MIKE SHE Code Verification and Validation for RFETS Site-wide Water Balance Model

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1.0 INTRODUCTION

After review of a number of computer codes, MIKE SHE (developed by the DHI-Water and Environment [DHI]) was selected to build a Site-wide Water Balance (SWWB) Model of the Rocky Flats Environmental Technology Site (RFETS or Site). To establish the suitability of the code and its ability to simulate the hydrologic processes that were identified in the conceptual model, a code verification and validation study was conducted. This report will summarizes code verification and validation testing of MIKE SHE code. These tests were designed to evaluate its performance and appropriateness for application at RFETS. This report is prepared by Dr. Tissa H. Illangasekare at the Colorado School of Mines in Golden, Colorado with the assistance of Mr. Robert Prucha of RMC Consultants. Dr. Torsten Jacobsen and Mr. Douglas Graham of DHI were responsible for the implementation of the validation simulations required in the testing.

In the development and application of the SWWB model, generally accepted methods and protocols are used. These include verification of the code, establishing the validity of the code and "*calibrating*" the model developed using the code for site-specific conditions. To avoid confusion with the terminology, appropriate working definitions are provided in this report. The focus of this report is on the <u>verification and validation of the code</u>. As a part of this effort, the equations/numerical methods that are used in the design of MIKE SHE code will be reviewed to evaluate their ability and appropriateness to represent the primary hydrological processes that are relevant to conditions at RFETS. The code verification is done by evaluating the code's ability to simulate setups that represent Site conditions. With proper assumptions and simplifications these can be solved using analytical methods (or closed form analytical solutions). As such analytical solutions do not exist for all the interactive processes between different components of the code, a validation methodology that rely on semi-quantitative evaluation of results from a set of test problems is presented. The code is also bench marked against other existing codes.

2.0 TERMINOLOGY

A "*model"* is a simplified representation of a physical *system*. A hydrologic model is always a simplified representation as it is not possible to reproduce the exact behavior of hydrologic systems that are very complex by their nature. The goal in developing a model is to use it as a tool to make predictions through "*simulations"* on how the modeled system is expected to behave when different *"excitations"* are applied on the system.
In this application, system refers to the hydrologic system whose components include the natural streams, canals, ground surface on which overland flow occurs and the unsaturated zone (UZ) (vadose zone) and saturated zone (SZ) of the subsurface. These components are in continuous dynamic interaction requiring the model to capture and simulate the integrated behavior the system.

The primary goal of the study at RFETS is to develop a water balance management tool to evaluate how the local hydrologic cycle is expected to change from current conditions as a result of various scenarios that will define the final Site configuration. The model in this case becomes a decision making tool that will be used to simulate the system response to different management scenarios. These scenarios will affect the model excitations and/or change the model parameters. The reliability and accuracy of the model predictions rely on how accurately the model captures the underlying natural processes of the hydrologic system. The term *"validation"* is widely used to define this process of testing models. However, because of the inadequacy of data in different spatial and chronological scales needed to understand, quantify and characterize all processes to be represented in hydrologic models, the question has been raised on whether such models could be validated. Oreskes and Beltiz (2001) states, "*validation is still widely used in ways that asserts or imply assurance that the model accurately reflects the underlying natural process, and therefore provides a reliable basis for decision-making*". The same authors, referring to reasoning by Konikow and Bredehoeft, 1992 and Oreskes et al, 1994, state that the usage of the term validation is misleading as models can not be validated. However, in the general modeling context as well as for groundwater modeling, definitions for model verification and validation have been provided (Schlesinger et al., 1979; Konikow, 1978; Tsang, 1991 and Anderson and Woessner, 1992). These definitions are used in a sequence of steps in hydrological model applications that is often referred to as a modeling protocol (Refsgaard, 1996). With the expectation that such a protocol will be used in the SWWB model development and application, a terminology for verification and validation is provided. These terms are largely similar to those proposed in the EPA guidelines (EPA, 1997), and with Anderson and Woessner (1991).

To introduce the terminology specific to integrated hydrologic models, it is necessary to provide clear and consistent definitions for *code* and *model* that will be used in this report. "*A code is a set of programming statements that solves the mathematical equations describing the flow processes in different components of the hydrologic system"*. In most hydrologic codes designed to simulate spatially- and chronologicallydistributed processes, the mathematical equations are first converted to a set of algebraic equations (linear or non-linear) using numerical methods that rely on spatial discretization of the solution domain. The most commonly-used numerical methods are finite differences and finite elements. Code by its definition is generic in the sense that it can be applied to any hydrologic system whose conceptual model requires the simulation of flow processes that are represented in the code. Refsgaard (1996) defines conceptual model as *"verbal descriptions, equations, governing relationships, or 'natural laws' that purport to describe reality."* A "*model*" on the other hand is designed for specific site conditions using a generic code. The specificity for a site comes from the incorporation of parameters of the site and its boundary conditions specific to the site. Hence, a model simulates the response of the hydrologic system to various excitations or stresses that are applied at the site. Figure 1 schematically shows how a code is used to develop a model. It should be noted that in the case of an integrated hydrologic code such as MIKE SHE, the code is developed by integrating (or coupling) independent modules that solve the governing mathematical equations of the primary components of the hydrologic systems (e.g. surface flow system, SZ, UZ, etc.).

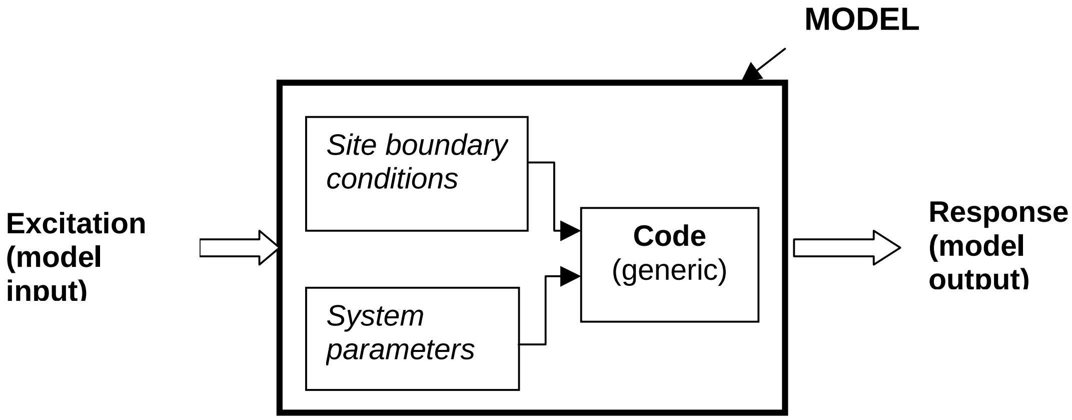


Figure 1: Definitions of code and model

The following working definitions are provided for code verification and code validation. This report will only address code verification and code validation. *"Model validation"* will not be considered, but will be performed as part of the RFETS SWWB Integrated Modeling effort using actual Site data. The overall approach that will be used in the numerical code validation is summarized in Figure 2.

