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Model Code and Scenario Selection Report
Site-Wide Water Balance
Rocky Flats Environmental Technology Site

February 19, 2001

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FINAL

February 19, 2001

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Executive Summary

The Rocky Flats Environmental Technology Site (RFETS or site), located 16 miles northwest of Denver, Colorado, encompassing approximately 6,500 acres, is owned by the Department of Energy (DOE), and is operated by Kaiser-Hill Company, L.L.C. (Kaiser-Hill). Before its current closure mission, RFETS was part of the nationwide nuclear weapons research, development, and production complex. The site contains a central Industrial Area (IA) surrounded by a Buffer Zone (BZ). The site is currently undergoing aggressive cleanup with a goal for site closure by the end of 2005.

As part of developing a detailed design basis for closure activities, RFETS is conducting a site-wide water balance (SWWB). The objective of the SWWB is to provide RFETS with a management tool to evaluate how the site-wide hydrology is likely to change from current to final site configuration.

An integrated model will be used to achieve this. An integrated hydrologic model is one that couples and simultaneously simulates all the principal components of the hydrologic regime, including: snowmelt, overland flow, channelized flow, unsaturated zone flow, saturated groundwater flow, and their interaction. As specified in the SWWB Statement of Work (Kaiser-Hill,1999), selection of the code shall be initiated after approval of the Work Plan (Work Plan). Kaiser-Hill formally approved the final Work Plan (Kaiser-Hill, 2000) on August 28, 2000.

The main body of this report documents the selection of the appropriate code for use in the integrated hydrologic model[1] that will be used for the SWWB. The last part of this report describes how the effects of final site configuration on the SWWB will be simulated in five modeling scenarios.

[1]In this report, "model" refers to the mathematical model that provides a simplified representation of the field situation, while "code" refers to the program or set of commands that is used to solve the model. A model is site- and objective-specific, whereas a code is generic and can be applied to many sites and problems.

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Code selection considerations

A systematic approach was followed in selecting the appropriate model code for use in the SWWB. The general considerations for selecting the SWWB code(s) were defined:

General considerations	Significance for selected code
Commercially-available	Code should be available for purchase by anyone who wants to run the model
Project objectives	Requires high resolution, predictive accuracy, and ability to work at various scales
Data quality and quantity	Both are high, not a limitation on code selection
Conceptual model	Site hydrology is very variable and complex, requiring a sophisticated code
Project constraints	Project schedule requires a flexible and efficient code
Applicable standards	Not a code selection limitation
Graphical Interface	Ability to be interfaced with GIS and graphical tools

Code identification

The available model codes potentially applicable to the project were reviewed. Only commercially-available, integrated, deterministic, distributed, physically-based, well-coupled, continuous codes were considered. The physically-based code flow equations to be solved include the following:

- One-dimensional Saint-Tenant flow equations for surface flow processes:
    - o Continuity equation, and
    - o Momentum equations (conservative and non-conservative forms);
- Two-dimensional diffusive wave for surface flow;
- Three-dimensional Boussinesq for saturated groundwater flow; and
- One-dimensional Richards for unsaturated vertical infiltration.

These equations are required based on the processes occurring at the site that affect the water balance.

Specific code selection criteria

Specific code selection criteria were determined, based on the general considerations and the available model code types. The 14 specific code selection criteria were weighted as follows:

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No.	Specific criterion	Weighting
1	Level of sophistication (physical & mathematical)	10
2	Spatial/temporal grid resolution capabilities	5
3	Spatial/temporal parameter/variable input/output capabilities	5
4	GIS capabilities, pre/post-processing	5
5	Boundary conditions (types, flexibility)	5
6	Documentation (current, complete, accurate, understandable)	4
7	Optional simplified process equations	3
8	Documented use	3
9	Ease of use, familiarity	3
10	Technical support (and access to code developers)	3
11	Animation/presentation capabilities, particle tracking	2
12	Internal consistency checks	2
13	Additional feature support (transport, erosion)	2
14	Hardware optimization	1
	Sum of weighting values (maximum possible)	53

Code evaluation and comparison

Based on these criteria, a wide variety of information sources were used to identify available distributed integrated hydrologic codes. Nine codes were evaluated and compared against the above 14 criteria using a weighted ranking system. The evaluated codes ranked as follows:

Acronym	Authors	Full name	Rank	% of max.
MIKE SHE	British Institute of Hydrology, Danish Hydraulic Institute, and SOGREAH (France)	MIKE SHE	49	92%
SWMM	US EPA	Storm Water Management Model	36	68%
TOPOG-Dynamic	CSIRO, Australia	TOPOG-Dynamic	35	66%
SWAT	USDA	Soil and Water Assessment Tool	33	62%
PRMS	USGS	Precipitation-Runoff Modeling System *(New code is MMS)*	29	55%
HSPF	US EPA	Hydrologic Simulation Program	27	51%
SWRRB	USDA	Simulator for Water Resources in Rural Basins	24	45%
DHSVM	DOE - Pacific Northwest Lab	Distributed Hydrology-Vegetation Model	23	43%
MODBRANCH	USGS	MODBRANCH	20	38%

Code selection

Finally, based on this evaluation, the MIKE SHE code was selected as the model code to be used to develop the SWWB model. MIKE SHE was developed by the British Institute of Hydrology, the Danish Hydraulic Institute Water and Environment (DHI)[2], and the French consulting company SOGREAH[3]. The code is named after Michael B. Abbott, the principal author of the code, and the Système Hydrologique Européen (SHE) (Abbott, Bathurst, 1986) (European Hydrologic System).

MIKE SHE represents each of the three main hydrologic processes and their dynamic interaction (surface flow, unsaturated zone flow, and groundwater flow) as well, or better than all other codes reviewed and, overall, meets model-specific criteria best. MIKE SHE possesses distinct advantages over other codes based on the complexity of the governing physical equations, which can, however, be simplified as justified for each hydrologic process, so that the overall computational efficiency of the integrated hydrologic model can be optimized. It utilizes spatial and temporal data easily, and is capable of providing a variety of output types. It also has several other advantages over other codes reviewed. Most notable are its Geographical Information System (GIS) interface capabilities, technical support (and access to code developers), documentation, and flexibility in defining boundary conditions and grid resolutions.

Five future scenarios

Five scenarios are planned to be simulated after model calibration (which, as described in the Work Plan, describes matching the behavior of the site hydrologic system under current conditions). Current conditions will be the basis of comparison with future five scenarios. The SWWB plans to model five future scenarios, designed to simulate the major changes between current and future conditions in a logical progression, so that the individual effects of specific changes can be evaluated alone and in combination. The five future scenarios are:

- Scenario 0 – discontinue imported water;
- Scenario 1 – Scenario 0, plus: seal or remove subsurface drain lines;
- Scenario 2 – Scenario 1, plus: convert 90 acres to engineered cover;
- Scenario 3 – Scenario 1, plus: regrade the surface in and near the IA; and
- Scenario 4 – Scenario 2 and 3 combined, plus: reconfigure the BZ.

Scenarios 0 through 4 will be simulated under a range of climatic conditions-- including extreme dry, extreme wet, and average conditions-- which will be varied for both initial

[2] The code is distributed in the US by DHI Water and Environment, Inc., Eight Neshaminy Interplex, Suite 219, Trevose, PA 19053.
[3] See www.sogelerg-sogreah.fr.

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(antecedent) conditions and boundary (event) conditions to create several combinations. Each scenario will be subject to an uncertainty analysis (varying the most sensitive parameters through a reasonable range) to determine a probabilistic range of predicted results. In conjunction with the climate scenarios, the uncertainty analysis will provide a large combination of probability-based results for each scenario.

1.0 Introduction

1.1 Background

The RFETS, located 16 miles northwest of Denver, Colorado, encompassing approximately 6,500 acres, is owned by the DOE, and is operated Kaiser-Hill. Before its current closure mission, RFETS was part of the nationwide nuclear weapons research, development, and production complex. The site contains a central IA surrounded by a BZ. The site is currently undergoing aggressive cleanup with a goal for site closure by the end of 2005.

As part of developing a detailed design basis for closure activities, RFETS is conducting a SWWB. The objective of the SWWB is to provide RFETS with a management tool to evaluate how the site-wide hydrology is likely to change as a result of changing the current site configuration to the final site configuration.

1.2 Code selection

The main body of this report documents the selection of the appropriate code for use in the integrated hydrologic model that will be used for the SWWB. There is a very important distinction between the terms "code" and "model". In this report, "model" refers to the mathematical model that provides a simplified representation of the specific field situation, while "code" refers to a generic program or set of commands that is used to solve the governing equations representing the physical processes. A model is site- and objective-specific, whereas a code is generic and can be applied to many sites and problems.

An "integrated" hydrologic model is one that couples and simultaneously simulates all the principal components of the hydrologic regime, including: (1) precipitation; (2) snowmelt; (3) overland flow; (4) channelized flow; (5) unsaturated zone flow; (6) groundwater flow; and (7) their interaction. Historically, and in current practice, individual processes are modeled using single-process codes. Such codes have been widely used and extensively tested, and may be considered "verified". However, these codes are limited to only one component of a hydrologic system, and other components are lumped, simplified, or ignored. One example would be saturated zone flow, which is represented using groundwater codes (e.g., MODFLOW). More complex codes couple two processes, such as unsaturated and saturated zone flow. There are only a few such coupled codes, and they are less standardized than single-process codes. Full integration of all important hydrologic processes has been standardized to a lesser extent than has been achieved for individual process codes. However, integrated codes offer the greatest benefit for simulating and linking all the components of a normal hydrologic system in a dynamic manner.

As specified in the SWWB Statement of Work (Kaiser-Hill, 1999), selection of the code shall be initiated after approval of the Work Plan. Kaiser-Hill formally approved the final Work Plan (Kaiser-Hill, 2000) on August 28, 2000.

Although the Work Plan was not developed assuming a specific model, the plan does assume that an integrated, physically-based, distributed parameter model would best simulate the hydrologic system at RFETS. Further, the selection process described here does not presume selection of one, stand-alone integrated model, but considers both integrated and coupled physical process codes.

This report describes the model code selection process. Review of the literature revealed no published "standard" protocol for selection of an integrated hydrologic numerical model code. Therefore, a site-specific protocol, which is described in this report, was developed for the SWWB project, based on the project objectives, data review, and conceptual model described in the Work Plan. The minimum criterion for code selection is the capability to achieve the project objectives. Code selection is also constrained by several other important and relevant factors, described in the following sections. A discussion of the code selection criteria is presented in Section 2.0. Various codes are identified and briefly discussed with respect to their capabilities in Section 3.0, and evaluated, compared, and ranked based on code-specific criteria in Section 4.0.

Within the scope of the SWWB project, detailed "hands-on" comparison of each code is not feasible, as each code and its documentation are usually substantial. In most cases, the code documentation or literature references describing the codes applicability were relied upon to determine capabilities and/or performance. However, recognizing the possibility for exaggeration of product capabilities in marketing materials, efforts were made in the code selection process to closely review documentation for the processes most important and relevant to the RFETS hydrologic system.

Simulating the integrated dynamics of the hydrologic system at RFETS is a complex task and requires an equally sophisticated code. The selection process sought to identify the best available code, based on its overall ability to meet all specified criteria well. Therefore, while a rejected code may meet one specific criterion better than the final selected code, the process was aimed at identifying the code that had the best overall balance of strengths. Based on this ranking, the selected code is discussed in more detail in Appendix A.

1.3 Five future scenarios

The last part of this report describes how the final site configuration will be simulated in five modeling scenarios. Details of the scenarios will be coordinated with the Kaiser-Hill Environmental Restoration Program.

1.4 Project Expectations and Model Capabilities

Although the planned model and the selected code are both sophisticated, and have potential for a number of applications at the RFETS, the current project is not unlimited in scope. Therefore, the expectations regarding anticipated results should be similarly constrained, specifically: (1) the current scope implies a regional scale model; and (2) the five future scenarios to be evaluated are limited to specific closure options.

The proposed model is regional in scale, comprising parts of two upland stream catchments. Therefore, the grid size, for computational efficiency, will be large, approximately 200 feet. As a result, fine-resolution details of site conditions will not necessarily be represented exactly. Features such as ground cover boundaries and road and building placement will be modified in the model to match the grid spacing. Within a grid cell, features at a smaller scale, such as individual drain locations, will be approximated or averaged. This is not a limitation of the code; the selected code has the capability to telescope into a local area, using boundary conditions established using the site-wide model, but detailed local refinement of the model is not part of this regional study. However, the databases for the current study have been set up so as to facilitate telescoping at a later stage if this is required. For example, the geologic model has been set up on 10-foot grid spacing.

Capabilities and limitations of the SWWB model, developed based on the MIKE SHE code, are discussed in this section. The MIKE SHE code was selected as the best available 'tool' for meeting SWWB objectives because of its specific capabilities. However, certain assumptions used in the MIKE SHE code, as in all codes, may limit the model's ability to accurately simulate specific hydrologic conditions in the RFETS SWWB model boundary. In addition, certain fundamental assumptions made in developing the SWWB model, like spatial and temporal discretizations, can also limit the model's ability to simulate some aspects of the system flow with a high level of accuracy. Although, the SWWB model is expected to simulate the larger scale hydrology of the system, it may not simulate more localized features. The more significant assumptions, capabilities, and limitations of both the MIKE SHE code and SWWB model are presented below to prevent potential confusion on its capabilities, applicability, and limitations.

