

SKB P-23-07

ISSN 1651-4416 ID 2006204 April 2023

Investigation of how changes in model structure affect runtimes and model performance for the MIKE SHE hydrological model of Forsmark

Jean-Marc Mayotte Svensk Kärnbränslehantering AB

Mona Sassner DHI Sverige AB

Keywords: MIKE SHE, Hydrology, Forsmark

Data in SKB's database can be changed for different reasons. Minor changes in SKB's database will not necessarily result in a revised report. Data revisions may also be presented as supplements, available at www.skb.se.

This report is published on www.skb.se

© 2023 Svensk Kärnbränslehantering AB

Abstract

This study focused on reducing the run-times of the MIKE SHE hydrological models used for the safety analyses. The study examined 10 different "calculation cases"; each case representing a unique model structure. In the context of this study, the combination of individual modelling procedures used within the MIKE SHE modelling framework was referred to as the "model structure".

The performance of each calculation case was assessed according to the models' ability to reproduce measured groundwater levels (in both the regolith and bedrock), lake levels and discharge data at Forsmark. The model runtimes of each calculation case were assessed against the runtimes of a "base case". The model structure and assignment of parameter values used for the base case followed that of the calculation cases were intended to represent a simplification of the model structure used for the base case. It was hypothesized that these simplifications would result in reduced runtimes of the models. In general, this study did not attempt to calibrate any of the calculation cases. Parameter assignments for each of the calculation cases followed those used in the base case.

Results showed that all of the calculation cases considered resulted in a reduction of model runtimes between 2% and 92% relative to the runtime of the base case. Model performance varied widely for each calculation case considered. None of the calculation cases considered performed better than the base case at reproducing all three data points (i.e. groundwater, lake and discharge data).

A preliminary calibration exercise was performed for the calculation case with the fastest runtime. Model performance for this calculation case improved significantly as a result of the calibration.

Sammanfattning

Denna studie har fokuserat på att minska beräkningstiderna för de hydrologiska modeller som sätts upp i MIKE SHE och som används för säkerhetsanalyser på SKB. Studien har fokuserat på ett tiotal beräkningsfall där varje fall representerar en unik modellstruktur. Inom ramen för denna studie avser ordet modellstruktur den kombination av individuella modelleringskomponenter som används i MIKE SHE:s modellsystem.

Varje beräkningsfalls förmåga att reproducera mätdata utvärderades. Utvärderingen gjordes för uppmätta grundvattennivåer både i jord och berg, samt för sjönivåer och flödesdata i ett utvalt antal mätstationer i Forsmark. Den totala simuleringstiden för varje beräkningsfall har jämförts med motsvarande för basfallet, d v s det ursprungliga beräkningsfallet. Basfallet är baserat på den parameteruppsättning av den kalibrerade MIKE SHE som använts i tidigare projekt, exempelvis FPSAR och PSAR SFR. Varje enskilt beräkningsfall i denna studie sattes upp för att representera en förenkling av den modellstruktur som finns i basfallet, med hypotesen att de uppsatta modellförenklingarna skulle resultera i reducerade simuleringstider. Syftet med denna studie har inte varit att försöka kalibrera om modellen för de uppsatta beräkningsfallen, utan modellparametriseringen för de olika beräkningsfallen följde den i basfallet.

Resultat visade att samtliga av beräkningsfallen resulterade i reducerade simuleringstider med mellan 2% och 92% jämfört med basfallet. En stor variation noterades i förmågan att reproducera mätdata. Inget av de genomförda beräkningsfallen gav bättre resultat än basfallet för de tre undersökta datatyperna (d v s grundvattennivåer, sjönivåer och vattendragsflöden).

En preliminär kalibreringsövning genomfördes för det beräkningsfall som resulterade i den kortaste simuleringstiden. Baserat på kalibreringsövningen kunde modellresultaten förbättras avsevärt.

Table of Contents

1	Introdu	ıction	3
2	Metho	ls	5
2.1		ing tools	
2.2	Calcula	tion cases investigated in this study	5
	2.2.1	Base case	
	2.2.2	CC1: Monthly time-steps	
	2.2.3	CC2: 10 computational layers	8
	2.2.4	CC2a: 10 computational layers / no MIKE 11	
	2.2.5	CC2b: 10 computational layers / no MIKE 11 / internal boundaries in lakes	
	2.2.6	CC3: Represent unsaturated zone with a two-layer water balance	
	2.2.7	CC4: Represent unsaturated zone using gravity flow	
	2.2.8	CC5: No overbank spill for surface water bodies	12
	2.2.9	CC5a: No overbank spill for surface water bodies / gravity flow for	
		unsaturated zone	12
	2.2.10	CC5b: No overbank spill for surface water bodies / gravity flow for	
		unsaturated zone / subcatchment method for overland flow	
2.3		nput data	
2.4	Perform	nance criteria	14
3	Results	·	17
3.1	MAE, N	ME, error in accumulated flows and relative runtimes for all calculation cases	17
3.2		cal presentation of results for selected calculation cases	
4	Autoca	libration test	35
5	Sugges	ted future work	38
Refe	erences		39
Арр	endix A		40
Арр	endix B.		41