(1) Code verification:

The process designed to establish that a generic code accurately solves the mathematical equations that describe the basic processes of the physical system. The standard approach of verification uses the code to simulate conditions for with simplifying assumptions (e.g., homogeneous parameters and simple geometry) are made

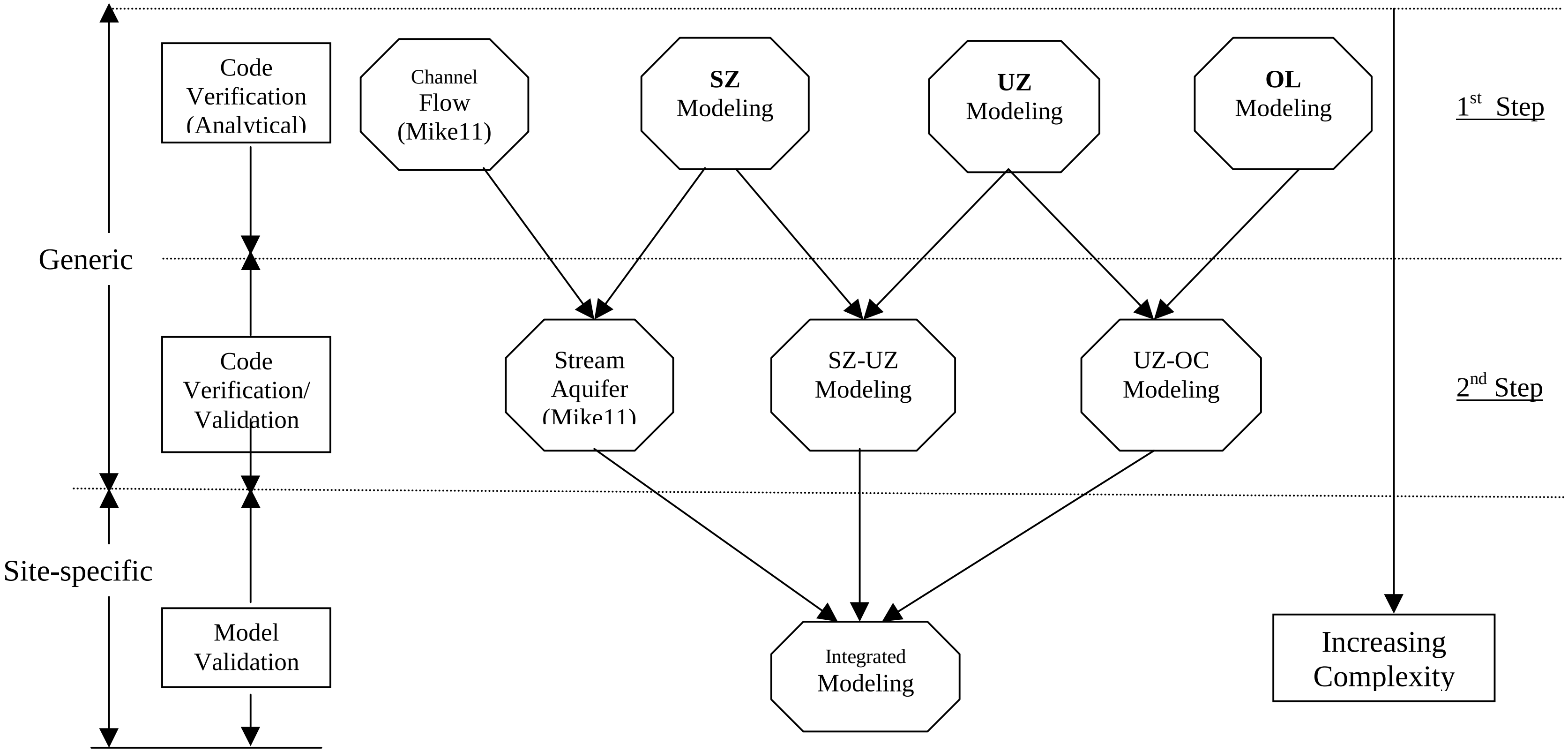


Figure 2. Code Verification and Validation Approach

Type of Verification

MIKE SHE Hydrologic Process/Processes

Description:**SZ** -- Saturated Zone Flow **UZ** -- Unsaturated Zone Flow **OL** – Overland to obtain closed form analytical solutions to the equations of the mathematical model. This approach does not evaluate whether the mathematical equations used in the code best represent the physical process, as the code and the closed form analytical solutions solve the same equations. It only checks whether the algorithms used to convert the mathematical equations to algebraic equations are solved with an acceptable accuracy and any coding errors (or programming "bugs") are introduced in the process.

(2) Validation of integrated code:

In this study, validation of integrated code is defined as the process of establishing whether the different components of the code are coupled properly to simulate the dynamic interactions accurately to represent the integrated behavior of the hydrologic system. For all possible cases of interaction between different modules of the code simulating the primary components if the hydrologic system, closed form analytical solutions do not exist. Ideally, the integrated code could be validated using either comprehensive field data or controlled laboratory data sets. In the absence of such data for validation of a generic code for its general applicability for all possible and anticipated field conditions, a code validation approach needs to be proposed.

3.0 MIKE SHE CODE REVIEW

The selection of MIKESHE, as the most appropriate code for the RFETS SWWB Integrated Modeling effort, is presented in the Model Code and Scenario Selection Report (Kaiser Hill, 2001). In this section, a review of equations/numerical methods used in MIKE SHE is presented evaluate whether it uses appropriate methods to represent the primary hydrological processes and the conditions of the Site.

According to MIKE SHE user's manual, the code has been designed with modular programming structure comprising of six process-oriented components, each describing major flow processes of the hydrologic cycle. Five of them are listed as: (1) Interception/evapotranspiration (ET); (2) Overland and channel flow (OC); (3) UZ; (4) Saturated zone (SZ); and (5) Snow melt.

This review is for four primary components of the code that are central to the proposed SWWB model. These include: (1) overland flow, (2) channel flow; (3) UZ of aquifer; and (4) SZ of aquifer. Where appropriate, the methods used in coupling of some of these components are also reviewed and commented on.

3.1 Overland Flow

The overland flow module is based on a kinematic wave approximation of the Saint Venant Equation. This equation, written for a two dimensional plane (x-y), fully describes the overland flow. Kinamatic wave approximation of Saint Venant Equation results in expressions that relate the flow velocities to depth of flow and ground surface elevation. Strickler coefficients defined for both x and y directions over the flow plane become the model input parameters.

Kinematic approximation is commonly used in the modeling of overland flow for its ability to simplify the input parameters. Complete solution of Saint Venant Equation without simplifying assumptions will need data for characterization processes that are not readily available. Use of a single parameter (Strickler coefficient) to characterize overland flow simplifies the solution of the overland flow processes at RFETS. These coefficients can be used as calibration parameters.

The simplified flow equations are solved using the finite difference method. This is an acceptable solution method that is used in the solution of flow equations. As an implicit method is used, the solution is unconditionally stable, thus allowing for the selection of any spatial and time discretization. However, as the relation between discharge and depth of flow is non-linear, second order terms in the Taylor series (a higher order term in the finite difference approximation of the first derivative that is generally truncated) are included for the correction of water levels. The method as used may produce internal mass balance errors. The methodology that is used to avoid these errors seem to place conditions for the selection of Δx, Δy and Δt. Also, in some cases the initially-calculated outflow has to be reduced by a factor of 0-1. The length of simulation time step is automatically reduced, when rapid changes occur in rainfall. The time stepping procedure prevents the solution from becoming unstable. The user manual presents the algorithm that is used to couple the overland flow and the SZ. Under normal conditions, the overland flow and the SZ are coupled through the UZ. That is, the depth of flow computed by the overland flow model is used as a boundary condition in the UZ model. The UZ equation is solved to provide the time-varying soil water distribution and compute the rate of infiltration that produce recharge to the SZ. In situations where the UZ from the ground surface to the water table becomes fully-saturated, MIKE SHE disables the UZ calculations. This situation can occur at RFETS close to the streams and at locations where the water table is shallow. Under these conditions, when there is ponded water on the ground surface, the vertical hydraulic conductivity of the upper layer of the SZ is used to estimate the recharge rate (application of Darcy's law using the saturated hydraulic conductivity and the gradient of head between the ground surface and the ground water table). In the RFETS application, caution should be exercised in selecting the appropriate hydraulic conductivity as the value based on the top layer of the SZ may not be representative of the conditions of the soil close to the ground surface. The manual suggests the use of a leakage coefficient that could be determined during calibration. If this option is used, it is important to check whether these leakage coefficients are compatible with the condition of the soil (soil type, macropores, etc.).