1.4.1 SWWB Model Capabilities and Limitations

The primary purpose of the SWWB model is to use it as a "management tool" for evaluation of the site-wide integrated hydrology under different initial and boundary conditions. The current hydrological conceptual flow model for the system indicates that subsurface flow is strongly affected by surface processes (i.e. precipitation, evapotranspiration, and surface flow), but it can also affect surface flow processes (seeps, gaining reaches of streams). The SWWB model should simulate the site-wide dynamic behavior of this interaction reasonably well because it includes all of the important flow processes and accounts for spatial distributions of parameters and time-

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varying boundary conditions. A considerable amount of data exists that will support both the model parameterization and development of appropriate boundary conditions.

Significant anticipated SWWB model assumptions and their implications are summarized below:

- Grid resolution for the site-wide model is anticipated to be 200 feet by 200 feet. This is a compromise between simulating the site-wide dynamics and mass balance reasonably well and preventing large simulation times. Several implications of this assumption are summarized below:

  - In general, flow associated with system components less than about 200 feet will not be accurately simulated (e.g., flow in, on, or around individual trenches, pipelines, building basements or roofs, and surface culverts). The average hydrologic effects of these features, however, will be accounted for within each grid cell;
  - Flows associated with the Denver Water Board inflow and distribution will not be explicitly simulated. The combined effects of leakage from all water supply lines within each model grid will be accounted for, so that the effects of turning it off in future scenarios can be evaluated. The amount of leakage from water supply lines will be based in direct proportion to the pipe density occurring in each grid cell and on the observed system response;
  - Flows in sanitary sewer lines will not be explicitly simulated in the model. The combined effects of groundwater inflow into sewers will be included in the model based on the density of pipeline and observed system response occurring in each grid cell; and
  - Surface flows in the more important channelized surface drainage features, within both the IA and BZ, will be modeled more accurately on a comparative basis. Surface flows are not constrained by the same 200-foot grid cell that governs subsurface and overland flow.

- Vertical resolution of the saturated zone will be constrained to four layers to account for important hydrologic features and to reduce computational inefficiencies. The assumption that vertical flow within each layer is uniform is reasonable based on review of current site data. Some areas, however, may exhibit more complex hydrostratigraphy. These features will be effectively averaged over a single layer.

- The vertical resolution of the unsaturated zone will be higher than the saturated zone, mainly for numerical stability and accuracy. The unsaturated zone material will be assumed homogenous over most of the model area. Review of site data generally support this assumption, though, some areas may experience perched groundwater conditions that only occur where underlying material has a lower hydraulic conductivity. The model will be able to simulate isolated saturated conditions in the unsaturated zone, but will not be able to simulate lateral flow in such perched conditions because of the code assumption that only one-dimensional vertical flow occurs in the unsaturated zone.

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- To capture the surface flow dynamics associated with the short duration, but high intensity precipitation events common in semi-arid western environments, the finest model time step will be 15 minutes. Climatic data and surface flow response data are available every 15 minutes.

- The precipitation and potential evapotranspiration (PET) will be simulated as boundary conditions. They will be spatially distributed over the model domain in zones based on available climatic data (nine precipitation stations, one met tower, five Colorado Department of Public Health and the Environment [CDPHE] wind and temperature stations) and observed trends. Snowmelt will be accounted for in the model and will be controlled by the spatial and temporal distribution of temperature and PET in the model area. PET will be distributed spatially and temporally. Its spatial distribution will be based on several factors including the temporal variation in wind and relative humidity, and the temporal and spatial distribution of temperature, and solar radiation. The distribution of topographic slope and aspect over the model area will be used to determine the incident solar radiation at the surface.

- The model will include watersheds in Woman and Walnut Creeks, but not Rock Creek, since this system is not hydraulically connected to the Woman and Walnut Creek flow systems.

1.4.2 MIKE SHE Code Capabilities and Limitations

The MIKE SHE code couples several partial differential equations that describe flow in the saturated and unsaturated zones with overland and channel flow. Different numerical solution schemes are then used to solve the different partial differential equations for each process. A solution to the system of equations associated with each process is found iteratively by use of different numerical solvers.

Several assumptions are associated with use of the specific partial differential equations. The significant assumptions that have direct implications to the application of the MIKE SHE code to the RFETS SWWB model include the following:

Unsaturated Zone — The main assumption is that flow is one-dimensional and vertical. In some cases-- for example beneath ephemeral streams, or near buildings/paved areas, or below trenches-- flow in the unsaturated zone may actually have local areas where flow is horizontal, causing this vertical-flow assumption to be violated. However, it is currently believed that these local areas will not significantly affect the interpretation of site-wide conditions.

Other Unsaturated Zone Processes — Other unsaturated zone processes not simulated in MIKE SHE include the following:

- Hysteresis;

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- Air entrapment;
- Vapor transport; and
- Freezing and thawing of soils.

Although, locally these processes exert strong influences on unsaturated zone flow, their effects will likely be much less pronounced on the site-wide model dynamics and mass balance than other factors (e.g., precipitation intensity and distribution, saturated hydraulic conductivities, and hydrostratigraphic structure).

Saturated Zone — Properties are uniform within a single grid cell. In reality, porous media properties likely vary by orders of magnitude within each grid cell. On average, however, these local scale variations are not expected to control the site-wide flow dynamics or mass balance, and it is reasonable to assume that properties can be averaged. Comparisons of model simulations with observed site-wide data will help to confirm this assumption.

Overland Flow — The kinematic wave approximation is used in MIKE SHE to simulate overland flow. This simplification to the full Saint Venant flow equations does not permit detailed simulation of backwater effects; however, given the anticipated grid resolution of the site-wide model the assumption is reasonable. Specific hydrologic processes like rill-flow are not considered in this code, but at the scale considered for application are not likely to be strong controls of flow.

2.0 Code selection criteria

As shown in Figure 2-1, the factors considered for selecting the SWWB code(s) include:

- Commercially-available code;
- Project objectives;
- Data quality and quantity;
- Conceptual model;
- Project constraints; and
- Applicable standards.

Each of these factors is described in more detail below.

2.1 Commercially-available code

The selected model code should be capable of being tested and verified by Kaiser-Hill, DOE, stakeholders, and other reviewing parties. Therefore, the code used should be one that is available for purchase by anyone who wants to run the model.

2.2 Project objectives

The project objectives laid out in the Work Plan and its appended data quality objectives (DQOs) define the most important factors to consider in the SWWB model code selection. These objectives constrain the modeling effort by specifying the following:

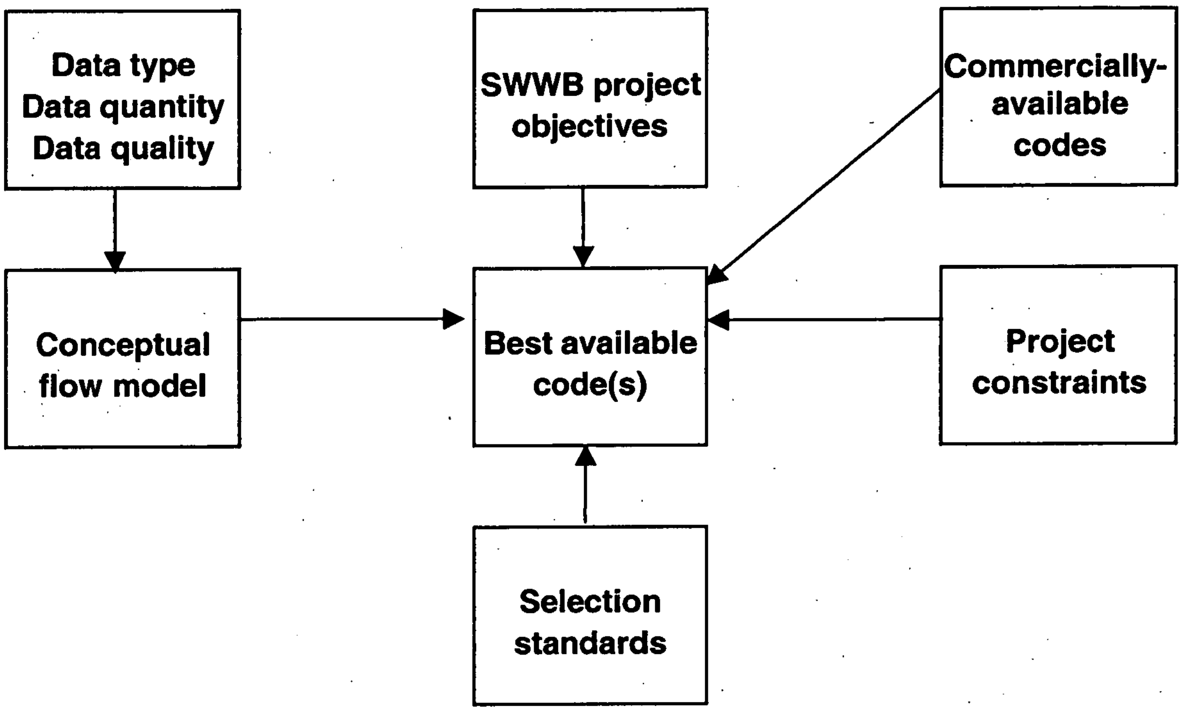
- General model boundary;
- Primary hydrologic components of concern;
- Level of spatial/temporal resolution desired; and
- Expected use of results.

The project objectives are the most significant constraint on model code selection. The primary objective of the SWWB is to provide RFETS with a management tool to evaluate how the site-wide hydrology, particularly groundwater and surface water flow, is likely to change from present to final site configuration ("present" indicates year 2000[1] site configuration) under various climatic and closure scenarios. SWWB results may also serve to provide information for final IA configuration to protect surface water quality (e.g., excavation, backfill, cover design, and land recontouring), and support preparation of the comprehensive risk assessment and RFETS Corrective Action Decision/Record of Decision. All objectives implicitly indicate that high levels of resolution and of predictive accuracy are desired attributes of the selected model.

[1] "Year" refers to calendar year unless otherwise indicated.

Figure 2-1

Model code selection criteria



The primary objective can be met through simulation of current site conditions to obtain a calibrated set of model parameters, followed by simulation of various final site configurations. Results from the current and final simulations will be compared to assess the overall change in conditions, and identify the implications of various changes to the RFETS parameters on the hydrologic flow system. The variability of these predictions due to uncertainties in site characterization and other input data will be explicitly addressed through uncertainty analysis. To meet this objective, it is critical that the selected code be sophisticated enough to simulate the complex dynamics of the entire site hydrologic system.

Specific modeling scenarios of conditions between present and final closure will also be performed with the SWWB model. These simulations will focus on the IA to evaluate the incremental effects of closure actions on the hydrologic regime. Therefore, the ability of a model to 'telescope' into a local area for further refinement, maintaining consistency between model scales, is a favorable attribute of the selected code.

New scenarios may be suggested by interim results of the modeling project, therefore the selected code must have the flexibility to be applied to different aspects of site closure.

2.3 Data quality and quantity

Reviewed data types are summarized in the data matrix provided in the Work Plan. Model input parameters and calibration target data types are summarized in Tables 2-2 and 2-3 of the Work Plan. A considerable amount of relevant site data is available providing an excellent spatial and temporal data distribution. In particular, meteorological records and surface water flow data are available across the RFETS model area at 15-minute intervals for at least one year (1999), and groundwater levels are collected every four hours at a large number of monitoring wells. As a result, data quality and quantity allow most hydrologic model codes to be considered for performing the SWWB.

Review of these data by the Water Balance Working Group (WBWG) indicates that, overall, existing data, supplemented by additional data were collected in 2000, are sufficient for developing a SWWB model of the study area using an integrated model code. While the quantity and quality of the data are generally adequate, lack of (or uncertainty in) data may cause greater uncertainties in the model predictions of some areas with any model used. For example, subsurface sandstone lenses (paleochannels) that notably influence groundwater flow have been identified in some areas on-site. Similar but unidentified sandstone lenses may exist in other areas within the model domain. Such localized data limitations would result in similar prediction uncertainties with any model code; therefore, these uncertainties are not a factor in the code selection.

2.4 Conceptual model

The current conceptual hydrologic model of the site is described in detail in the Work Plan. Some of the most important features of the conceptual model are summarized below:

- There has been a significant modification of the natural hydrologic conditions in both the IA and BZ. Modification in the IA is mainly due to changes in surface cover, rerouting of overland flow, subsurface construction, imported water, and subsurface treatment systems, while modification in the BZ is mainly due to construction of channels and dams and rerouting of channel flows;
- Annual precipitation is generally low (semi-arid), coupled with high evapotranspiration during summer months;
- Precipitation exhibits a high degree of spatial and temporal variability and, during winter months, occurs as snowfall that can be redistributed by wind;
- Most of the annual precipitation that is intercepted within RFETS is lost through direct evaporation at the surface, or through evapotranspiration via phreatophytes along streams or at springs on steeper slopes;
- Lateral inflow and outflow of groundwater to RFETS is relatively small compared to direct recharge, mainly from spring precipitation events, when evapotranspiration is lower;
- Groundwater recharge strongly responds to early spring precipitation;
- Groundwater levels respond to antecedent recharge events with a time lag that is affected by soil type and is proportional to the unsaturated zone thickness;
- Surface water base flows and seep locations respond to spatial and temporal variations in groundwater levels;
- Surface water flows respond rapidly to precipitation events;
- Surface water inflow and outflow within the site boundaries are currently managed by RFETS in the IA and with the ponds immediately downstream;
- Groundwater beneath the IA interacts with various subsurface pipes, utility conduits, and building basements, and is subsequently redirected, or discharged to the surface flow system (e.g., pressurized pipe leakage, storm and sanitary sewer lines, and footing drains);
- A substantial amount of imported Denver Water Board water is distributed through pipes within the IA, and is used in various applications;

- Most imported water is routed through the wastewater treatment systems and discharged to the managed series of ponds;
- A component of the imported water leaks from piping and adds to groundwater beneath the IA; and
- Groundwater is intercepted by several IA remediation systems.