1 Introduction

It is the responsibility of the Swedish Nuclear Fuel and Waste Management Company (SKB) to manage the management of both radioactive waste and spend nuclear fuel in Sweden. The existing Repository for Short-Lived Radioactive Waste (SFR) and the site for the planned Spent Fuel Repository is located in Forsmark (Figure 1-1). An extension to the SFR facility is planned to extend the capabilities of the repository. As a part of the license applications for the extension of SFR and the construction of the final repository for spent fuel, SKB is continually assessing the long-term radiological safety of each repository.

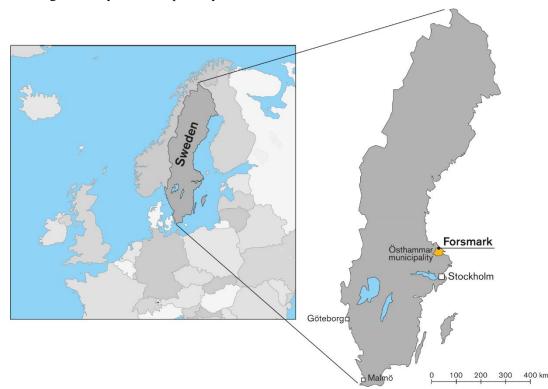


Figure 1-1. Location of the Forsmark site in Sweden (right) and in context with the countries in Europe (left). The site is situated in the Östhammar municipality, which belongs to the County of Uppsala.

Hydrological and hydrogeological modelling is an important part of the safety assessments for the existing and planned repositories at Forsmark. Comprehensive analyses of the future hydrology and future near-surface hydrogeology of the Forsmark area were performed for the license application for the SFR extension (Werner et al. 2013, Sassner et al. 2022) and site-selection for the Spent Fuel Repository (Bosson et al. 2010). A key point of these modelling studies was that they were required to examine the hydrology as affected by a postulated future climate and landscape over very large time-spans (10⁵ years for SFR and 10⁶ years for the Spent Fuel Repository). The time-spans under consideration are so large that geological events such as large-scale bulk transports of sediment via erosion processes, shore-line retreat due to isostatic rebound and future ice ages must be accounted for. Geological events like these can cause significant changes to quaternary geology and topography of an area; the nature of these changes is generally only understood at regional scales. For the hydrological and near-surface hydrogeological investigations for Forsmark, models are parameterized using topographical and geological information with a spatial resolution which varies between <10 m² up 80 m². There are significant uncertainties regarding the topographical and geological characteristics of a landscape in the very far future at these smaller spatial scales which can affect the predictive capacity of the hydrological models.

A review of the SR-Site project (i.e. the safety assessment for the Spent Fuel Repository as implemented at Forsmark; main findings reported in SKB 2011) conducted by the Swedish Radiation Safety Authority (SSM) stated that the deterministic nature by which the future landscape at Forsmark was considered in the safety analyses was insufficient and they recommended that uncertainties in the future landscape be accounted for when examining the future hydrology at

Forsmark (Section 7.1.2.2 in SSM 2018). This implies that landscape development modelling needs to be conducted within an uncertainty framework which can account for several possible realizations of the possible future landscape at Forsmark. This further implies that several hydrological and near-surface hydrogeological models may also need to be examined as these models are highly dependent on landscape and geological inputs. Historically, a move towards a Monte Carlo hydrological modelling approach has not been practical within the context of the safety analyses at SKB due primarily to the long set-up and run-times of the hydrological models.

The primary purpose of this study is focused on reducing the run-times of the hydrological models used for the safety analyses. Historically, the hydrological and near-surface hydrogeological modelling has been conducted using the MIKE SHE modelling suite. This study focuses on MIKE SHE in order to stay consistent with previously used modelling methodologies. This is an experimental modelling study which examines how changes in the model structure affects both model performance and model run-times when modelling the hydrology and near-surface hydrology at Forsmark. The study examines different spatial and temporal discretization of the MIKE SHE hydrological model affects model performance. This study also explores how different modelling assumptions surrounding key hydrological processes such as unsaturated, overland and channel-flow, affect model performance. Results of this study will help inform how future modelling work within MIKE SHE can be conducted in a manner more conducive to an uncertainty framework which is capable of considering multiple model realizations while operating within the time and resource constraints typical of earlier safety analyses performed at SKB.

This study is not meant to provide conclusions with which to update the current modelling methodology used for the hydrological modelling within the context of a post-closure safety assessment. Rather, this study is only meant to present the results of the modelling exercise undertaken herein. Any concrete conclusions based the results presented herein, conclusions that, for example, could be used to modify the current modelling methodology used for the hydrological modelling within the post-closure safety assessment(s), would require a thorough analysis of modelling results; this analysis does not take place in this study.