In summary, MIKE SHE uses generally accepted mathematical representation of the flow processes and numerical solution methods for the modeling of the overland flow. Attention should be given when the UZ become fully-saturated to determine what parameters need to be used to describe the recharge process to the ground surface and affects overland flow (such as near streams and seeps).

3.2 Channel Flow

The original channel flow module of MIKE SHE adopts the diffusion approximation of the Saint Venant equation. The MIKE SHE version that is used in the REFTS water balance model contains the river module MIKE 11 HD that has all the capabilities of the original module as well as additional features that allow for higher order fully-dynamic wave approximation of the Saint Venanat equation. MIKE 11 HD allows for the inclusion of a suite of hydraulic structures and has the ability to simulate flood plains. This version also allows for the full dynamic coupling of the surface and subsurface processes. All these features make it possible to use MIKE SHE to simulate the surface flow component at RFETS. In this section we will review the methods used in MIKE SHE to couple the channel flow to other surface flow components and the subsurface.

3.2.1 *Lateral inflow into river*

At many locations along the main flow channels in REFTS, the overland flow will supply lateral inflow to the stream network. The code estimates the lateral flow to a segment of the river using thewater level of the grid cell adjacent to the river and the river bank elevations described by the river section.

3.2.2 Surface water and aquifer exchange

Two options for water exchange between the surface water and aquifer are considered: (1) river-aquifer exchange where the river is considered as a line source and (2) an area-inundation flood plain approach used for wide rivers (flood plains), lakes etc. Both these conditions exist at REFTS.

The river-aquifer flow is calculated using a conductance and the head difference between the river and the aquifer. This approach is similar to that is used in the river module of MODFLOW. Three options are available for estimating the conductance. The first option (option A) assumes that there is no clogging layer at the river bottom and the flow resistance only comes from the soil in the SZ. In the second option (option B), the flow resistance in a clogging layer and the underlying aquifer are considered. The third option (option C) allows for the flow resistance only in the clogging layer. At RFETS, either options B or C could be used. In using options A and B, it will be necessary to use the hydraulic conductivity of the soil in the SZ. If grid refinement is not performed close to the river, the saturated conductivity (estimated during calibration) of the underlying cell should not be used as the river exchange will be controlled by a hydraulic conductivity local to the river. For the options B and C where a clogging layer is assumed, its hydraulic conductivity should be determined during calibration. In most practical situations, data for the leakage coefficient that represents the permeability of the river lining does not exist and hence should be treated as a calibration parameter.

To determine the infiltration from flood plains, the user needs to delineate areas that may be flooded. The locations that have been identified as inundation grid points gets flooded when the water levels are above the ground surface. The exchange rate is calculated using a Darcy's law approximation similar to what was adopted to estimate recharge in overland flow module. The comments that were made with respect to the proper use and selection of the parameters in the overland flow-SZ coupling are also relevant in this case.

3.3 Unsaturated zone

The UZ processes play a critical role at RFETS because it couples the surface flow system to the SZ. Even though the UZ does not store significant volume of water, it acts as a conduit for water flow. The dynamics of how the water table responds to precipitation, evaporation, and surface flow depends on the UZ flow and storage processes. As the flow in the UZ is primarily vertical, MIKE SHE uses the one-dimensional unsaturated flow equation (Richard's Equation). Accurate solution of this equation to simulate unsaturated flow in response to short duration precipitation events requires the use of small computational time steps. As this non-linear partial differential equation in some cases has to be solved at all grid cells, the UZ module may become most computing intensive component of MIKE SHE. The code offers a computationally-efficient option that provides a simplified solution to the Richard's equation. In this simplified formulation, the capillary (or tension) terms are neglected thus assuming only gravitational forces control flow. This may have implications on the accuracy of the model in simulating semi-arid zone conditions that exists at REFETS.

The input parameters needed in the solution of Richard's equation are: (1) soil moisture retention function (capillary pressure versus water content); and (2) unsaturated hydraulic conductivity function (partially saturated hydraulic conductivity versus water content). In most models of unsaturated flow Brooks-Corey (1964) and/or Van Genuchten (1980) models in combination with pore network model by Burdine (1953) or Mualem (1976) are used to provide these inputs. The fitting parameters of the Brooks-Corey or Van Genuchten models are used with Burdine or Mulalem models to obtain the unsaturated hydraulic conductivity functions. MIKE SHE uses similar functional relationships as Burdine (1953) or Mualem (1976), but a parameter *n* that defines this relationship has to be estimated during calibration. The retention function is provided independently in the form of table (interpolated using cubic splines). As the parameter *n* in MIKE SHE is not related to the retention function, the calibrated *n* may be incompatible with the retention function of the soil (during the progress of the study, MIKE SHE was updated to include tabular values for the effective conductivity relationships). MIKE SHE can only handle monatomic retention functions that will not allow for the modeling of hysteresis.

MIKE SHE uses a fully-implicit finite difference formulation to solve the Richard's equation. This technique provides stable solutions that converge. Two types of boundary conditions at the soil surface can be simulated: (1) constant flux; and (2) ponded water. The transition from one type of boundary condition to the other can also be simulated. These conditions exist at RFETS. The lower boundary condition is a specified pressure as determined from the elevation of the water table. It is expected that the vadose zone simulation results will be sensitive to the initial conditions (this determines the antecedent moisture conditions in the soil profile before a storm event). MIKE SHE assumes equilibrium soil moisture pressure profiles as the initial conditions. The retention function of the soil has to be used get the moisture content from the assumed hydrostatic pressure distribution. In heterogeneous systems, it may take very long time periods for the soil profiles to attain hydrostatic conditions. However, the re-initialization capability of UZ component allows for the generation of non-equilibrium initial conditions that may occur for the conditions at RFETS.

For the full coupling of the surface water system to the SZ, the UZ may have to be simulated in all grid squares. Use of small time steps and spatial discretization to get accurate solution to the non-linear equations results in long computational time. A feature in MIKE SHE allows for the lumping of grid cells with homogenous physical characteristics. Caution should be exercised in using this feature at REFTS in areas where the ground slope changes and in zones where the water table fluctuations are different.

One of the most critical processes that need to be represented accurately in the REFTS water balance model is the coupling of the UZ and SZ. The recharge to the water table determined by how the code algorithm solves the unsaturated flow equations (soil moisture distribution or head) while the water table is fluctuating as a result of recharge. The developers of MIKE SHE have recognized this and have employed an iterative procedure that tracks the mass balance in the unsaturated column. In the scheme used, the coupling is done between the entire UZ column and the uppermost calculation layer of the SZ. It is not clear from the documentation in the manual how the coupling is performed if a situation occurs where the water table drops below the bottom of the uppermost SZ layer. However, the coupling appears to be rigorous enough to capture the dynamics through the use of small computational time steps. At RFETS the groundwater table fluctuates across a number of geologic model layers. Hence, in the semi-quantitative evaluations a problem was developed to evaluate the code's coupling performance for this condition.

The simplified solution to Richard's equation ignores the tension terms. This simplification makes the numerical scheme more efficient by allowing for the selection of larger time steps and computational cells. Neglecting the capillary terms will not allow the model to capture the dynamic UZ processes accurately. Hence, this option should be used with caution at REFTS, as coupling of surface systems to SZ that occur through the dynamics in the UZ has to be modeled accurately.