The variety and complexity of the hydrologic system further supports the requirement for a sophisticated model code. A discussion of the appropriate level of sophistication is presented in Section 3.0.

2.5 Project constraints

Software costs, project budget, and project schedule must be taken into consideration in the model selection process. A holistic evaluation of software costs includes not only the initial procurement and technical support costs, but also consideration of software robustness, computational efficiency and flexibility, ease of data import and export, documentation, technical support, etc. Deficiencies in any of these areas inevitably lead to a significantly greater level of effort and resulting higher cost.

2.6 Applicable standards

The American Society for Testing and Materials (1998) standards were reviewed for code selection criteria. However, no selection criteria are available for integrated codes. Only a standard guide for selecting a groundwater modeling code is provided (Designation 6170). This guide is very general and is more of a checklist of boundary conditions and specific capabilities of the selected model, rather than a set of criteria on which to base selection. Therefore, formal third-party standards were not used specifically in the model code selection; however, the general guide that the model must be capable of simulation of site processes was used.

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3.0 Code identification

Many of codes have been developed and used to solve many types of hydrologic and hydraulic flow problems, many of which are similar to those that occur at RFETS. In the past few decades, dramatic improvements in computer hardware (notably in storage capacity, processing speed, and graphics handling ability), coupled with improvements in computer software (GIS, database, programming environments), have led to the development of more sophisticated hydrologic codes capable of solving increasingly complex problems. Such codes are typically the result of many years of continued development and application. Because of the sophistication of many hydrologic codes, it can take a considerable amount of time to understand the physical equations and mathematical methods used to simulate the numerous possible processes. To simplify the selection of an appropriate code for the SWWB, it is necessary to identify the different types of codes that have been developed and are available for use.

Section 3.1 provides a brief description of the types of available codes that, based on a standard classification scheme, could be used to simulate hydrologic processes at RFETS. This classification provides a means by which a select type of code can be identified and further evaluated for its capability of simulating site conditions. In some instances, model code documentation may describe its applicability and/or capability using terms meant to be consistent with this classification. Often, however, under closer scrutiny, certain capabilities or portions of the code are inconsistent with its stated classification. This makes evaluation of a specific code more difficult and requires that details of the code be reviewed (a time-consuming process). Nevertheless, the classification scheme is useful in eliminating certain types of codes from the selection process, either because they are too simple, or because they do not consider processes and details important to the RFETS flow system.

Section 3.1 also presents the main physical equations to be solved by the selected model code.

Following this brief summary of code types, the detailed model code selection criteria are presented in Section 3.2. This is followed in Section 3.3 by an initial screening of all possible hydrologic codes, based on the classification presented in Section 3.1 and the criteria presented in Section 3.2. Sources of information used to identify potentially applicable and relevant codes (including Internet addresses), and their features, documentation, and use are summarized in Section 3.4. Potential hydrologic codes are identified and their capabilities are summarized in Section 3.5.

3.1 Hydrologic model cod types

Hydrologic model codes vary greatly in their complexity and purpose. At the simplest level is a steady-state, lumped-parameter model. This type of model describes a process, such as streamflow into and out of a reservoir, without regard for spatial geometry or timing of flows. This model's operation is governed by the statistical

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correlation between input and output, and could be represented by an empirical equation.

Model codes solve increasingly more complex hydrologic problems with an increase in the sophistication of the code itself. At a basic level, the time dimension is not considered, and processes are assumed to be steady-state. At the next level of complexity, transient model codes treat only the time dimension explicitly and the solution becomes 'unsteady' in time. As the time resolution of interest becomes finer, different processes become dominant. For example, summer precipitation events over RFETS typically occur in less than one half hour. Runoff and channel flows respond quickly to these events, but groundwater flows may take hours to days to respond if at all. Increased model complexity incorporates storage within the model domain. At further levels of complexity: (1) the parameters controlling the processes become more transparent; (2) the model is driven by system parameters rather than empirical constants; (3) the parameters become spatially distributed at finer spatial resolution throughout the study area; and (4) simulated processes become more integrated. At each stage, the number of equations to be solved at each time step increases. The most complex codes are limited in their applicability by the cost of the computational power required to solve the equations within a reasonable time.

For model code selection, simpler types of code were eliminated. The process of elimination is illustrated through the following discussion of types of hydrologic code.

3.1.1 Integrated versus coupled individual process codes

Simulating hydrologic processes independently, using individual process codes, was considered to determine the feasibility of such an approach to meet the specified SWWB objectives. The primary advantage to using individual process codes is the modeling team's familiarity with the codes. A number of the codes have already been used at RFETS to model different areas, or hydrological processes. Some of the codes include MODFLOW, Storm Water Management Model (SWMM), Hydrologic Simulation Program (HSPF10), HEC-2, HydroCAD, HELP, and TR-20. Other variable saturation codes were used to simulate unsaturated zone flows in specific areas of the site. Another advantage to using individual process codes would be that the existing applications of these codes could be simply modified to meet the objectives of the SWWB. Two of the codes, HSPF and SWMM, were selected for further evaluation and are discussed in more detail in Section 4.1.

None of the individual codes considers all processes simultaneously in any detail. This is considered a major limitation because the RFETS hydrologic system responds in a very integrated manner. Coupling process codes to simulate the integrated system at RFETS would be difficult to implement because new code and programming would have to be developed for this method. Therefore, the selected code should be *integrated.*

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3.1.2 Deterministic versus stochastic codes

Figure 3-1 illustrates the general types of hydrologic flow codes currently available. Codes are defined as being either deterministic or stochastic (Singh, 1988; Refsgaard and Abbott, 1996), depending on whether or not the input is specified in terms of a probability distribution. Deterministic codes input unique values for specific parameters and produce output with apparent "certainty". Stochastic codes incorporate uncertainty in the model input parameters. However, stochastic codes are not appropriate for the SWWB project, as they can only be applied to relatively simple systems. Because of the hydrologic complexity of the site, the selected code should be *deterministic*.

3.1.3 Joint deterministic-stochastic codes

The substantial data requirements of deterministic distributed codes (see Section 3.1.4), and the common uncertainty related to many of their input parameters, have led to development of joint deterministic-stochastic codes that attempt to incorporate stochastic representations of uncertainty in input parameters. Stochastic analysis typically has focused on linear systems, where the input parameters are parameterized in terms of their mean and standard deviations to account for their uncertainty.

Stochastic analysis of non-linear systems is uncommon, because of the inherent complexity associated with solving the partial differential equations when stochastic representations of the parameters are incorporated within them. The accepted alternative is to perform a Monte-Carlo analysis on a deterministic model, running multiple simulations, and generating a probabilistic distribution of results. This is the approach that will be used for the SWWB uncertainty analysis. Therefore, stochastic and joint deterministic-stochastic codes are not considered further.

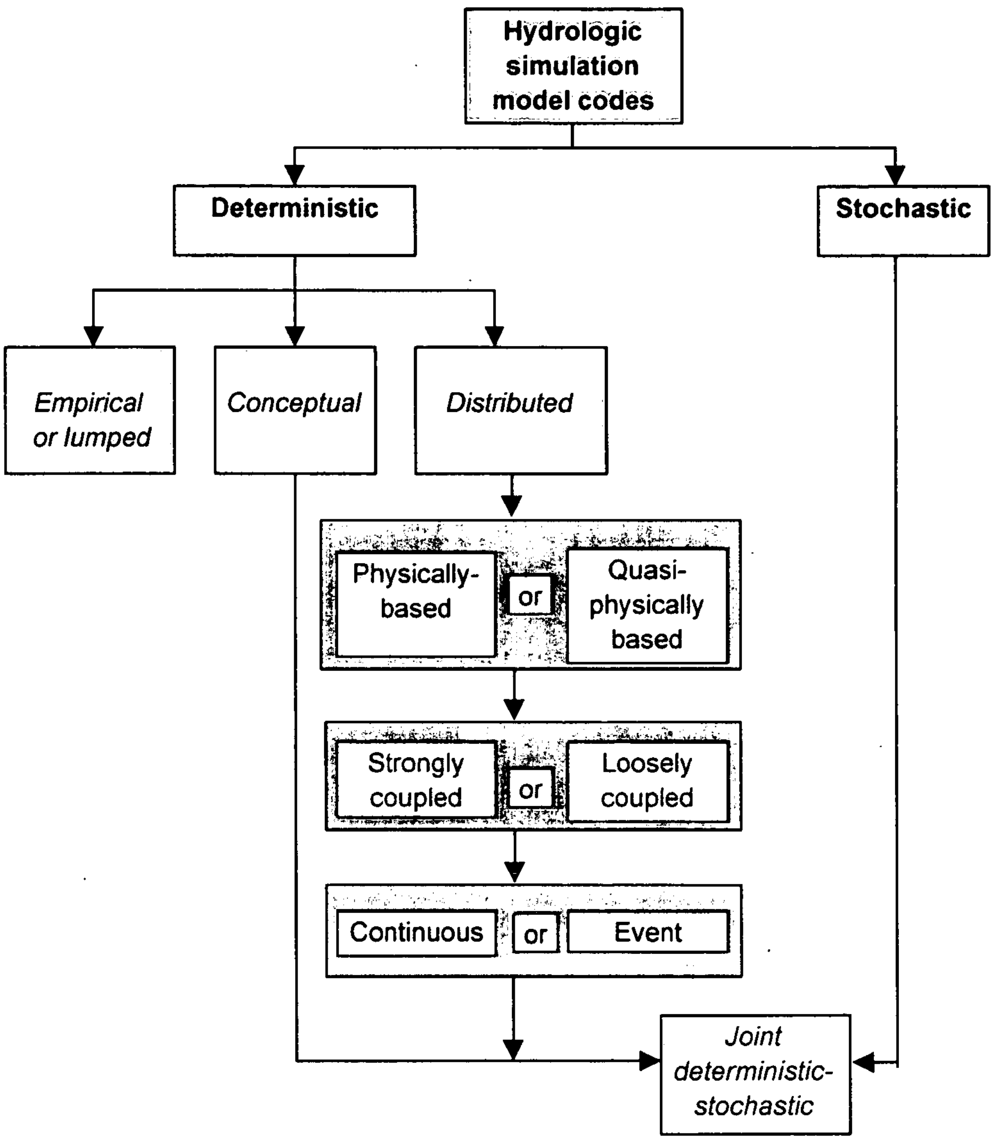
3.1.4 Types of deterministic code

Deterministic codes can be classified as empirical, conceptual, or distributed, based on the degree of spatial distribution of input parameters. Empirical codes (also termed "lumped") treat the entire system as a single control volume, in which the parameters controlling the flow within the system are effectively lumped into a single value. Conceptual codes incorporate more physical reality, but also tend to represent the system by a series of lumped parameter models that do not consider the explicit spatial variability of input model parameters within each sub-model. For example, most rainfall-runoff (unit hydrograph) models fall into this category. The obvious limitation of both empirical and conceptual codes is that they do not address the considerable and very significant spatial variation in properties (e.g., hydraulic conductivity) across the site.

Unlike the empirical and conceptual models, distributed codes (also termed "distributed parameter" codes) require a distribution of input parameters in both space and time that more realistically relates to their actual field distribution. In a distributed code, the hydrologic system is assumed to behave as a continuum, and flow within the system is defined by governing physical equations. These equations and their numerical solution

Figure 3-1

Types of hydrologic model code[1]



[1] Modified from Refsgaard, J.C., Danish Hydraulic Institute, "Terminology, Modeling Protocol and Classification of Hydrological Model Codes" in *Distributed Hydrological Modelling,* Abbott, M.B., Refsgaard, J.C., 1996, Water Science and Technology Library, pp. 321.

require a distribution of input parameters in both space and time. These codes represent the most data-intensive types of hydrologic models that can be used to simulate a system.

Only *distributed* codes were considered for code selection because only these codes simulate the distributed effects of input on output, and they are considered most capable of simultaneously simulating the hydrologic processes most important to the SWWB.

3.1.5 Distributed codes

Distributed codes can be subdivided as follows:

- Physically-based or quasi-physically-based;
- Strongly- or loosely-coupled; and
- *Continuous* or *event*.

The term "physically-based" is often misused in the literature. There is a tendency by many code developers to use this term to describe their code, because it implies that it was developed on the basis of sound physical and mathematical representations. However, in reality, sophisticated codes have a substantial number of physical processes to be simulated, and there is a tendency to sacrifice more rigorous physical and mathematical representations of a given process for a simplification that will permit a more rapid solution. Therefore, although a code may be described as a physically-based, distributed code, in reality certain processes may be simulated by equations that are less physically-based than could be described based on current research. Such simplified codes are referred to as "quasi-physically-based".

This is an area of significant differences between codes, and also one which can make it difficult to compare the differences between two codes that make similar claims as to their capabilities. In the model selection process, preference was given to those codes that are truly considered *physically-based* for all significant hydrologic processes.

The second distinction between distributed codes is how they integrate, or couple, the hydrologic processes throughout the simulation. In other words, how do they actually account for transfers, for example, from surface water to the unsaturated or saturated zones? Ideally, the partial differential equations should be solved simultaneously and exactly so that mass is conserved and each state variable (e.g., system pressure) is updated as a function of how input variables change. However, very rigorously coupled codes are extremely inefficient computationally, and are typically used only for research, or applied to much smaller areas, such as test plots. Therefore, the selected code should be *well coupled*, but retaining computational efficiency at the scale of the study area.

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The third distinction among distributed codes is continuous versus event code types. Event codes simulate the results of only one event (e.g., one storm with its corresponding hyetograph and, typically, one or more streamflow hydrographs). Continuous codes simulate all events and the system relaxation period between events. Therefore, event codes are subsets of continuous codes. The selected code for this project should be *continuous*, for the following reasons:

- Event-response relationships are affected by antecedent conditions;
- A period of at least one year should be simulated for calibration; and
- The future scenarios may extend over several years.

