)
IEC	Intera Environmental Consultants, Inc. (Austin, TX)
IGWMC	International Groundwater Modeling Center
ISWS	Illinois State Water Survey
ITASCA	ITASCA Consulting Group, Inc
LANL	Los Alamos National Laboratory
LMNO	LMNO Engineering, Research, and Software, Ltd.
MEND 2000	Mine Environmental Neutral Drainage
LU	Laval University
NCEA	National Center for Environmental Assessment
NWRI	National Water Research Institute.
NWS	National Weather Service River Mechanics Models
OECD	OECD Nuclear Energy Reserch

ACRONYM	COMPANY NAME
Ohio University	Ohio State University
ORNL	Oak Ridge National Laboratory
OSU	Oklahoma State University
PG	Princeton Groundwater
RASI	Resources & Systems International, Inc.
REM	Register of Ecological Models
Rockware Inc.	RockWare Inc. Earth Science Software
SDC	Shell Development Corporation
SEC	Slotta Engineering Consultants
SFIT	Swiss Federal Institute of Technology - Institute of Hydromechanics and Water Resources Management
Soil Vision	Soil Vision
SSG	Scientific Software Group
SSPA	S.S. Papadopoulos & Associates
SU	Stanford University
Tetra Tech Inc	TETRA TECH Research and Development
TICAM	The University of Texas at Austin - Texas Institute for Computational and Applied Mathematics
TRRP	Texas Risk Reduction Program
U of T	University of Texas
U of W	University of Waterloo
U.S. Department of Energy	United States Department of Energy
UCF	University of Central Florida
UFIS	Universitaet Braunschweig, Institute of Geography andn Geoecology
UOA	University of Arizona
UOC	University of California

ACRONYM	COMPANY NAME
USACE	United States Army Corps of Engineers
USDA -ARS	United States Department of Agriculture - Agriculture Research Service
USGS	United States Geological Survey
USSL	United States Salinity Laboratory - George E Brown Junior Salinity Laboratory
VCE	Vatnaskil Consulting Engineers
WASY	WASY Software
Watermark	Watermark Numerical Company
WCGR	Waterloo Centre for Groundwater Research
WHI	Waterloo Hydrogeologic Inc.