3.4 Saturated Zone

The SZ module of MIKE SHE simulates three-dimensional groundwater flow under both unconfined and confined conditions. An implicit finite difference scheme is used in the numerical solution of saturated groundwater flow equation (Boussinesq equation). Implicit solution schemes allow for the use of any grid size and computational time steps without affecting convergence and stability of the solution. The formulation and solution schemes are closely similar to the saturated groundwater flow simulator MODFLOW, developed by the US Geological Survey (USGS). MODFLOW is well-accepted as a simulator. As the SZ component is very similar, in this report we will not provide a separate review. Later in the report benchmark tests will be performed comparing MODFLOW with SZ component of MIKE SHE.

4.0 CODE VERIFICATION

The objective of this task is to verify whether the mathematical equations are solved accurately using the stated numerical methods. Four primary code components will be verified, specifically: (1) code simulating the SZ processes; (2) code simulating the UZ processes; (3) code components simulating overland flow processes; and (4) code for channel flow. Even though a large number of other secondary (but important) processes are simulated by the code, the code accuracy as determined by the errors in the numerical solution schemes will likely be of most significance for the model performance.

Several MIKE SHE code verification tests were identified. These test cases are analytical solutions selected from a verification test matrix. The matrix listed many different potential test problems that could be used to verify the code against. However, only a subset of these problems was selected to meet the needs and time constraints of the RFETS project. These test problems with some of system characteristics at REFTS were provided to DHI. DHI conducted the simulations and the simulation results were provided in a report prepared by them (Appendix A). In the main text of this report, we will only summarize the analysis of the results of the tests that are presented in detail in Appendix A.

4.1 Verification of SZ module

Three test problems were used to verify the ability of the SZ module of MIKE SHE to solve the saturated flow equation. A close match of steady and transient solutions will demonstrate that the numerical approximation of the saturated flow equation is accurate and the algorithm used to march forward in time to solve the transient behavior is working correctly. Also, this verification test will check the solution accuracy of the method used to solve the linear system of equations.

4.1.1 A single well pumping in a homogenous aquifer bounded by a river

A closed-form analytical solution to calculate the transient piezometric head in a semi-infinite aquifer bounded on one side by a stream (constant head), due to pumping from a single pumping well is available (Theis, 1941 and Hunt, 1999). Both steady-state and transient head distributions were simulated and compared with the analytical solution. The match between MIKE SHE and the analytical solution for steady-state flow was found to be almost exact. The maximum error in the transient drawdown calculated at an observation point half way between the pumping well and the stream was found be by 1 mm (i.e. 0.01 % of saturated thickness). The maximum error at a point closer to the stream (1/10 the distance between stream and well) was less than 1 cm (i.e. less than 0.1% of saturated thickness).

4.1.2 A single well pumping in a homogenous aquifer bounded by a river with a semi-permeable boundary.

A similar comparison was done for this as for the previous case. Only steady-state solutions were compared. The match was very close with errors ranging from 2-3 cm (0.2 –0.3 % of saturated thickness) close to the stream and 1-2 cm rest of the aquifer.

4.1.3 A single well pumping in a circular island

A steady-state solution for a case where a well is pumping in an circular aquifer with a constant head boundary condition was available. In addition to the pumping, a steady recharge is applied on the ground surface. The code simulated and the analytical solution matched closely except at points close to the well. This is expected as the closed form solution assumes that the well is a point singularity (well with zero radius), Where as, the finite difference formulation used in MIKE SHE, the well is represented as a uniformly distributed withdrawal (negative recharge) over a grid cell (100 m x 100m). This suggests that the code computed drawdowns in cells where there is a pumping well, should not be used to predict the point drawdowns within the cell. However, if an accurate drawdown is needed, a finer grid system could be superposed (grid refinement).

The results of the above comparisons verify the computational accuracy of SZ module of MIKE SHE. It should be noted that in the first example it is assumed that the drawdowns are small compared to the saturated thickness of the aquifer (transmissivity remains constant with time).

4.2 Verification of UZ module

Closed form solutions that are of interest in this case are solutions to the one-dimensional Richard’s equation. The analytical solution used in this verification exercise uses a simple analytical model by Gardner (1957) to define the unsaturated hydraulic conductivity as a function of pressure head. One empirical fitting parameter defines this functional relationship. Where as, UZ module in MIKE SHE as in other similar codes use a hydraulic conductivity versus water content (or pressure) and pressure versus water content (retention function) as code inputs. In this case more than one parameter characterizes the inputs. To use MIKE SHE to compare with the analytical solution for a one-dimensional infiltration problem, it is necessary to obtain a relation between the fitting parameter of Gardner model and the fitting parameter n of MIKE SHE. The approach that was used attempts to fit the best value of n for the Gardner model. The comparison of the curves shows that only the pressure head values match at low suction values. A modification was made to input the Gardner model in tabulated form (instead of using the fitted n) in to MIKE SHE. The results as presented were generated using this modified version.

Infiltration of water through a one-dimensional homogeneous soil column was simulated. A flux boundary condition at the soil surface produces unsaturated and unsteady infiltration through the column. The code simulation and the analytical solution matched exactly for both hydrostatic conditions (zero flux at the soil surface) and with boundary flux. The results of this test verify that the UZ model solves the steady state infiltration problem accurately. However, it should be noted that this test does not verify the accuracy of modeling of transient behavior. The stability of the solution can only be verified by conducting a test under transient conditions. Ability to model transient behavior of soil moisture profiles is important at REFTS as the groundwater recharge from storm events is sensitive to antecedent soils moisture conditions.

4.3 Overland Flow

An appropriate analytical solution was not available for the verification of the overland flow module. However, this model component was tested as a part of semi-quantitative analysis.

4.4 Coupled processes

Closed form analytical solutions to some of the coupled processes between different components of the hydrologic system are available. Three such solutions were selected for the following cases: (1) stream and aquifer; (2) overland flow and UZ; and (3) lake and SZ.

4.4.1 Stream/aquifer coupling

Hunt (1999) provided an analytical solution for transient drawdown due to pumping in an aquifer with a stream represented as line source (river loosing or gaining water due to the coupling). The pumping from the well lowers the water table at the river and the head gradient between the river and the aquifer produces leakage. The model was setup by the SZ component of MIKE SHE to the channel flow model MIKE 11. The river/aquifer exchange option where the leakage is calculated using a leakage coefficient of the river lining was used. The steady-state and the solution for the drawdown 23 days into the simulation were compared. They showed perfect agreement with the analytical solution. The transient drawdown at an observation point 50 m from the pumping well was compared. The analytical solution and MIKE SHE again showed close agreement (maximum error less than 0.01% of saturated thickness).

The verification exercise tests the coupling of the flow exchange between the river and the aquifer. However, it should be noted that this test does not evaluate the full dynamic coupling of the two components as the analytical solution assumes that the water level in the river remains constant. In a fully-coupled system, the river stage has to be adjusted for the gain/loss into the river. MIKE SHE when coupled with MIKE 11 has this capability, but this verification test does not evaluate this feature.

4.4.2 Lake and unsaturated zone coupling

An analytical solution for the three-dimensional, steady-state flow to a hemispherical lake in a confined, homogeneous aquifer with a uniform regional gradient and infinite extent and depth was available (Kacimov, 2000). This test case is suitable for testing the interaction between large body of surface water and an unconfined aquifer. This comparison requires utilizing the three-dimensional solution capabilities of MIKE SHE. In the previous verification tests, the groundwater flow was two-dimensional. In the simulation setup, the surface water model MIKE 11 is coupled to the SZ component of MIKE SHE.

For the case where the lake is defined as a constant head boundary, the model compares favorably with the analytical solution, except in zones immediately upstream of the lake and an area below the lake. Still these errors are very small (in the range 1-3 cm head differences). The errors were found to be slightly higher for the case where the lake was defined as a river in MIKE 11. DHI attributes these errors to model discretization along the steep side of the lake. Using relatively thick layer for the first layer adjacent to the lake, it was possible to minimize the errors.