3.1.6 Physically-based code flow equations

Typically, distributed parameter, physically-based model codes are based on a set of partial differential equations that describe the flow and mass conservation for each hydrologic process within a given flow system. The primary processes include: (1) surface flow, which consists of channelized and overland flow; (2) groundwater flow; and (3) unsaturated zone flow. A brief description of the physical equations that are used in the more rigorous, physically-based hydrologic models is presented below. Figure 3-2 illustrates conceptually how the three-dimensional hydrologic processes are related.

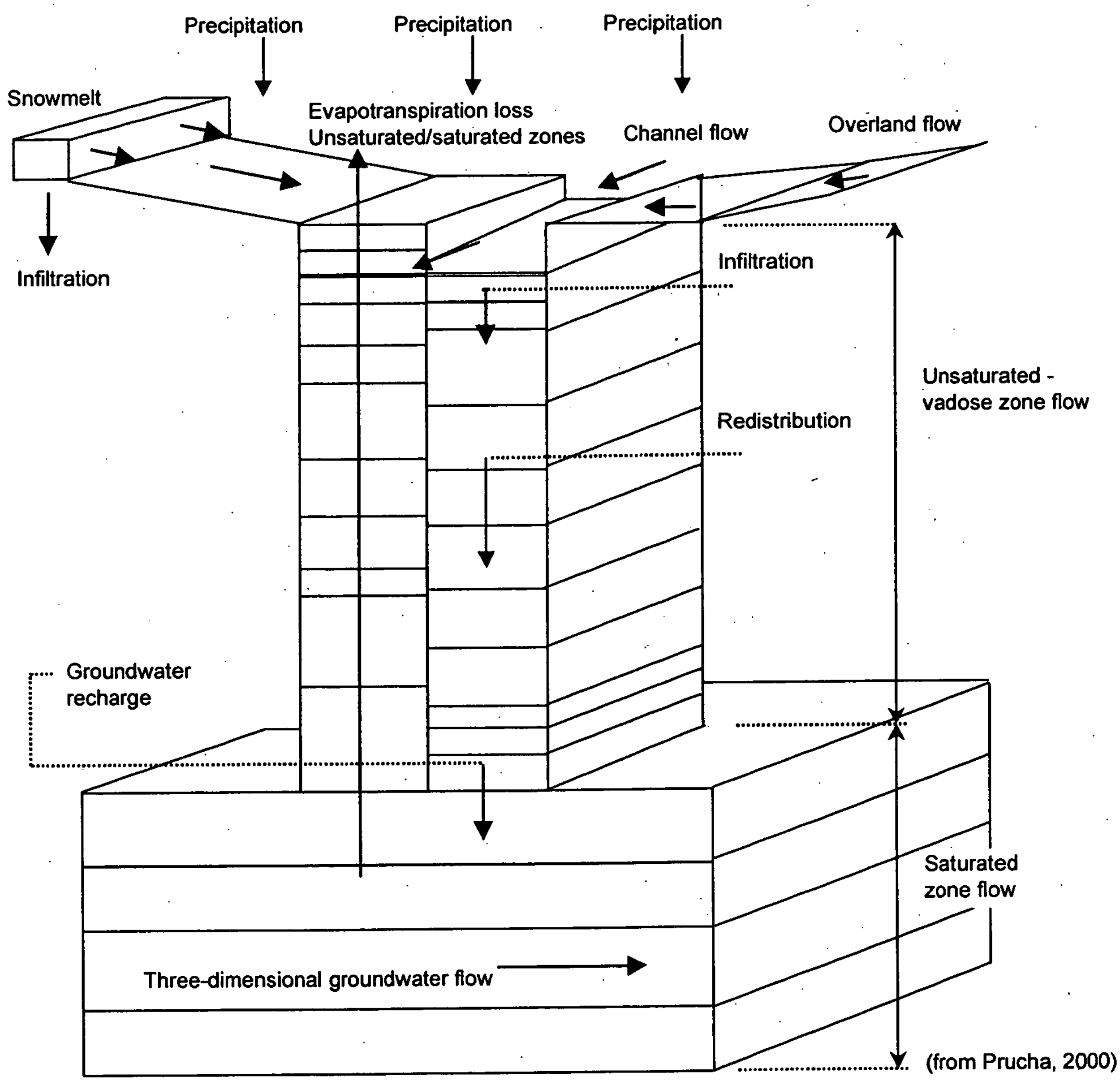
Overland flows respond to direct precipitation or snowmelt and feed into channels. Infiltration occurs between overland flow planes, or through the bottom of channels. Evapotranspiration acts to remove all, or some of the infiltration from the unsaturated zone before it becomes recharge. Evapotranspiration can also remove water directly from the groundwater zone. Groundwater is recharged by the fraction of infiltration that exceeds evapotranspiration losses, and subsequently flows laterally out of the system, or discharges directly to a channel or to an overland flow plane.

Surface water flow

Distributed physically-based hydrologic codes typically use the one-dimensional Saint-Venant flow equations to simulate the physical routing of water through surface channels within the model domain. These equations neglect lateral inflow, wind shear and eddy losses. They are used extensively in practice and are actually simplifications of the much more complicated three-dimensional Navier-Stokes flow equations. Despite their simplification, they still represent unsteady, non-uniform flow conditions within a stream under most watershed conditions.

Figure 3-2

Three-dimensional hydrologic flow system



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The conservative form of the Saint-Venant equations is presented in Chow (1988) as follows:

Continuity Equation:

$$\frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t} = 0$$

Momentum Equation (Conservative Form):

$$\frac{1}{A}\frac{\partial Q}{\partial t} + \frac{1}{A}\frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right) + g\frac{\partial y}{\partial x} - g(S_o - S_f) = 0$$

Local Acceleration Term	Convective Acceleration Term	Pressure Force Term	Gravity Force Term	Friction Force Term

Momentum Equation (Non-Conservative Form):

$$\frac{\partial V}{\partial t} + V\frac{\partial V}{\partial x} + g\frac{\partial y}{\partial x} - g(S_o - S_f) = 0$$

Kinematic Wave: $g(S_o - S_f)$ terms
Diffusion Wave: from $g\frac{\partial y}{\partial x}$ term onward
Dynamic Wave: all terms

where A is the cross-sectional area, Q is flow rate, g is the gravitational acceleration, V is flow velocity, x and y are distance along the channel and water depth, respectively, and S_o and S_f are channel slope and friction loss, respectively.

Often, simplifications to the momentum equation distinguish various distributed hydrologic codes from one another. For example, some codes only provide for the simplest surface routing capabilities and use the kinematic wave assumption (see above). More complex codes permit routing that includes the diffusive, or even the fully dynamic wave equations. Kinematic and diffusive wave approximations appear to work well under different conditions, whereas the fully dynamic wave approximation (full Saint-Venant equations) provides the highest level of surface prediction under most conditions (hydrostatic pressure distribution, small channel bottom slope, and uniform cross-sectional flow velocity), but is also the most computationally intensive. Another advantage of using the full dynamic approximation is that backwater effects can be simulated.

Overland Flow Equation (Two-dimensional Diffusive Wave):

$$\frac{\partial h}{\partial t} + (8g)^{1/2}\frac{\partial}{\partial x}\left(\frac{S_o^{1/2}h^{3/2}}{F^{1/2}}\right) - q - r + f = 0$$

where h is flow depth, r is rainfall rate, f is infiltration loss rate, q is lateral inflow rate, t is time, and f is the Darcy-Weisbach friction factor.

Groundwater flow

Groundwater flow equation (Three-dimensional Boussinesq):

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial x}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) - W = S_s\frac{\partial h}{\partial t}$$

Where K_{xx}, K_{yy}, and K_{zz} are principal hydraulic conductivity tensor values, h is the hydraulic head, W represents sources or sinks, S_s is specific storage and x, y, and z are Cartesian coordinates.

Unsaturated zone flow

Unsaturated Zone flow equation (One-dimensional Richard's Equation):

$$C(\psi)\frac{\partial \psi}{\partial l} = \frac{\partial}{\partial z}\left(K(\psi)\frac{\partial \psi}{\partial z} + K(\psi)\right) - S$$

where $C(\Psi)$ is the specific water capacity, $K(\Psi)$ is the unsaturated hydraulic conductivity, S is a sink term, and Ψ is the pore-water pressure.

3.2 Model code selection criteria

Based on the general constraints described in Chapter 2 (project objectives, conceptual flow model, data quality and quantity, standards, and schedule) and those presented above (available model code types), the selected code, at a minimum, should possess the following features:

- Adequate sophistication to simulate all relevant hydrologic processes at RFETS for short and long time periods (described by the three-dimensional conceptual flow model presented in the Work Plan, and details associated with future scenarios outlined in Section 1.0). In particular, unsaturated zone and groundwater flows and their interactions with surface water flows should be explicitly accounted for in the selected model;

- Allows spatial and temporal variability in model parameters and inputs across the site;

- Permits a variety of time-variant boundary conditions;

- Able to incorporate variable spatial resolution within the model domain, or the ability to 'telescope' into desired area (grid refinement);

- Rigorously couples different hydrologic processes (e.g., surface and groundwater flows) that operate simultaneously;

- Has built-in code options that permit simplified process solutions where appropriate to improve computational efficiency; and

- Well documented use, available documentation on use, and easy to use.

A set of secondary model code selection criteria were also developed to reflect the overall 'capabilities' of a given model as a decision-making or management tool. Though not absolutely necessary for application, these additional criteria are considered nearly as important as those above because they can dramatically improve the efficiency (time and complexity) in overall SWWB model development, or the ability to visualize, interpret or evaluate complex spatial and temporal distributions of model input and output. These criteria can reflect a code's ability to rapidly modify or develop a complex set of hydrologic conditions (e.g., a specific future scenario) and to accurately and efficiently interpret and evaluate a potentially large and complex set of model output. These secondary model code selection criteria are:

- Graphical User Interface (GUI);

- GIS capability;

- Internal consistency checks; and

- Pre- and post-processing capabilities.

Finally, additional code selection criteria specified below are not within the SWWB scope of work, but are considered relevant to the secondary objectives outlined in Section 2.1:

- Ability to simulate erosion and sediment transport; and
- Ability to simulate dissolved species transport.

3.3 Initial code screening

It is clear that the response of the hydrologic flow system at RFETS is a strong function of many spatially- and temporally-distributed parameters based on the three-dimensional conceptual model presented in the Work Plan and summarized in Section 2.4 of this report. It is, therefore, essential that the code selected for simulating the RFETS SWWB have, at a minimum, the ability to incorporate this spatial and temporal variability for the most significant system parameters. Neither empirical nor conceptual model codes are considered further in this model selection process. Empirical and conceptual codes do not provide the needed degree of resolution or sophistication to adequately simulate current or future conditions at the site to meet the project objectives. They do not consider the spatial distribution of model parameters-- like hydraulic conductivity, evapotranspiration, or precipitation-- at the level required to adequately predict system response to meet project objectives.

Stochastic model codes are not considered because system parameters are known relatively well in both space and time. This is particularly true for precipitation, which is a critical model parameter because it is responsible for most of the system's temporal response. Often, distribution of precipitation in space and time is considered a stochastic process because it is not known well. However, at RFETS it is considered reasonably well known in space and time. Chow et al. 1988) indicate that use of a deterministic model code (compared to a stochastic model code) is appropriate where the output variability is small in comparison to the variability resulting from known parameters.

As a result of this initial screening of codes, only distributed parameter codes will be considered further for use in the SWWB project. Only these types of codes incorporate the spatially and temporal variability necessary to meet project objectives and to simulate important conceptual flow model details.

3.4 Information sources

Based on the initial screening described in Section 3.3, only distributed parameter, integrated hydrologic model codes are considered for the SWWB modeling. A variety of information sources were used to identify potential distributed hydrologic codes that could be used for the SWWB. A substantial amount of the information on available integrated, physically-based hydrologic models and their capabilities was obtained from in-progress Ph.D. dissertation research (Prucha, 2000).

Several source texts were used to identify and review capabilities of available codes. These sources are briefly summarized below:

- Singh, 1995. This reference is a fairly comprehensive summary of more sophisticated hydrologic models, but fails to discuss comparison or evaluation of codes;

- Abbott and Refsgaard, 1996. This discussion, by the principal authors of MIKE SHE, is somewhat slanted towards use of that code for hydrologic modeling, but overall they identify a number of codes, their objectives and capabilities for different types of problems, including agrochemical, soil erosion modeling, and multi-species reactive transport modeling;

- United States Bureau of Reclamation (USBR), 1991 USBR summarized available hydrologic codes nearly 10 years ago, to facilitate selection of an appropriate hydrologic model code from the many existing codes. The list of codes in this reference represents those supported by USBR, but not necessarily developed through this institution. For each code listed, relative strengths and weaknesses are provided;

- Bedient and Huber, 1992. This reference presents several hydrologic models, with greatest focus on urban hydrology related models like SWMM and HEC models;

- Viessman, 1977. This reference is a little outdated, but provides a good overview of existing 'major' hydrologic simulation models as of the publication date. Many of these codes still exist today, but have been updated; and

- Ponce, 1989. This reference provides an excellent discussion on catchment hydrology at various scales, and discusses a few physically-based, distributed parameter models in some detail.

The rapid development associated with distributed hydrologic models makes many hardcopy text references of code capabilities outdated; therefore, Internet sources were also relied upon for obtaining the current information on code capabilities and applications. Several software developers' Internet sites offering trial codes and documentation were also consulted. A number of specific hydrologic model references were identified on the Internet. These are summarized in Table 3-1.