Even though, the situation represented in this problem with a large lake coupled to the aquifer does not exist at REFTS, pond/aquifer and flood plain/aquifer interaction have to be simulated. These interactive processes are modeled using the same coupling of MIKE 11 and SZ module of MIKE SHE that was used in this verification exercise. Hence, attention should be given to the grid geometry issues that were identified in this test when the pond/aquifer and flood plain/aquifer interactions are modeled at REFTS.

5.0 CODE VALIDATION

Code validation is done in two steps. First, the code is compared with other accepted codes such as MODFLOW used for saturated flow simulations or VS2DT used for unsaturated flow simulations. Bench marking the code against other codes allows for the evaluation of the code by conducting simulations of situations that are much more realistic and complex than the ones that were used in code verification. The second method involves a semi-quantitative performance evaluation where the coupling of the various model components is evaluated through a set of simulations. This is the only viable way to test the code's performance for more complex hydrologic conditions (i.e., where simple analytical solutions are not available) in the absence of highly controlled field or laboratory tests.

5.1 Code validation through bench marking

Two commonly used models are used in this exercise. They are: (1) MODFLOW, a modular three-dimensional saturated flow model developed by the USGS, and (2) VS2DT, a two-dimensional variably saturated flow code developed by the USGS. The results of the comparison of these codes to MIKE SHE are evaluated. The details of the problem setup and results are given in Appendix A to this report prepared by DHI.

5.1.1 MODFLOW-Water table conversion

When confined aquifers are pumped, it is possible for the piezometric surface to drop below the top confining layer resulting in unconfined conditions in the aquifer. The yield from the aquifer under confined conditions is controlled by the storage coefficient (generally a very small number defined by the compressibility of the soil matrix and water). Under unconfined conditions, the water is yielded through drainage from pores. In this case the specific yield defines the volume of the water yield. This test is designed to test MIKE SHE's ability to convert from confined to unconfined conditions. An example problem that was used by EPA was used. In this problem, a fully-penetrating well pumps water from a large uniform aquifer. The pumping rate and the problem parameters are such that the aquifer converts from confined to unconfined conditions.

The results show that MIKE SHE and MODFLOW produce exactly the same results. This suggests that MIKE SHE simulates the flow and conversion process as same as the well accepted code MODFLOW.

5.1.2 MODFLOW – Two-dimensional flow in an irregular aquifer

In all the code verification tests, the simple aquifer geometries were assumed. In this problem selected from a EPA test case for a hazardous waste site, an arbitrary aquifer geometry is used.

In the MODFLOW simulation a variable grid size was used. Where as MIKE SHE can only handle uniform grid cells, thus making it not possible to reproduce the solutions at same locations using both models. When the contour map of the water table elevations were compared, they show close agreement except at the boundaries. However, it should be noted that these solution discrepancies at the boundaries are very small. DHI modelers attribute this discrepancy at the boundaries to the differences in the grid sizes.

The simulation of a second EPA test problem for the case of transient flow in an aquitard showed perfect agreement.

5.1.3 VS2DT – steady vertical infiltration

The same test problem that was used in code verification was used in this bench marking test. The algorithms used by VS2DT and UZ component of MIKE SHE to solve the Richard’s equation are very similar. Except, VS2DT uses Van Genuchten moisture content and hydraulic conductivity relationships as inputs. Where as, UZ component of MIKE SHE uses tabular data. Also, VS2DT is a more general model that can solve flow in two-dimensional systems where as UZ is restricted to one-dimensional flow.

In the test, Van Genuchten model was fitted to the tabular data used in MIKE SHE. The simulations of both the vertical distribution of water content and the pressures using the two models for the cases of zero boundary flux (hydrostatic) and specified boundary flux matched exactly.

5.1.4 VS2DT- transient vertical infiltration

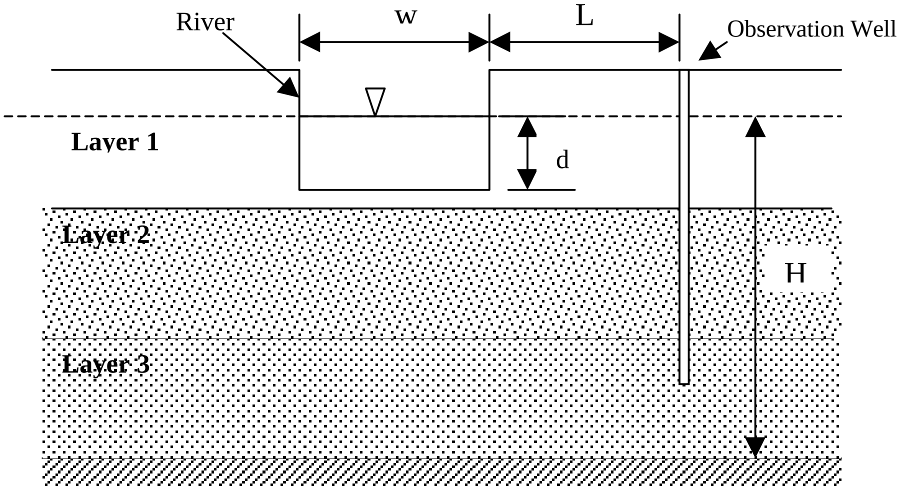
This test problem is similar to the previous steady-state simulation, but soil parameters, the depth to the water table and the precipitation rates are all selected to more closely represent those found at a semi-arid field site such as RFETS. To create transient conditions, an intermittent rainfall event was created by first applying an intense rainfall followed by two longer rainfall events. Each rainfall event was followed by dry period. The simulations of both transient vertical distributions of pressure and moisture contents match exactly with the two codes.

5.2 Semi-quantitative performance evaluation

The tests conducted and presented so far mainly focus on the individual components of the hydrologic cycle and do only to a limited extent test the ability to model some of the complex interactions that occur at REFTS. Based on some of the critical processes and interactions that were identified during the development of the conceptual model for the site, a set of hypothetical problem setups was developed. As no laboratory or field data are available to compare the results against, an approach that relied on a semi-quantitative analysis of the code simulations was used. In this approach, the model predictions were analyzed using these criteria: (1) the predictions qualitatively capture the coupled behavior; (2) the predictions make physical sense; (3) the solutions are stable; (4) mass balance is maintained.

Eight test problems were designed and provided to DHI. DHI conducted the simulations and the input data files were provided to us with the results. After evaluating the results, additional clarifications were requested from DHI. Also, in some cases the data files were used by the reviewers independently to simulate variations of the test problems for QA/QC purposes. The findings from this semi-quantitative performance evaluation are summarized.

5.2.1 Saturated groundwater / surface water model with a transient river stage



Given:

Geometry	*W, L, and layer thickness*
Aquifer parameters	*K and S for layers*
Initial conditions	*H*
Boundary conditions	*Constant head at infinity*
River stage	*Transient d(1), d(2), and d(3)*

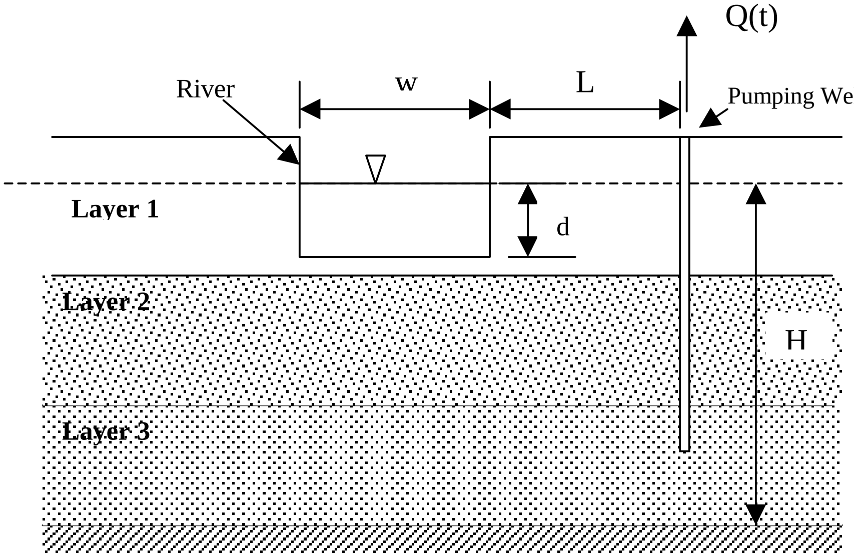
Simulate and provide:
1. Transient water level in the observation well.
2 Transient river gain/loss.
3. Mass balance/water budget.