Many sources of currently-available hydrologic models were found on the Internet. The USGS provides a comprehensive lists of hydrologic models developed through federal government agencies at http://smig.usgs.gov/SMIG/model_archives.html. The USBR also provides another comprehensive listing of hydrologic models at http://www.usbr.gov/hmi/invlist99.htm#1999_List. Text references included in Table 3-1 are downloadable from the associated Internet site.

Table 3-1
Hydrologic model references available on the Internet

Hydrologic Model	Reference
MIKE SHE Danish Hydraulic Institute, British Institute of Hydrology, and SOGREAH (France)	http://www.dhisoftware.com/mikeshe/index.htm
Precipitation-Runoff Modeling System (PRMS) USGS New Version is MMS	http://wwwbrr.cr.usgs.gov/projects/SW_precip_runoff/mms/
Hydrologic Simulation Program (HSPF) USEPA	http://www.scisoftware.com/products/hspf_model_details/hspf_model_details.html http://www.epa.gov/ceampubl/hspf.htm Bicknell, B.R., Imhoff, J.C., Kittle, J.L., Jr., Donigian, A.S., Jr., and Johanson, R.C., 1997, Hydrological Simulation Program--Fortran: User's manual for version 11: U.S. Environmental Protection Agency, National Exposure Research Laboratory, Athens, Ga., EPA/600/R-97/080, 755 p.
Simulator for Water Resources in Rural Basins (SWRRB) USDA Agricultural Research Service	http://dino.wiz.uni-kassel.de/model_db/mdb/swrrbwq.html http://www.cee.odu.edu/cee/model/swrrbwq.html
Storm Water Management Model (SWMM) US EPA	http://www.ccee.orst.edu/swmm/
TOPOG-Dynamic (CSIRO, Australia)	http://www.clw.csiro.au/topog/
MODBRANCH (USGS)	http://pubs.usgs.gov/publications/1996-08/books.shtml#twri Swain, E. and E. Wexler.1996. A coupled surface-water and groundwater flow model (ModBranch) for simulation of stream--aquifer interaction. Chapter A6. Techniques of Water-Resources Investigations of the United States Geological Survey. p. I 125.
SWAT (USDA, Agricultural Research Service)	http://www.brc.tamus.edu/swat/versdif.html
Distributed Hydrology-Vegetation Model (DHSVM) (DOE, PNNL)	http://www.ce.washington.edu/~nijssen/docs/DHSVM/

3.5 Code identification and capability summary

A number of physically-based, distributed, integrated hydrologic codes were evaluated, but eliminated from the initial list because they failed to meet certain aspects of the selection criteria. These codes include the following:

- ISGW-SDI (HSPF + MODFLOW);
- SWATMOD (SWAT + MODFLOW);
- MODFLOW-Surfact 2000 (HydroGeoLogic);
- SWATCH (CSU); and
- MOGROW (DLO-Netherlands).

3.5.1 ISGW-SDI

The ISGW code developed by SDI Environmental Services, Inc. out of Tampa, Florida (Davis, P.R., 1998) couples HSPF and MODFLOW. Although, this sounds appealing, the main limitation for this code is its implementation of time-stepping, which does not offer the flexibility necessary to simulate the type of rapid precipitation events and runoff at RFETS. Furthermore, it does not consider unsaturated zone flow as rigorously as other codes. This is important in arid and semi-arid zone hydrology.

3.5.2 SWATMOD

The previous discussion is also true for the SWATMOD code (Ramireddygari, 1998), which also couples an existing code, SWAT, with MODFLOW.

3.5.3 MODFLOW-Surfact 2000

MODFLOW-Surfact 2000 (Panday and Huyakorn, 1998) was eliminated from further consideration because it is still being developed. Further, it has no documented use and would not be efficient in solving all of the complexities associated with flow at RFETS. The code represents the most physically-based code identified to date; however, the three-dimensional variably saturated approach used for subsurface flows, rigorously coupled to surface flows would be incapable of solving system complexities over the site, due to numerical solver limitations over the spatial and temporal scales of interest in the SWWB at RFETS.

3.5.4 SWATCH

SWATCH (Alhassoun, 1987) was developed as a Ph.D. dissertation in a comparatively physically-based approach, but does not appear to have been applied outside of an academic capacity.

3.5.5 MOGROW

MOGROW (Querner, 1997), developed in the Netherlands, couples two codes, SIMWAT and SIMGRO, to integrate surface and groundwater flow. It was eliminated because it simplifies features of MIKE SHE, and it does not appear to have as broad a history of application as other codes.

3.5.6 Other eliminated codes

Other distributed parameter hydrologic codes like TopModel (Beven and Kirkby, 1979), Thales (Grayson et al, 1992), or KINEROS (Woolhiser et al, 1990), adequately handle only some but not all of the hydrologic processes at RFETS. For example, groundwater is typically handled too simply, where the partial differential equation describing flow is greatly simplified to the point where it is a lumped or conceptual model component.

The US Army Corps of Engineers supports development of GMS, SMS, and WMS codes that respectively deal with groundwater, surface water, and watershed management. These codes do not currently permit the direct coupling of the surface and groundwater flow modules.

As discussed above, integrated codes are preferred over individual hydrologic codes to independently simulate various aspects of the conceptual model. However, in the following discussion, one combination of individual codes is included for comparison. Table 3-2 summarizes the distributed hydrologic model codes considered for use in the SWWB project. This table includes those codes that appear to meet all the model selection criteria specified in Section 3.2. The organization of Table 3-2, and each code's purpose, description, and the specific methods it uses to represent physical processes, are described below in Sections 3.5.7, 3.5.8, and 3.5.9, respectively.

3.5.7 Code name, author(s), and purpose

Table 3-2 first presents the code name(s) and the author(s) or sponsoring organization(s). Most codes listed were first developed as research codes by universities or government institutions, and have been subsequently updated over many years. Next, the primary purpose of the code is described. The purpose is significant because each code has been developed to address a specific problem, or suite of problems (e.g., water quality issues, water balance, land-use effects, or soil erosion). Often these problem types do not overlap, and one code may be better than another for addressing a given problem.

3.5.8 Spatial representation

Table 3-2, describes the spatial representation of the hydrologic flow system, indicating the degree to which the code allows its parameters or variables to be distributed. As noted previously, there is some degree of subjectivity in defining codes; but in general, a code is considered distributed if it permits most or all of its input variables and parameters to be specified as spatially distributed. All codes are lumped to some degree, because even the most distributed codes must define a minimum grid cell size in which the model parameters, or variables, are effectively lumped to remain computationally feasible.

If a coarse grid is used to describe the model domain using a distributed code, there might be little difference between results obtained by simulating the entire system with a "lumped watershed" code or a "distributed" code. However, the "distributed" code typically permits a finer grid resolution of the system, which can represent the system more accurately.

The "lumped watershed", or "contour-based," codes are basically constraints imposed on the code by the methodology used to solve the surface flow within the hydrologic system. Typically, sub-watersheds, or areas of uniform streamline, are defined based on topography (derived from a digital elevation model). This permits the two-dimensional overland flow process to be represented by a one-dimensional. That describes the hydrograph response from the sub-watershed or streamline.

3.5.9 Physical processes

The remainder of Table 3-2 provides descriptions of how each code simulates physical processes. The following processes are considered the most important components of the SWWB conceptual flow model:

- Surface flow as overland flow and channel flow;
- Subsurface flow as unsaturated zone flow and ground water flow;

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Table 3-2
Selected distributed continuous hydrologic model codes

		Surface flow			Subsurface flow					
Hydrologic model code	**Primary purpose**	**Spatial representation**	**Overland flow**	**Channel/reservoir routing**	**Infiltration/unsaturated flow**	**Evapotranspiration Plant growth**	**Snow melt**	**Sediment transport**	**Water quality Chemical transport**	**Additional features/ considerations?**
MIKE SHE Danish Hydraulic Institute, British Institute of Hydrology, and SOGREAH (France)	Simulation of interrelationships among hydrologic processes in relation to watershed modifications	Fully Distributed in space and time. (Limited to square grid)	2-dimensional kinematic wave routing. Uses DEM data directly.	complete dynamic flow routing equations with various control structures (gates, culverts). 'Floodplains' used to simulate ponds and their interaction with unsaturated zone & groundwater. Muskingham routing option.	*1-Dimensional Richard's* Equation Solution with time varying water table (Simplified gravity-only method or, spatial lumping of 1-D columns allowed for increased efficieny)	*Potential ET from* Kristensen and Jensen Method where actual ET based on calculated soil moisture. Penman-Monteith to be added in Spring 2001.	*Degree-Day* Snowmelt Model (Temperature-based model)	Physically-based sediment transport module for both cohesive and non-cohesive sediments	Separate Modules Available for both water quality and chemical transport	Yes, several other options are available. Additional graphical features (i.e., MikeSHE GIS) are available to improve efficiency. Includes Macropore Flow
TOPOG-Dynamic (CSIRO, Australia)	Variable Source Area Representation of Streamflow Generation	Contour Based Elements. (Flow trajectories determined for each sub-watershed).	I-D kinematic wave flow	I-D kinematic channel network routing	1-D Richard's Equation Solution (3 numerical methods, mixed form very efficient) Simplifications Available	Potential ET from Penman-Monteith, actual ET based on moisture accounting	Snow component not yet coupled with model	Based on boundary sheer strees of overland flow, no channel sediment transport component	Chemical transport included.	Includes Macropore flow. Only runs on Unix OS. Authors indicate intended use if for 'research'.
Precipitation-Runoff Modeling System (PRMS) USGS New Version is MMS	Streamflow response to climate and land use conditions. Primarily intended for Large-scale hydrologic basins.	Hydrologic Response Unit (HRU)	not included in continuous simulation	no flood routing for continuous simulation (see note to right)	2-layered reservoir accounting model based on Green-Ampt	Potential ET from Empirical Methods, Actual ET based on Soil Moisture	Temperature-based model	No sediment transport for continuous simulation	No Chemical Transport No Channel Routing in 24 Hr Time Period.	Integrates with the USGS Modular Modeling System (MMS) graphical user interface based on X-Windows Environment
Hydrologic Simulation Program (HSPF) USEPA	Effects of land-use change, reservoir operations on flow and water quality (joint deterministic-stochastic)	Lumped subareas	lumped empirical routing	Kinematic wave routing through channel reaches	Physical & empirical formulas with reservoir accounting model	Empirical method for Potential ET; with moisture accounting adjustment	Uses physical & empirical formulas	Based on ARM & NPS models	Simulates contaminant runoff with instream water quality and sediment interactions. Code also simulates complex chemical processes *including hydrolysis*, biodegradation, and oxidation.	No Information
Simulator for Water Resources in Rural Basins (SWRRB) USDA Agricultural Research Service	Hydrology, erosion and nutrient predictions for large-scale, agricultural, or ungaged basins	Lumped subwatershed areas	Rational Formula or SCS TR-55 empirical-based methods	no flood routing	Infiltration calculated using SCS curve number. Flow routing through soil layres.	Potential ET from Empirical Methods, actual ET based on *moisture accounting*	Temperature-based model	MUSLE and sediment routing, no channel sediment component	No Information	Time steps only in 24 hour periods.
Storm Water Management Model (SWMM) US EPA	Storm-water flow (and quality) within natural drainages and/or storm sewer in urban areas	Up to 100 subwatershed areas	Non-linear reservoir routing	Kinematic flow or complete dynamic flow routing equations In Extran Block	Infiltration modeled using Green-Ampt or Horton approach. Flow routing using lumped reservoirs with rising water table.	ET from Empirical Methods and soil moisture accounting	Temperature-based model	Modified USLE for sediment load.	yes	This code has been applied in a substantial number of sites across the U.S., primarily for Urban environments that include complex storm drain analysis.
MODBRANCH (USGS)	coupled groundwater (MODFLOW) and surface water (Branch)	Distributed	storm runoff must be provided by another model	Dynamic flow equations for *open-channel networks*	Recharge estimate must be provided	ET from groundwater only. Not from Unsaturated Zone	not considered	not considered	Not included, but MT3D, or other transport code could be used separately.	No Information

- Evapotranspiration and plant growth;
- Snowmelt;
- Chemical transport (unsaturated and groundwater zones) and water quality (surface water); and
- Macropore flow.

These processes are discussed in detail in the Work Plan and will not be described further here. The selected code should be able to simulate all of these processes well.

4.0 Model code evaluation, comparison, and selection

Section 4.1 summarizes how codes were evaluated and then compared to identify the code that best meets the model code selection criteria set forth in Section 3.2. A relatively simple, but useful ranking scheme, developed as a means of comparing overall features of each code, is also presented in Section 4.1. The model code selected for use in the SWWB modeling based on this ranking is presented in Section 4.2.

4.1 Code evaluation and comparison

Comparisons and evaluations of each model code presented herein are made using available manuals or documentation (Section 3.4), literature references describing actual performance or application, and direct experience using the model. Foremost in the effort to identify the most well-suited model code for the SWWB, is the need to remain unbiased towards selection of any one code. There is often a tendency for scientists and engineers to simply use the code with which they are most familiar instead of using a code that may offer a better solution to the specific problem at hand. There are several reasons for this, one of which is that it takes a significant investment in person-hours to become familiar enough with a specific code to apply it correctly to a given problem. Furthermore, each code in Table 3-2 was developed through a large government, or academic institution and there is a strong tendency for users within such institutions to sponsor their own code. There is little motivation for users to switch to another code because models for most complex sites take months, and even years to develop. Users become familiar with features of a particular code, such as the procedures for data input, how the model performs, or the sensitivities of a particular numerical solver, and are reluctant to give up this experience by using another code.

It is felt that no "absolute" comparison can be made whereby one code is considered more accurate, or better than another, particularly for a given site. No standardized method is known to exist. Instead, each code should ideally be compared against one another using the same assumptions and site parameters and variables. However, this type of comprehensive comparison of the physically-based distributed parameter model codes (Table 3-2) has not been performed to date in any rigorous fashion (El-Kadi, 1989). To rigorously demonstrate how one code may perform better than another for a specific physical problem is well beyond the scope of this report. Instead, the approach taken in this report is to evaluate and compare codes identified in Table 3-2 using a simple, but objective numerical ranking scheme based on the model code selection criteria specified in Section 3.2. The intent of the ranking scheme is to:

- Numerically rank each code's capability against each criteria;
- Remain unbiased toward use of a specific code; and
- Identify the best model code for the RFETS SWWB based on professional judgement.

Once this ranking template was developed, specific code features and capabilities were evaluated in greater detail. Table 4-1 presents the model code selection criteria and ranking scheme used to compare codes. Model code selection criteria occur in columns with labels at the top. Numerical rankings are provided in each column, corresponding to the specific codes listed in the left column of the table. The second row beneath the model code selection criteria shows the total possible score for each criterion. The last two columns on the right sum the total for each code, and provide a percentage of the maximum possible. The total possible value for a given criterion varies according to the relative importance of that criterion to the overall model selection. For example, the "physically-based" criterion has a maximum possible score of 10 points (pts), compared to the "Technical Support" criterion, which has a maximum possible score of three pts. In this case, the assigned points reflect the relative importance of a physically-based code to a code having excellent technical support.

Other important criteria listed in Table 4-1 include the following code capabilities:

- To provide spatial and temporal variability for input and output (5 pts);
- To provide flexible boundary and initial conditions (5 pts);
- To provide flexible grid resolution capabilities (5 pts); and
- To provide GIS and pre- and post-processing capabilities (5 pts).

The remaining criteria have lower point values:

- Available documentation that is current, complete and accurate (4 pts);
- Documented use (successful, difficulties etc.) (3 pts);
- Ease of use, or code familiarity (this is somewhat subjective and is based on user experience and qualifications) (3 pts);
- The type and availability of technical support (3 pts);
- Animation and particle tracking (2 pts);
- Internal consistency checks (2 pts);
- Whether the code supports additional features like chemical or sediment transport, or erosion modeling (2 pts); and
- Hardware optimization for PC-based processor (1 pt).

Table 4-1
Model evaluation matrix

Hydrologic model code	Level of Sophistication (Physical & Mathematical)	Spatial/Temporal Grid Resolution Capabilities	Spatial/Temporal Parameter/Variable Input/Output Capabilities	GIS capabilities Pre/post-Processing	Boundary Conditions (types, flexibility)	Documentation (Current, Complete, Accurate, Understandable)	Optional Simplified Process Equations	Documented Use	Ease of Use Familiarity	Technical support	Animation/ Presentation Capabilities Particle Tracking	Internal Consistency Checks	Additional feature support (transport, erosion)	Hardware optimization	Total Score	Percent
Total Possible Rank	10	5	5	5	5	4	3	3	3	3	2	2	2	1	53	
MIKE SHE Danish Hydraulic Institute, British Institute of Hydrology and SOGREAH (France)	10	5	3	5	5	3	3	2	3	3	2	2	2	1	49	92%
TOPOG-Dynamic (CSIRO, Australia)	7	3	3	4	4	3	1	2	2	2	1	1	2	0	35	66%
SWAT Soil and Water Assessment Tool (USDA)	7	3	3	4	3	3		1	2	2	1	2	2	0	33	62%
PRMS Precipitation-Runoff Modeling System (USGS) *New code is MMS*	7	3	2	3	3	1		2	1	2	2	2	1	0	29	55%
SWMM Storm Water Management Model (US EPA)	8	4	2	3	4	3	2	2	2	2	1	1	2	0	36	68%
DHSVM Distributed Hydrology-Vegetation Model (DOE) Pacific Northwest Lab	7	3	3	1	3	1		1	1	1	1	0	1	0	23	43%
HSPF Hydrologic Simulation Program (US EPA)	8	3	2	2	4	1		1	1	2	0	1	2	0	27	51%
SWRRB Simulator for Water Resources in Rural Basins (USDA)	5	3	2	3	3	2		1	2	1	0	0	2	0	24	45%
MODBRANCH (USGS)	5	3	1	1	2	2		1	2	1	1	0	1	0	20	38%

4.1.1 Physically-based criteria

The first selection criteria listed in Table 4-1 is the model code's level of sophistication, or specifically, the degree to which it is physically-based. This column summarizes the physical capabilities for the primary processes listed in Table 3-2 for each code. MIKE SHE was given a 10 because it has the capability to simulate all physical processes using the most physically-based approach possible. The most significant distinction between MIKE SHE and other codes is how flow within the unsaturated and groundwater zones are calculated. Both of these subsurface processes are considered very important at RFETS in controlling the interaction between surface water and subsurface water.

The Richard's equation and three-dimensional Boussinesq equation are generally considered to be the most physically-based equations currently used for simulating unsaturated and saturated zone flows, respectively. Only the MIKE SHE and TOPOG codes simulate unsaturated zone flow using a one-dimensional Richards-based solution. All of the other codes reviewed, except for ModBranch (USGS), simplify the representation of groundwater flow, typically with a lumped reservoir model. While this approach may be reasonable over large areas, or over long time periods, this approach will not provide detailed information on short-term, localized system response (e.g., hydraulic heads, flow rates).

Both TOPOG and MIKE SHE simulate overland flows explicitly using a kinematic wave approximation, though MIKE SHE simulates flows using a two-dimensional approach. This is seen as a unique advantage over other codes since no assumptions are required for how system flows are routed within the model domain (e.g., sub-basin delineation). Instead, the model will automatically determine how water flows on overland planes based on topographic digital elevation model (DEM) data. TOPOG relies on defining many flow paths based on topographic data, but must rely on this analysis to actually route the water through the system.

Other codes use less physically-based equations. For example, SWRRB, SWAT, HSPF, SWWM, and PRMS all require definition of sub-watershed areas, and use one-dimensional flow equations. SWRRB and SWAT both use the SCS curve method, a well known, but empirical flow equation. This method appears limited for future scenarios, where system responses will not be known beforehand (see Section 1.0). The two-dimensional overland flow feature used in MIKE SHE will likely show much greater functionality for future scenarios where hydrologic divides must be determined prior to simulating the scenario. In some instances, (for example during high precipitation events or flood events), the pre-designated hydrologic divides used in overland planes will not permit flows across these boundaries.

4.1.2 Climate

In codes like SWAT and SWRRB, climate can vary over different sub-basins, but not within a given sub-basin. At RFETS, the precipitation is known to vary significantly over relatively small areas, and surface runoff is known to respond rapidly to precipitation and strongly to its spatial variation. This would likely be a major limitation of these model codes. MIKE SHE permits both the spatial and temporal variation in precipitation, though, its distribution in space is limited to the spatial grid discretization over the model domain. Most codes appear to include snowmelt as an option except for TOPOG and Modbranch. HSPF and DHSVM appear to have the most sophisticated simulation of snowmelt. HSPF includes features that simulate snowdrift as well.

4.1.3 Documented use

All of the codes listed in Table 4-1 appear to have been applied to a variety of hydrologic problems, although most have been applied to basin-scale flow systems that are larger than at RFETS. All of the codes appear to have had extensive applications, not only within the United States, but worldwide. For example, the SWAT model has been applied to a variety of problems (http://www.brc.tamus.edu/swat/swatapp.html) within the United States, including arid/semi-arid environments (Rio Grande/Rio Bravo Watershed). The MIKE SHE model has been successfully applied mostly in international locations, but within the past few years it has been applied to sites within the U.S (see Section 4.2 for more details). TOPOG was developed in Australia, but usage in a variety of applications (water yield, erosion, salinity etc.) is well distributed internationally, with nearly 100 users in North America. Only ModBranch and DHVSM do not appear to have been applied to any significant number of sites. DHSVM has been applied primarily to mountainous areas in the northwestern U.S. (Cascades) where precipitation rates are high. PRMS has typically been applied more often to larger scale hydrologic basins than other codes.

4.1.4 Documentation

SWAT, TOPOG, SWMM, and MIKE SHE all appear to have good documentation to support code use and learning. Theory, data manipulation (input/output), and illustrations are clearly stated in the documentation associated with these codes. Example problems and setup are provided. For being the most data intensive, the HSPF code has the poorest quality documentation of all the codes and is very difficult to understand (Donigian et al, in Singh 1995). The PRMS model documentation provides no information on theory or application, but offers an accurate format for input. The Modbranch code provides basic theory, history, and data input features, but does not go into detailed application of the code.

4.1.5 GIS/Graphical capabilities/animation

The SWAT code has been interfaced with both ArcView (ESRI) and Grass, and provides a strong GIS interface capability. The PRMS code uses the recently developed USGS X-Windows Modular Model System (MMS) feature to provide pre- and post-processing capabilities, although it is uncertain how seamless or reliable this method is. TOPOG also utilizes X-Windows and Motif graphic routines. HSPF is perhaps the weakest of all the codes regarding graphical GIS, or pre- and post-processing capabilities. As a result it is given the lowest score (one pt) for this criterion, because it is probably one of the most data intensive of all of the codes reviewed. MIKE SHE uses ArcView as the basis for most of its graphical interfacing, and has several extensions written directly in ArcView for contouring and data visualization and manipulation. Animations and particle tracking are also features available in MIKE SHE. MIKE SHE animations can be developed showing several graphs and plan view scenarios where parameters change in time.

4.1.6 Technical Support

Technical support is somewhat difficult to assess without direct experience. MIKE SHE ranked highest for this factor, primarily because its initial cost includes rapid and helpful technical support that is confirmed through direct experience with this code. MIKE SHE also has a dedicated group of computer programmers that support worldwide efforts and continued model development. Code modifications for particular issues have been quick and effective. Other codes appear to have training courses and web pages where authors could be contacted, but they likely don't offer the same level of support as MIKE SHE. These were scored a possible two points out of three, while Modbranch, SWRRB, and DHSVM all scored only one point, because none of these appears to support even a web page.

4.1.7 Other Criteria

Other criteria, such as ease of use and WBWG familiarity with the code, internal consistency checking, hardware optimization, other features like chemical transport or sediment erosion capabilities are ranked in Table 4-1, but are not discussed here at great length. Most codes appear to offer advanced features like transport of chemicals, pesticides, or nutrients (general water quality parameters), with the exception of PRMS and ModBranch, which were not designed for this purpose. HSPF, SWMM, and MIKE SHE probably have the greatest number of additional transport parameters. Most codes can be run on various computer operating systems.

4.2 Code selection

Based on the evaluation against other codes (presented below), MIKE SHE will be used to develop the SWWB model. It meets the model-specific criteria best. It also utilizes spatial and temporal data easily and should be capable of providing output to satisfy the SWWB objectives. Based on rankings assigned in Table 4-1, MIKE SHE appeared to have several advantages over other codes reviewed. Of the notable advantages are its GIS capabilities, technical support, documentation, and flexibility in defining boundary conditions and grid resolutions. MIKE SHE also possesses distinct advantages over other codes based on the complexity of the governing physical equations. Additionally, recent efforts by DHI to improve the functionality of MIKE SHE have involved adding various simplifying equations for each hydrologic process, so that the overall computational efficiency of the integrated hydrologic model can be improved.

MIKE SHE represents each of the three main hydrologic processes (surface flow, unsaturated zone flow, and groundwater flow) as well as, or better than, all other codes reviewed. The way in which unsaturated zone, groundwater, and surface water flow processes are treated is discussed below.

Unsaturated zone flow is a very important process at RFETS, because of its strong influence on evapotranspiration, surface runoff, and groundwater recharge. MIKE SHE simulates unsaturated zone flow using a Richards-based equation, which represents the unsaturated zone flow rates and moisture distributions more accurately and realistically than other approaches. Only MIKE SHE and TOPOG use this equation.

Three-dimensional groundwater flow is also represented by MIKE SHE better than the other options. With the exception of ModBranch, other codes treat the groundwater zone as a linear reservoir flow model. At the RFETS site groundwater flow is strongly controlled by three-dimensional aspects of the system (e.g., sloping geologic surfaces, subcropping sandstones, variable-depth weathered bedrock zone).

Surface water is handled better by MIKE SHE than most other codes. It provides for a fully dynamic solution of channelized flow, and accounts for flooding and the dynamic interaction between surface water and unsaturated and/or groundwater zones. This capability provides for more realistic solution of surface flows, stage heights, and groundwater levels, particularly during intense precipitation events. Other codes do not have this complexity available. Furthermore, MIKE SHE allows the user to simplify the surface flow equations, if conditions allow, optimizing computational efficiency. MIKE SHE simulates overland flow as a two-dimensional kinematic wave solution determined by topographic data. This gives it a strong advantage over other codes that pre-process topographic DEMs into either sub-watersheds or streamlines that effectively reduce the overland flow process into a one-dimensional solution. The MIKE SHE code is the only code reviewed that does not require any simplification to solving overland flow and calculates it as a two-dimensional process.

Current U.S. based modeling efforts using MIKE SHE include the South Florida Water Management District, which is applying the code to develop an integrated model for the Caloosahatchee reservoir, primarily to assess strong interactions between groundwater and surface water (http://www.sfwmd.gov/org/exo/cwmp/mikeshe/index.html). MIKE SHE is also being used in an integrated model for the semi-arid Hemet-San Jacinto Valley in southern California, and is being used to model hydrologic conditions within a large scale arid/semi-arid basin flow system, the Black Mesa basin flow system in northeastern Arizona (Prucha, 2000). Various universities (University of Nevada, Reno; Desert Research Institute, Reno, Nevada; San Diego State University, California; Massachusetts Institute of Technology; Cornell; and University of Colorado, Boulder, Colorado) are also using the code for research. MIKE 11 (MIKE SHE's channel flow component, which is also available in stand-alone form) is one of the currently supported hydrologic models within the USBR (http://www.usbr.gov/hmi/hmi.html).