Figure 3: Problem setup for two-dimensional river-aquifer interaction-river stage fluctuation

Figure 3 shows the problem setup. The goal in this test is to evaluate the code for its ability to simulate the response of the aquifer due to the variation of stage in the river. The three aquifer layers with different properties represent the three model layers that are used in the SWWB model. The situation as represented in this example is important at REFTS as at some locations in the stream system is in hydraulic connection with the aquifer and base flow contributes to the flow in the stream. The simulation results show that the aquifer responds to the stage variation in the river. The lag in the response is controlled by the hydraulic conductivity (K) and storage coefficients.

Using the data files provided by DHI, a number of other simulations were conducted by changing the aquifer properties. When the storage coefficient in the aquifer was changed from 0.25 to 0.01, the water table responded faster as the aquifer acted like a confined aquifer. When the K value in the second layer was increased, as expected the lag in the peak got smaller and the amplitude got bigger. When the observation well was moved further, the responses dampened. When the river stage was dropped and maintained at a constant level, the well drawdown reached a steady value. Based on the results of this analysis, we conclude that the river-aquifer interaction is modeled by the code correctly. The coupling maintained mass balance in the system.

5.2.2 Saturated groundwater / surface water model with transient pumping and river / aquifer interaction



<u>Given</u>:

Geometry	*W, L, layer thickness*
Aquifer parameters	*K and S for layers*
Initial conditions	*H*
Boundary conditions	*Constant head at infinity*
River stage	*Constant d*
Pumping	*Transient Q(1), Q(2), and Q(3)*

<u>Simulate and provide</u>:

1. *Transient water table profile.*
2. *Transient river gain/loss.*
3. *Mass balance/water budget.*

Figure 4: Problem setup for two-dimensional river aquifer interaction-well pumping

The problem setup is similar to the previous case. In this case, the code is evaluated for its ability to simulate the river response to pumping in the river. This exact situation of wells pumping from the aquifer does not exist at REFTS. But, the conditions as represented are conceptually similar to a case where the stream responds to a local recharge event (negative pumping).

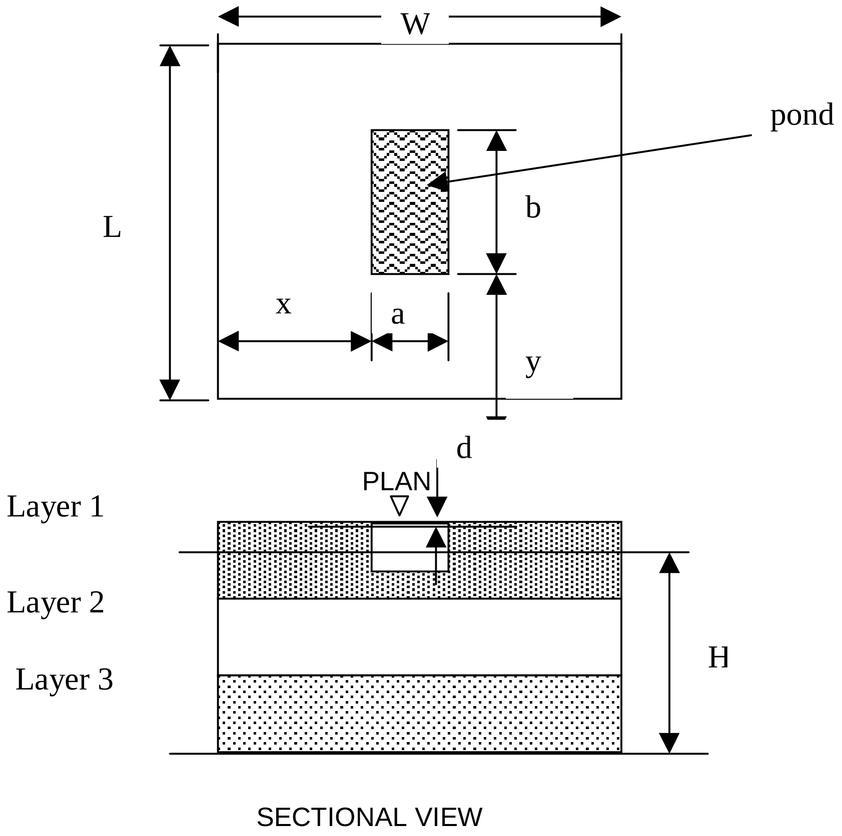
For the problem parameters used, the effect of pumping is primarily seen in the upper layer and a delayed and dampened response was observed in the lower two layers. The lowering of the water table due to pumping resulted in the river loosing water to the aquifer. The water balance analysis shows that the water withdrawal from the well and the return flow from the river to the aquifer balance the net change in storage in the aquifer at any time.

A number of independent simulations were conducted by changing the aquifer parameters and the boundary conditions. These include, increasing the pumping, changing pumping schedule, change in leakance and change in storage coefficient. Based on the results of this analysis, we conclude that the river-aquifer interaction is modeled by the code correctly. The coupling maintained mass balance in the system.

In the previous two test cases, the aquifer flow had to be simulated in two dimensions (x and z). This test is designed to check the ability of the code to simulate three-dimensional flow in response to the water level changes in an isolated pond. The pond is in dynamic interaction with the aquifer. In the problem setup, we requested an isolated pond that acts as a recharge area. However, DHI modelers in setting up the input data files included a river branching from the upstream boundary to a pond represented by wide cross sections and a canal segment to allow surface water flow from the pond across the downstream boundary. They used this method to use MIKE 11 to set the water level in the pond by controlling the upstream and downstream boundary conditions. It is not clear whether this is a limitation in the code that it is not able to represent an isolated pond. At REFTS, it is possible to have situations where an isolated pond (when streams are not flowing) will be in hydraulic connection with the SZ.

The head response in the aquifer seems to capture the interactive behavior well as reflected by correct slopes of the head responses, lag in the peaks, and damping at lower layers.