Internationally, MIKE SHE has been used successfully in a variety of applications of variable size and complexity. A comprehensive list of many of these projects is located on the DHI web site (www.dhi.dk). Details of the MIKE SHE code are provided in Appendix A.

4.3 Code verification program

The selected code, MIKE SHE, has been widely used internationally but is less well known in the United States, and is relatively unfamiliar to many workers in the U.S. In addition, benchmarking tests (described in the Work Plan, Section 2.7) have not yet been performed. To increase client, peer reviewer, stakeholder, and public confidence a separate Code Verification Program (CVP) will be implemented. The CVP will consist of, at a minimum, the following three components:

- Verification tests; and
- Dossier of published tests and applications.

4.3.1 Verification tests

This will include three separate tests, in which simulations made using the selected code will be compared with either:

- Established analytical expressions for the simulated condition;
- Published lab/field data; or
- The same simulation run using well-known, long-established, open-code, public-domain software.

The verification tests will separately evaluate the selected code's performance in simulating:

- Overland flow;
- Saturated zone flow; and
- Unsaturated zone flow.

The channel flow module of the selected code (available as a stand-alone code called "MIKE 11") has already been accepted for use by two U.S. Government agencies, the USBR and Federal Emergency Management Association, and is, therefore, considered to be "benchmarked".

4.3.2 Dossier of published tests and applications

In addition, a dossier of 50 internationally-published peer-reviewed papers, describing the operation and numerous applications of the selected code, will be submitted to the site.

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5.0 Future scenarios

The SWWB plans to model five future scenarios, as summarized in Figure 5-1. These future scenarios are a clearly-defined focused set of achievable targets for the SWWB. They are designed to simulate the major changes between current and future conditions in a logical progression, so that the individual effects of specific changes can be evaluated in isolation and in combination. The scenarios to be performed, and the underlying rationale for this approach, are presented below. These scenarios are the highest priority scenarios as determined by RFETS management.

A considerable number of parameters and inputs can be changed within the model, either individually or in combination, to evaluate effects of these changes on the site's hydrologic system. This could represent a very large number of scenarios. The focus of the SWWB scope of work is to meet the primary project objective. Therefore, the most critical future scenarios that can be reasonably simulated within the scope, budget, and time frame of the SWWB project have been identified. The general framework for defining other future scenarios, outside of the present SWWB project scope, is also defined. This provides a useful template for potential application of the SWWB modeling "tool" to other future scenarios.

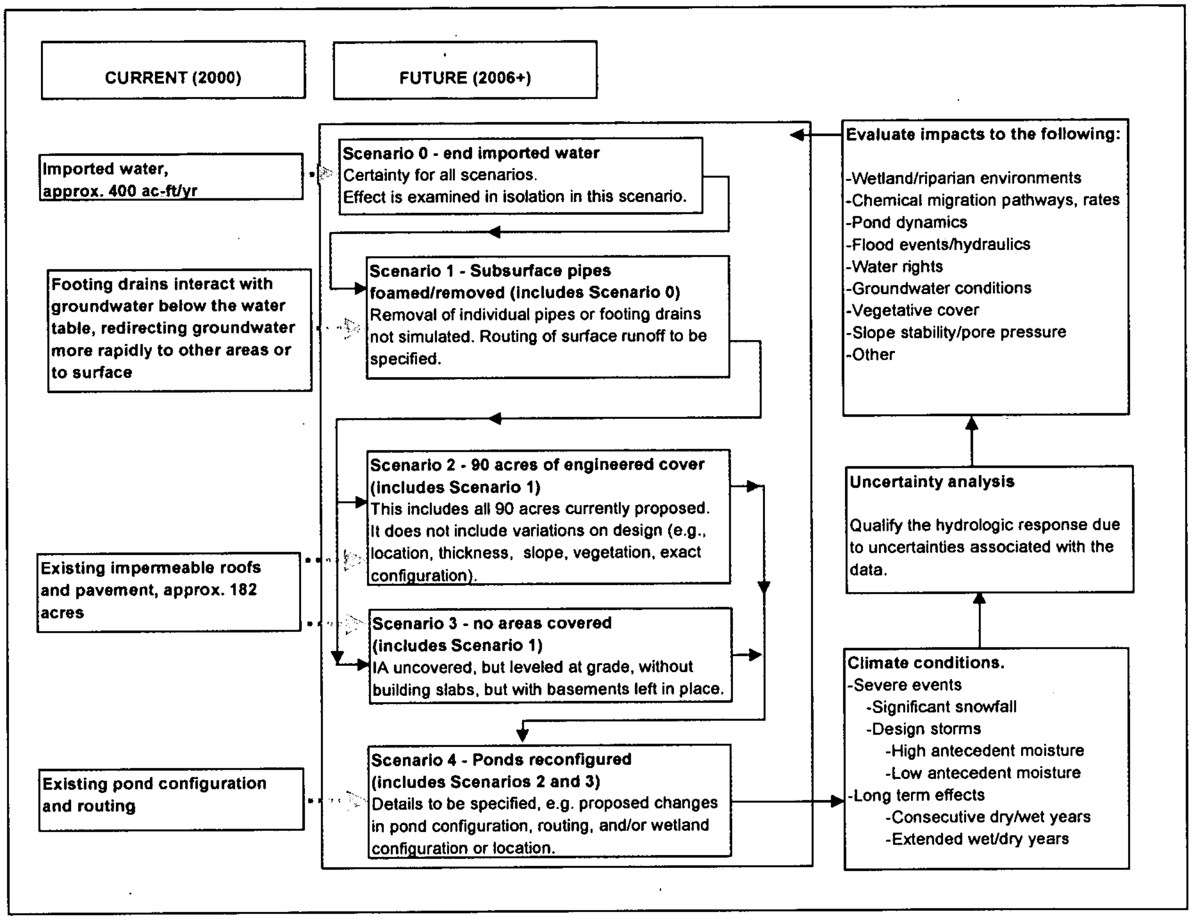
The five future scenarios to be evaluated as part of the SWWB work focus on site-wide objectives rather than on smaller-scale issues. These scenarios also reflect more extreme conditions that are likely to result in the largest change from current and future (closure) hydrologic conditions. In other words, conservative estimates of maximum change are expected from these simulations. Simulating these types of scenarios may eliminate the need to simulate other, less extreme, future scenarios. For example, if the model results indicate that covering a significant area of the IA only has a minimal effect on the downstream hydrologic regime, it can be inferred that less cover would result in even less significant effects. The details of the five scenarios will be coordinated with the RFETS Environmental Restoration Program and the Land Configuration Design Basis Project.

5.1 Scenario 0 – Discontinue imported water

Scenario 0 is to be performed first and is termed Scenario 0 because it is a certain closure condition and will be included in all following scenarios. This scenario consists of discontinuing the import of water (supplied by Denver Water Board) into the RFETS. Initial evaluation of the site water budget indicates that imported water is a significant component of the total inflow to the RFETS hydrologic system. Imported quantities are approximately 400 acre-feet of water per year (ac-ft/yr). Imported water contributes to surface water flow through discharge of used water to the surface water system via the wastewater treatment plant, and contributes to groundwater through piping leakage. After closure, these contributions will no longer exist.

Figure 5-1

Future Scenarios



This situation will be simulated first, because it is anticipated that this change will have a significant impact in reducing surface water base flows, and these results may be useful for planning future pond configurations and surface flow routing important to planning other scenarios. This change may also lower the water table beneath the IA, due to the loss of recharge from leaking pipes.

Scenario 0 is extreme because it incorporates the effect of ceasing all water import. In practice, the volume of imported water will be reduced in stages during the closure process. The effects of these incremental changes may be logically construed to lie between current conditions and Scenario 0.

5.2 Scenario 1 – Subsurface pipes foamed/removed

This scenario includes conditions of Scenario 0. Like Scenario 0, this scenario applies to all further closure scenarios. In this scenario, all subsurface footing drains, storm sewers, and sanitary sewers are either plugged or removed and replaced with backfill material. To consider the most extreme effect of this process, it is assumed that this backfill will be low permeability, equivalent to plugging. Channelized surface runoff that previously would have entered the subsurface storm sewer system will be rerouted; rerouting is to be specified to the SWWB model.

Plugging these pipes will probably result in a higher water table beneath the IA. The current effect of the subsurface conduits is to lower the water table beneath the IA, because the subsurface sewers and drains currently reroute intercepted groundwater from areas of high potentiometric head, either to areas of lower potentiometric head groundwater, or to the surface water system. This is the opposite effect to that in Scenario 0, but may be lower in magnitude, because Scenario 0 results in a net reduction in recharge, whereas Scenario 1 only redistributes the reduced recharge over the same area.

The effect of Scenario 1 on surface water flows is difficult to predict, due to the complexity of the current storm runoff and drainage system. For example, footing drains currently drain groundwater in the IA into the surface water system which is a complex process. Therefore, this scenario will provide useful information on the runoff volumes that need to be rerouted if storm drains are plugged, and will be evaluated for further scenarios in which rerouting is likely to be important.

Scenario 1 is an extreme, because it incorporates the effects of plugging all subsurface piping. In practice, only selected pipes may be plugged. Also, in practice, plugging pipes does not necessarily plug permeable backfill that may surround or underlie the pipes. The effect of these lesser changes may be logically construed to lie between current conditions and Scenario 1, and may be more localized.

5.3 Scenario 2 – 90 acres covered

This scenario includes all conditions of Scenario 1, and will be part of the conditions of Scenario 4. This Scenario will be coordinated with the Land Configuration Design Basis Project. Ninety acres, consisting of selected buildings and other areas in and near the IA, will be covered with an engineered and vegetated surface. The intent of this cover is to reduce infiltration to groundwater at those locations in Scenario 2, which may lower the groundwater table. Design of the engineered cover, and runoff rerouting will also be specified to the SWWB model.

Scenario 2 will simulate the existing buildings and pavement that are included in current conditions (and Scenarios 0 and 1). The existing buildings and pavement make up about 180 acres of effectively impermeable cover. The areas of engineered cover substantially overlap with the existing impermeable cover (i.e., some buildings and pavement will be covered with an engineered surface). The engineered cover may have lower infiltration compared with native soils, but is unlikely to be impermeable.

Scenario 2 is an extreme, because 90 acres of engineered cover is likely to be the maximum area that may be covered. In practice, a smaller area of engineered cover may be installed. The effect of lesser changes may be logically construed to lie between current conditions and Scenario 2, and may be more localized.

5.4 Scenario 3 – Surface regrading

This scenario includes all conditions of Scenario 1. It is planned that this Scenario will be coordinated with the Land Configuration Design Basis Project. In Scenario 3, all existing roads, pavement, and buildings within and near the IA will be leveled at grade and covered with native soil and compatible vegetation. This will remove approximately 180 acres of effectively impermeable cover, which will significantly reduce runoff response to precipitation events and maximize infiltration to groundwater. The east and west access roads and the northern perimeter road will remain. Runoff rerouting, if any, is to be specified to the SWWB model. This scenario will result in a higher groundwater table than Scenario 0 and Scenario 1 (although it may still be lower than current conditions) and will be evaluated for any changes in groundwater flow direction and/or flow rates that may affect the existing groundwater treatment systems.

Scenario 3 will simulate the effects of the building basement foundations remaining lower than three feet below grade, which will likely direct recharge and control groundwater flow in localized areas. This scenario will also provide useful input into planning future pond configurations and surface flow routing for Scenario 4.

Scenario 3 is an extreme, because it considers the maximum recharge over the regraded IA, which may result in a higher water table. In practice, because engineered cover will be added to the regraded area, recharge will likely be less than that predicted by this scenario.

5.5 Scenario 4 – Buffer zone reconfiguration

This scenario includes a combination of conditions of Scenarios 2 and 3, plus the anticipated BZ reconfiguration. Scenario 4 will be coordinated with the Land Configuration Design Basis Project and the Water Management Closure Strategy. Up to 90 acres will be completed with engineered surface cover, and the remainder of the IA buildings and pavement will be leveled at grade. Surface materials, regrading (if any), and rerouting will be specified to the SWWB model. In addition, anticipated reconfiguration actions in the BZ will be included. These may be based in part on the results of previous scenarios and are not currently known. They may include changes in pond configuration, operational routing, and/or wetland configuration.

Scenario 4 includes previous extreme scenarios, but is the most probable of the scenarios because it incorporates a realistic combination of effects, and may be expected to produce less extreme results due to opposing effects of multiple included scenario conditions. This scenario is expected to be the basis for any future applications of the SWWB model.

5.6 Climate scenarios

As shown in Figure 5-1 and described in the Work Plan, all modeled scenarios will be run for a range of climatic conditions. These will include:

- Average conditions (typical long-term climatic conditions);
- Extremely wet conditions (maximum surface and subsurface flow conditions); and
- Extremely dry conditions (minimum surface and subsurface flow conditions).

Model-specified climatic conditions consist of:

- Initial conditions; and
- Boundary conditions.

The Initial hydrologic system (antecedent) state specified for the three climate conditions mentioned above will include the following:

- Groundwater levels;
- Surface water levels;
- Surface soil moisture content; and
- Soil moisture distribution with depth.

Initial conditions are affected by antecedent climate and weather patterns. Each component of the site hydrologic system has a different hydrologic "memory" depending on its internal dynamics and storage capacity. Typically, the groundwater system has the slowest response to perturbations (e.g., precipitation events), while the unsaturated zone exhibits a fast response but can dampen effects on groundwater depending on soil type and depths. Surface water responses (i.e., pond stage and storage, overland flow, and surface channel flow) all respond rapidly to such events. Surface water elements, except for the ponds, have relatively 'short-term' storage capacity compared to the subsurface system.