5.2.3 Saturated groundwater / surface water model with a transient pond stage



<u>*Given*</u>***:***

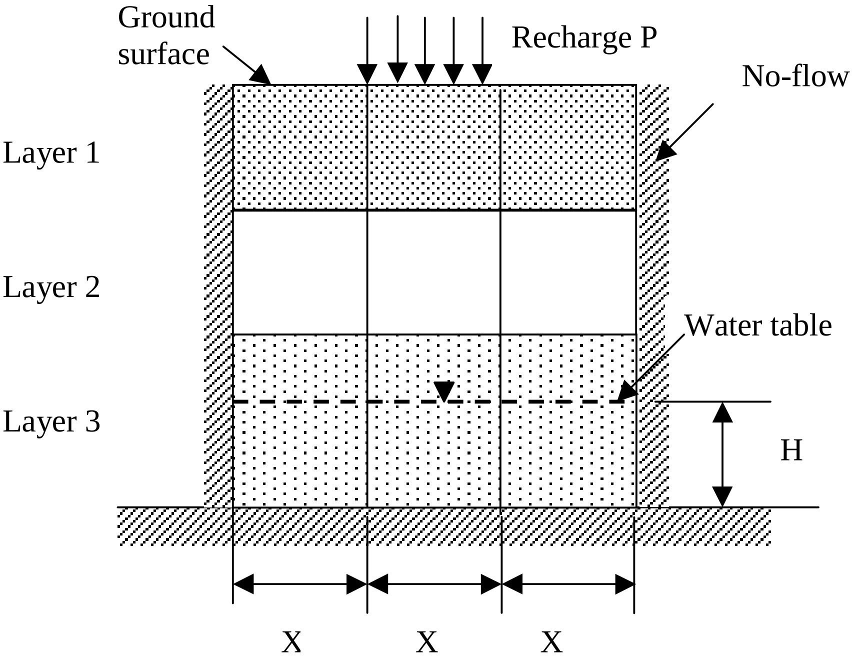
Geometry	*W, L, a, b, x, y and layer thickness*
Aquifer parameters	*K and S for layers*
Initial conditions	*H*
Boundary conditions	*Constant head at H*
Rainfall	Transient d(1), d(2), and d(3)

<u>*Simulate and provide*</u>***:***

1. *Transient water table profile.*
2. *Transient river gain/loss.*
3. *Mass balance/water budget.*

Figure 5: Problem setup for fluctuating water table due to water level changes in a pond

5.2.4 Unsaturated zone / saturated groundwater model with transient recharge without ponding



Given:

Geometry	X and layer thickness
Aquifer parameters	*1. K and S for layers* *2. Retention functions*
Initial conditions	*H*
Boundary conditions	*No-flow*
Recharge	*Transient P(1), P(2), and P(3)*

Simulate and provide:

1. *Transient water table profile.*
2. *Transient soil moisture profile.*
3. *Transient water table recharge.*
4. *Mass balance/water budget.*

Figure 6: Problem setup for recharge to aquifer with specified flux at the ground surface

This test is designed to evaluate dynamic coupling of the UZs and SZs by MIKE SHE. Water infiltrating through the UZ recharges the aquifer. As a result of recharge, the water table rises. The UZ model uses the water table as the lower boundary condition. Accurate representation of this process is critical at REFTS as the water table response to storm events and snow melt has to be simulated.

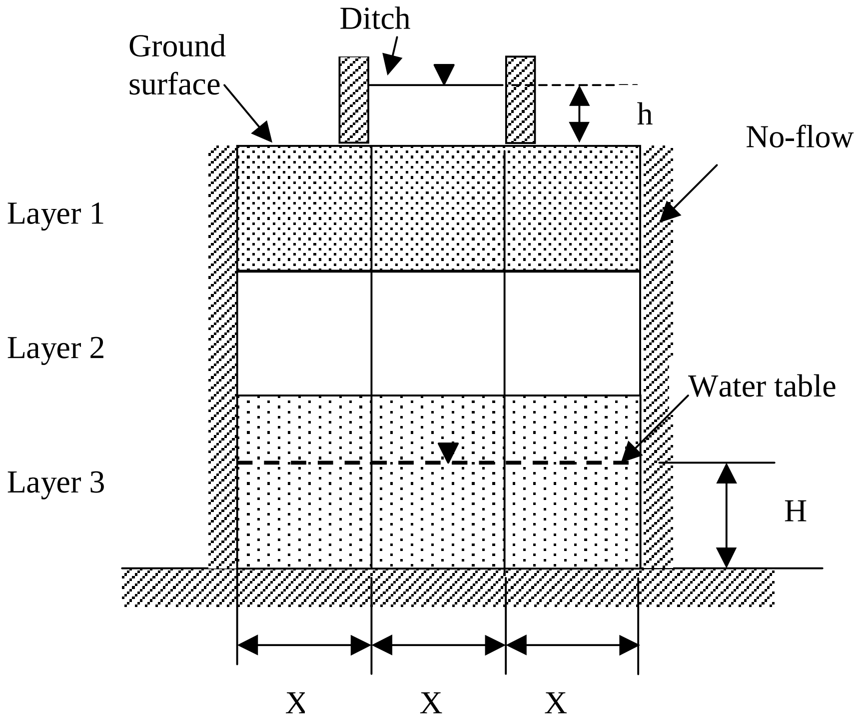
In the problem setup, the initial water table was at a depth –2.5 m thus placing it in the first layer. The shallow water table conditions resulted in the water table rising to the ground surface as a result of infiltration from rainfall. The heads in the three aquifer layers responded to the infiltration event as expected.

The test case shows that MIKE SHE simulations capture the unsaturated and SZ coupling. The situation DHI simulated represents shallow water table conditions. The behavior of the model for situations when the water table is deep and in the third aquifer layer was tested. The test results show that the unsaturated model directly transmits the infiltrating water from the first layer to the water table assuming unit head gradient. This approach of coupling the UZ and water table assumes perched conditions at the bottom of the first layer that may not occur in reality. It is our recommendation that the accuracy of this approximate way of coupling the UZ and SZ under conditions of deep water table should be further tested during the model calibration and validation.

This test case was designed to evaluate MIKE SHE's ability to couple a surface system (a ditch) to the SZ when ponding occurs at the ground surface when the infiltration capacity of the soil column is less than the rate of supply. DHI modelers setup this problem by using the overland component to represent the ditch. Rainfall to the ditch was used to create ponded conditions. Overland flow to the surrounding areas was disabled by using a high value for detention storage. A flux boundary condition was used to bring the UZ to full saturation. Ponding can occur on the ground surface when the infiltration capacity is less than the rainfall intensity. Under these conditions, the soil still remains unsaturated.

We make the same recommendation as for the case of section 5.24 for cases where the water table is deep attention should be given during model calibration and validation to make sure the infiltration process is captured adequately.

5.2.5 Unsaturated zone / saturated groundwater model with transient surface pond water levels



Given:

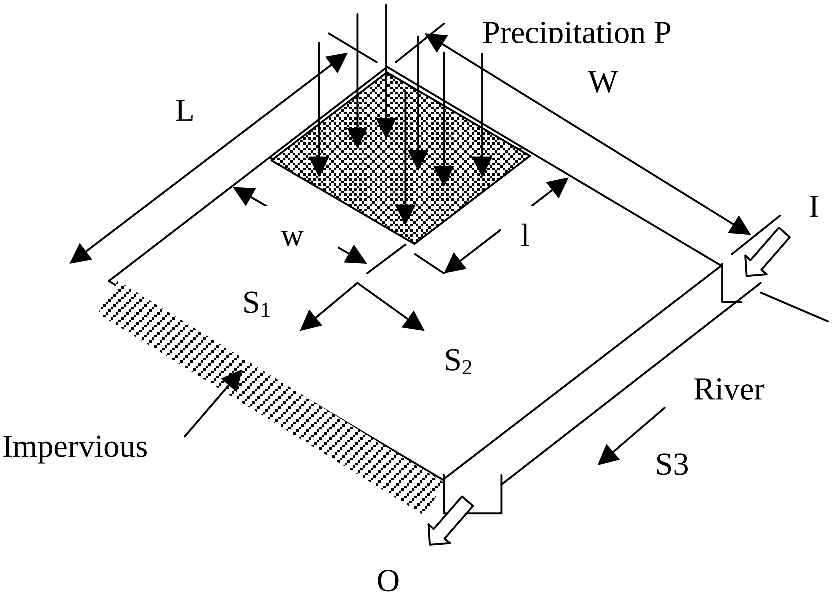
Geometry	X and layer thickness
Aquifer parameters	*1. K and S for layers* *2. Retention functions*
Initial conditions	*H*
Boundary conditions	*No-flow*
Water table	*Transient H(1), H(2), and H(3)*
Ponded depth	*Transient h(1), h(2),and h(3)*

Simulate and provide:

1. *Transient water table profile.*
2. *Soil moisture profile.*
3. *Transient water table recharge*
4. *Mass balance/water budget.*

Figure 7: Problem setup for recharge to aquifer with through specified ponded depth at the ground surface

5.2.6 Overland flow / surface water model with an impervious surface



Given:

Geometry	*W,L.w,l, and river section*
Slopes	*S_1,S_2 and S_3*
Initial conditions	*dry*
Boundary conditions	*Impervious*
Inflow hydrograph	*Transient I(1), I(2), and I(3)*
Parameters	*Strikcler coeff. K, and river routing*

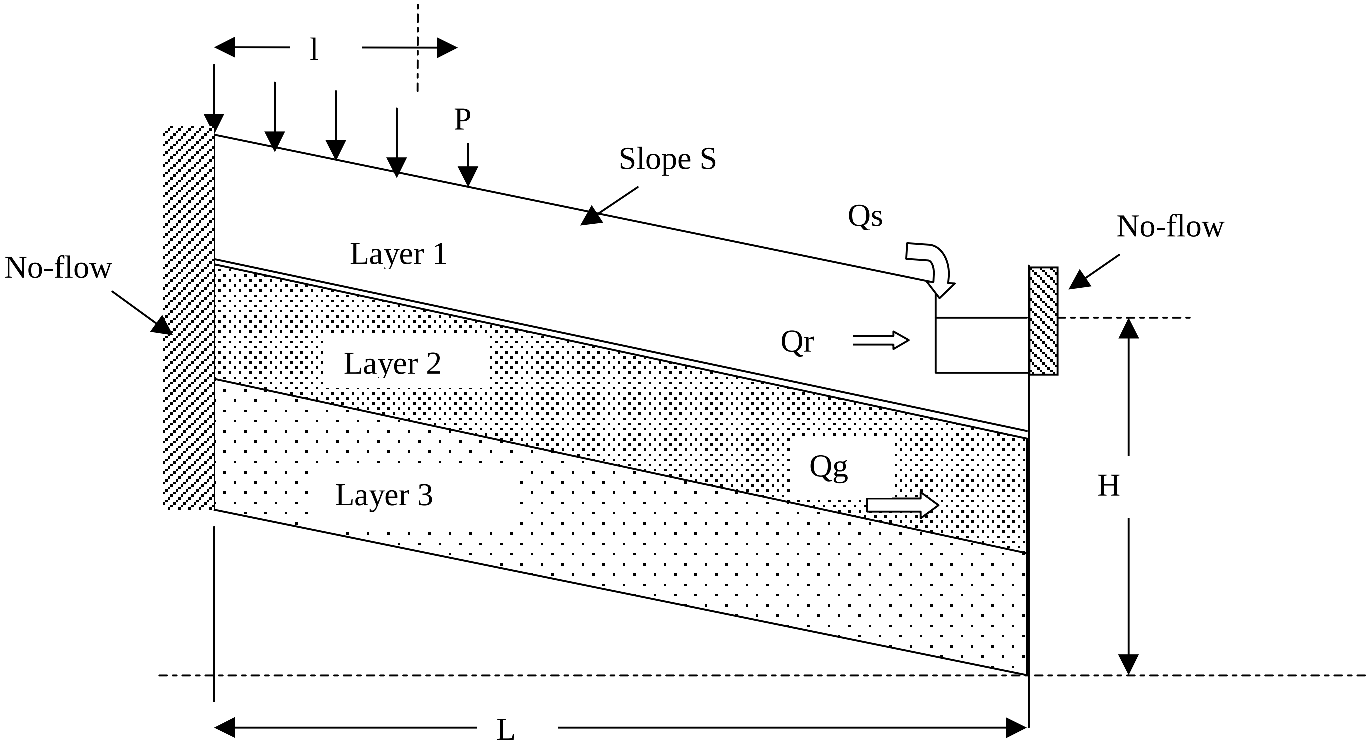
Simulate and provide:

1. *Outflow hydrograph.*
2. *Water budget.*

Figure 8: Problem setup for overland flow-channel coupling

This test case was designed to test MIKE SHE's ability to simulate overland flow in response to a localized rainfall event applied on an inclined surface bounded by a channel. The channel receives lateral flow from the adjacent overland planes. The simulations show mass balance is maintained. The hydrograph of channel flow shows proper lag from the rainfall events. However, the problem was setup causes some water flow across the no-flow boundary. We found there are two options to prevent flow out the boundaries, controlling topography or using overland flow boundaries. A set of independent simulations showed that the model functions well and the surface water gets routed over the ground surface.

5.2.7 Overland flow / unsaturated zone model with a pervious surface



Given:

Geometry	*L, l, S and layer thickness*
Aquifer parameters	*1. K and S for layers* *2. Retention functions*
Initial conditions	*H*
Boundary conditions	*No-flow and H*
Precipitation	*Transient P(1), P(2), and P(3)*

Simulate and provide:

1. *Water table profile.*
2. *Transient Qr.*
3. *Transient Qs.*
4. *Transient Qg.*
5. *Soil-moisture profile.*
6. *Mass balance/water budget.*

Figure 9: Problem setup for overland flow-unsaturated zone coupling

This problem was designed to test MIKE SHE's ability to couple overland flow and UZ. Three aquifer layers were created and simulations were requested to show how return flow to a bounding stream is created as a result of a rainfall event. The model was set up using the SZ component, the UZ component, overland component, and the MIKE11 river component. Overland flow is generated by four rainfall events. The groundwater model includes three layers dipping towards the river. For the condition that was simulated, the model captured the coupling behavior of the overland zone and UZ. We suggest DHI to perform a simulation for the case where the water table is deep if it becomes necessary that such a condition be found to occur at RFETS.

6.0 CONCLUSIONS

This report documents the results of a code validation study conducted to evaluate the suitability of MIKE SHE as an integrated hydrologic modeling code for the development of a water balance model at RFETS. The tests were carefully designed to not only evaluate the strengths but also possible weaknesses of the code. To our knowledge very few codes have been subjected to this level of rigorous testing. The model developers at DHI were very cooperative and supportive of this effort. The authors of the report are very appreciative of this, as without the full cooperation of the code developers and their expertise, it would not have been possible to conduct such a detailed evaluation. Additional tests would have provided more information to conduct further evaluations of many possible combinations of the interactions between the different components. However, the authors are very comfortable that the test cases captured the most important processes to make an evaluation of the suitability of the code to be applied at RFETS. It is also important to note that the authors used the data files provided by DHI for the test cases to conduct independent tests. These independent tests allowed meeting the QA/QC requirements for code validation.

It is the opinion of these authors that integrated modeling of dynamic systems is not a trivial exercise, and no code will be able to capture all the processes accurately to the point that the model becomes an exact representation of the physical system. A comparative analysis was not conducted to evaluate the performance or the accuracy of MIKE SHE in comparison to other similar integrated modeling codes. In addition, we are not aware of any other code that is as comprehensive and user friendly as MIKE SHE to be available to simulate complex semi-arid hydrologic conditions such as the ones that exist at RFETS. Based on the results of the tests and the knowledge we have of other codes that are reported in literature, we conclude that MIKE SHE will be the best code that is currently available to conduct this complex study. We are confident that a model based on this code when properly calibrated will be the best decision tool that could be developed for the Site. The feature of MIKE SHE that can be used for the simulation of contaminant transport will make the SWWB model to be the best flow simulator that could be used in any future decision tools that may become necessary to conduct water quality analysis at the Site.

7.0 REFERNCES

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