Initial conditions for each of these components will be established by modeling antecedent events (particularly for the shorter-memory components such as pond storage and surface soil moisture), or by making conservative assumptions based on historic site data.

Different types of boundary conditions will be imposed on the future SWWB model scenarios. These will include the following:

- Rainfall and snowfall;
- Various design event intensities and durations; and
- Average long-term precipitation events (one year).

Overall, the hydrologic system responds quickly to external forcing (e.g., precipitation events) and as such the 'memory' of the system is not expected to last for even a full year (some areas might respond very slowly, but these areas would not be expected to greatly affect the overall system hydrology). Therefore, 1-year simulation times are appropriate for average 'long-term' conditions for a given scenario. These boundary conditions will be applied to the unique combinations of the initial conditions indicated above to create several initial/boundary combinations for each future scenario (0 through 4).

5.7 Scenario implementation

Modeled scenarios will be processed through an uncertainty analysis (varying the most sensitive parameters through a reasonable range) to determine a probabilistic range of predicted results. In conjunction with the climate scenarios, this will provide a large combination of probability-based results. These will be evaluated for specific decisions as described in the Work Plan.

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Appendix A

MIKE SHE description

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MIKE SHE description

The general features of MIKE SHE were presented in Table 4-2. This appendix presents additional information about the code including development history, simplifications, and limitations. The approach to apply MIKE SHE to the SWWB is presented. This supplements the flow chart showing the general modeling approach that was presented in the Work Plan. Details of additional modules for both MIKE SHE and related software are presented last. More specific details on code performance and capabilities can be found at http://www.dhi.dk.

A.1 MIKE SHE code development history

The development of MIKE SHE is summarized in the following table. Fuller details are available from the DHI website.

1975	Code formulated (University of Newcastle, DHI, and SOGREAH)
1975 - 1980	Development/testing, mainly by DHI
1980s	Internal use on DHI projects
1990	First official release of MIKE SHE
1990 - 2000	Continual upgrades and improvements

The MIKE SHE code has been used on about 200 projects in 50 countries around the world, and between 1994 and 1999; 50 articles have been published in the technical literature describing its use, testing, and application.

A.2 General calibration approach using MIKE SHE

- Develop a saturated groundwater flow model under long-term steady-state conditions (calibrate against average annual groundwater surface contours);
- Develop a surface flow model consisting of overland flow and channel flow. This is inherently transient and will simulate various precipitation events. Results will be compared against observed values of flow for target calibration points;
- Develop an unsaturated zone model; and
- Couple each of the hydrologic components.

A.3 SWWB MIKE SHE modules

The main components of MIKE SHE to be used for the SWWB are the pre- and post-processor (PP), the water movement (WM) modules, the particle tracking (PT) module, the MIKE 11 hydrodynamic (HD) module, and the converter for GIS files.

A.3.1 Pre- and post-processor (PP) module

This module handles all data entry and output.

A.3.2 Water movement (WM) module

The Water Movement module (WM) is the core of MIKE SHE. WM contains several process simulation modules which, in combination, describe the entire land phase of the hydrological cycle, including:

- ET;
- Unsaturated zones;
- Saturated; and
- Overland and channel flow (OC), this will be combined with the more sophisticated MIKE 11 (see below) channel flow code, to incorporate floodplains and structures; and
- Irrigation (IR).

A.3.3 Particle tracking (PT) module

The main purpose of particle tracking is to estimate flow paths and transport times in the groundwater. Subsequently, groundwater delineation zones, ground water age and pollution risk may be calculated. This information may be useful for future planning and management. The basic principle of particle tracking is to release a number of notional particles at different locations and times in the model area. The origins of the introduced particles are recorded, and flow velocities calculated in the main water movement module (MIKE SHE WM) are applied to project the flow paths of the individual particles. This is performed for each time step for the duration of the simulation.

When particles are entered with infiltrating water, ground water age may be estimated. For species transport predictions, the random walk method is applied, which includes a deterministic advective term and a deterministic/stochastic dispersive term in analogy to the advection/dispersion equation solved in MIKE SHE AD (see below). This approach provides an estimate of the first appearance of a constituent at a point or receptor.

Alternatively, if only average flow rates are of interest, the dispersive term may be excluded, in which case the calculated flow paths correspond to the mean streamline.

A.3.4 MIKE 11 hydrodynamic (HD) module

The HD module contains an implicit, finite difference computation of unsteady flows in channels. The formulations can be applied to branched and looped networks and quasi two-dimensional flow simulation on flood plains.

The computational scheme is applicable to vertically homogeneous flow conditions ranging from steep stream flows to tidally influenced estuaries. Both subcritical and supercritical flow can be described by means of a numerical scheme that adapts according to the local flow conditions.

The complete non-linear equations of open channel flow (Saint Venant) can be solved numerically between all grid points at specified time intervals for given boundary conditions. In addition to this fully dynamic description, a choice of other flow descriptions is available:

- High order fully dynamic;
- Diffusive wave ;
- Kinematic wave; and
- Quasi-steady state.

Within the standard HD module, advanced computational formulations enable flow over a variety of structures to be simulated, including:

- Broad crested weirs;
- Culverts; and
- User-defined structures.

A number of add-on modules exist for the MIKE 11 Hydrodynamic Module:

- Flood Forecasting Module (FF);
- Dam break Module (DB);
- Structure Operation Module (SO);
- Quasi Steady State Module (QSS); anD
- Advection-Dispersion Module (AD).

The AD module is based on the one-dimensional equation of conservation of mass of a dissolved or suspended material (e.g., salt or cohesive sediments). The behavior of conservative materials that decay linearly can be simulated. The module requires output from the hydrodynamic module, in space and time, of discharge and water level, cross-sectional area and hydraulic radius. The advection-dispersion equation is solved numerically using an implicit finite difference scheme, which has negligible numerical dispersion. Concentration profiles with very steep fronts can be simulated accurately. The module includes a description of the erosion and deposition of cohesive sediment. Erosion and deposition are modeled as source/sink terms in the advection-dispersion equation. Whereas the erosion rate depends primarily on the local hydraulic conditions, the deposition rate depends also on the concentration of suspended sediment.

Finally, it is possible to simulate erosion, transport, and deposition of non-cohesive sediments with the AD module. Here the transport of the suspended sediment is described with the advection-dispersion equation, and the erosion and deposition terms are described by conventional sediment transport formulations. Both the Advanced Cohesive Sediment Transport Module (ASC) and the Water Quality Module (WQ) are add-on modules, which require a functioning AD module.

A.3.5 GIS converter

The GIS coverter allows ArcView GIS data to be imported and exported. This will allow for the extensive ArcView coverages available for the site to be used as direct input to the model. The ArcView compatibility of MIKE SHE and MIKE 11 is an extremely valuable feature for use at RFETS because so much of the environmental data at RFETS is in the form of ArcView coverages. It also makes MIKE SHE a strong planning tool in its own right.

A.4 Potential additional modules

Additional modules for MIKE SHE and MIKE 11 have been developed and are available from DHI. When installed, they create optional program switches that can be turned on and off to include or exclude specific processes or effects. While it is not planned to use these for the SWWB project, they illustrate potential applications of the final model outside of the SWWB, and additional functionality of the MIKE SHE group of codes. For example, modules are available to simulate particle tracking in all hydrologic zones (i.e., groundwater, unsaturated zone and surface flows), chemical transport (advection/dispersion), water quality associated with surface flows, geochemistry (PHREEQC-based equilibrium model), sorption, and degradation. A brief summary of some potentially useful modules follows.

A.4.1 Advection/dispersion (AD) module

Based on the flows computed by MIKE SHE WM, the MIKE SHE AD module simulates distributed concentrations of dissolved species in overland flow, rivers, the unsaturated

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zone, and groundwater. In integrated studies, this module accounts for the migration of contaminants from surface water to subsurface water or vice versa. It is possible to include various types of point or area chemical impact sources with a fixed or time-varying chemical load in the model. The advection/dispersion equation is solved by an explicit scheme (QUICKEST). A simpler alternative to performing full transport simulations is the application of the particle-tracking module (MIKE SHE PT).

A.4.2 Geochemistry (GM) and biomass (BM) modules

The geochemistry module (GM) includes equilibrium calculations for the following reactions:

- Ion exchange;
- Complexation;
- Mineral precipitation and dissolution; and
- Redox reactions.

The processes are modeled as equilibrium reactions using the PHREEQC program. A full description of the core program can be found at http://h2o.usgs.gov/software/phreeqc.html.

A related biomass module (BM), which can run simultaneously, simulates biodegradation (respiration or fermentation) reactions for the breakdown of organic chemicals. The BM module represents the sequential use of electron acceptors (oxygen, nitrogen, iron, manganese, sulfur, and inorganic carbonate), growth of microorganisms, nutrient availability, and environmental limitations (temperature, pH, and other species concentrations). Degradation follows Monod/Michaelis-Menten degradation kinetics. Growth in biomass and in daughter-product concentrations is accounted for, and co-metabolic or inhibited systems can be represented.

A.4.3 Sorption/degradation (SD) module

The SD module includes the following features:

- Water flow and solute transport in both the saturated and unsaturated zone;
- Attenuation, retardation, and degradation using the standard advection-dispersion equation, including decay and sorption;
- Sorption - equilibrium sorption isotherms include linear, Freundlich, and Langmuir and kinetic sorption isotherms are also available;
- Dual porosity sorption (i.e., macropore effects);
- Decay - biological, radioactive, or other are described by a first-order degradation process, which can be dependent on soil moisture and soil temperature; and

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- Plant uptake of solutes.

A number of processes relevant for simulating reactive solute transport in a simple manner have been included in MIKE SHE. These processes include water and solute transport through preferential pathways. The physically-based description of macropore flow assumes a secondary pore domain through which water is routed separately as gravity flow, but within which chemical exchange with the surrounding bulk (or matrix) porosity is possible. Sorption of solutes is described by either equilibrium sorption isotherms (Linear, Freundlich, or Langmuir) or kinetic sorption isotherms, which can also include effects of hysteresis in the sorption process.

In situations where preferential flow is considered, it is possible to distribute the available sorption sites unevenly between the soil matrix and the macropore porosity. Attenuation of solutes is described by exponential first order decay, influenced by soil temperature and soil moisture content. Degradation of solutes transported in a macroporous media with diffusion from and to the soil matrix may be different in the two domains (e.g., due to differences in oxygen availability). For this situation, it is possible to specify a different half-life of the solute for each domain. Plant uptake of solutes is described as passive transport along the transpiration stream.

A.4.4 Underground sewer flow (MIKE MOUSE)

Future modifications include adding features of the MOUSE code to MIKE SHE; this is expected to be released in the Spring 2001. This will permit pipe flow in sewer lines to be simulated simultaneously with MIKE SHE.

A.4.5 Water quality (WQ) module

The water quality module (WQ) is coupled to the AD module and simulates the reaction processes of multi-compound systems including the degradation of organic matter, the photosynthesis and respiration of plants, nitrification, and the exchange of oxygen with the atmosphere. The mass balance for the parameters involved are calculated for all grid points at all time steps using a rational extrapolation method in an integrated two-step procedure with the AD module. A number of additional modules have been developed describing:

- BOD-DO relationships;
- Nitrification;
- Bottom vegetation influences;
- Sedimentation and resuspension; and
- Oxygen consumption from reduced chemicals.

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- Oxygen consumption from reduced chemicals.

Two add-on modules are available for the Water Quality Module:

- Water Quality Heavy Metals Module (WQHM); and
- Eutrophication Module (EU).

A.4.6 Sediment transport (ST) module

The non-cohesive sediment transport module (ST) can be used to study the sediment transport and morphological conditions in rivers. Features include:

- Five models for the calculation of sediment transport capacity:
  - Engelund-Hansen;
  - Ackers-White;
  - Engelund-Fredsøe;
  - Van Rijn; and
  - Smart-Jaeggi.
- Sediment description by an average particle size and standard deviation of the grain size distribution;
- Explicit (no feedback with HD);
- Morphological (with feedback via sediment continuity and bed resistance) models; and
- Output of sediment transport rates, bed level changes, resistance numbers and dune dimensions.

An add-on module (GST) is available for simulating transport of graded sediments.

A.5 Simplifications

The authors of MIKE SHE acknowledge that using a physically-based distributed parameter code like MIKE SHE can be very data intensive and computationally complex (compared to a code like MODFLOW). As a result, they have made a noteworthy effort to provide simplifications for the main hydrologic processes simulated – surface water, unsaturated zone, and groundwater flows. These simplifications permit the user to develop the integrated model in increasingly more complex stages before full implementation. For example, the groundwater system can be greatly simplified, or even eliminated from a surface flow simulation, allowing the surface flow details to be evaluated without the additional complexity of the groundwater system. Once a stable configuration for the surface flow is established, the groundwater system can be incorporated. In this fashion, numerical instabilities caused by poorly constrained conceptual models or initial parameterizations can be reduced. The ability to avoid such instabilities can save considerable calibration and simulation time.

A.6 Limitations

- Resolution may be limited due to computational inefficiency. The result may be to increase model cell size;
- Numerical instabilities may limit the ability to simulate certain dynamic conditions.
- The unsaturated zone assumption of one-dimensional flow may be limiting along steep slopes, or near the edge of paved areas or structures;
- Some simplifications are not available (e.g., the Green-Ampt solution);
- Snowmelt is treated relatively simply; and
- The code is relatively expensive (about $10,000) compared with more familiar less-sophisticated groundwater codes.