2 Methods

2.1 Modelling tools

The hydrological modelling tool investigated in this study is MIKE SHE. MIKE SHE is an integrated hydrological model system that is capable of describing the main processes in the terrestrial hydrological cycle. The MIKE SHE model distribution version used in this study is 2020. A detailed description may be found in DHI (2022) and in Graham and Butts (2005). A conceptual presentation of the different model components capable of being accounted for in MIKE SHE is presented in Figure 2-1.

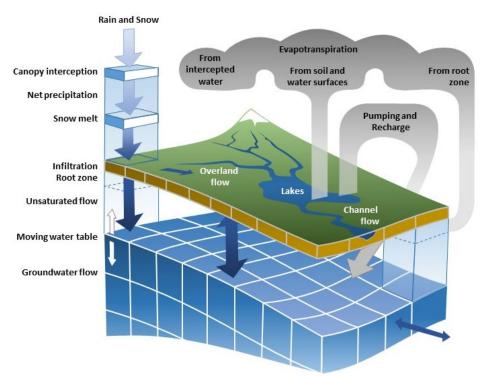


Figure 2-1. Hydrological processes modelled by MIKE SHE. Figure taken from DHI (2022) (Figure 1-1) with permission from DHI.

MIKE SHE is a comprehensive hydrological modelling suite which describes the primary components of the terrestrial hydrological cycle. Several individual hydrological processes, each with their own governing equations and modelling framework, are incorporated into a coupled hydrological model. MIKE SHE provides several different modelling procedures for many of the individual hydrological processes represented in the modelling suite. The decision of which modelling procedures are used is problem-specific and it is up to the modeler to decide how each process is represented. Differences between individual modelling procedures are most often centered around the assumptions taken in the formulation of the numerical representation of the hydrological component in question. In the context of this study, the combination of individual modelling procedures'.

2.2 Calculation cases investigated in this study

Sections 2.2.1-2.2.10 detail the 10 unique model structures investigated in this study. These model structures are referred to as "calculation cases" in the context of this study.¹ All calculation cases are chosen with the explicit purpose of reducing model run-times. Model run-times and model performance of each calculation case is then compared to the base case. The calculation cases are investigated in the order they are presented below. The two calculation cases presented in sections

¹ "Calculation case" is used instead of "scenario" so as not to confuse the modelling exercises pursued in this study with the scenarios investigated within the context of the SKB safety analyses.

2.2.2 and 2.2.3 investigate changes to the temporal and spatial discretization of the model. All computational processes in these calculation cases are identical to those used in the base case (i.e. representation of unsaturated conditions, open-channel flow and surface water inundation of the watershed). These calculation cases were performed first to help inform which spatial and temporal simplifications may be worth investigating in tandem with simplifications in computational processes.

The calculation cases presented in sections 2.2.6-2.2.10 were investigated after examining the results of the first two calculation cases. All the calculation cases presented in these sections investigate alternatives to one or many of the modelling processes used in the base case and most of these calculation cases represent a combination of prior calculation cases.

In general, no calibration of the individual calculation cases is considered in this study as this was seen to be outside of the scope of the study. A "base case" is considered as a benchmark to compare results. The base case is based on the calibrated model used during the FPSAR and PSAR SFR presented in Werner et al. (2013) (see Section 2.2.1). For each calculation case, parameter assignments are taken from the base case for each of the common parameters. An exception is made in this study for one particular calculation case which attempted to calibrate the model using the MIKE SHE auto-calibration tool (see Section 4), however, the calibration focused on parameters that are not present in the base case; all parameters in common between the base case and the model being calibrated have the same values as that of the base case.

Within the context of this study, each individual calculation case can be viewed as an alternate model structure. Using the base case as a benchmark, each individual calculation case examined in terms of how "sensitive" the model is to changes in the model structure used to define the base case in the absence of iterative calibration steps (i.e. the individual calculation cases are not calibrated again following the changes made to the model structure).

For ease of reading, the names of the calculation cases have been given unique IDs. The names of the calculation cases and their corresponding IDs are shown in Table 2-1. It is recommended that the reader have this table readily available when reading the report.

Table 2-1. Unique IDs for the calculation cases investigated in this study. Note that the "base case" does not have a unique ID. This is because this calculation case is referred to by name throughout the report. Copies of all of the models are stored on SKB servers (G:\SKB\modellering\Ber\MIKE_SHE-P-23-07).

ID	Calculation case name
-	Base case
CC1	Monthly time-steps
CC2	10 computational layers
CC2a	10 computational layers / no MIKE 11
CC2b	10 computational layers / no MIKE 11 / internal boundaries in lakes
CC3	Represent unsaturated zone with a two-layer water balance
CC4	Represent unsaturated zone using gravity flow
CC5	No overbank spill for surface water bodies
CC5a	No overbank spill for surface water bodies / gravity flow for unsaturated zone
CC5b	No overbank spill for surface water bodies / gravity flow for unsaturated zone / subcatchment method for overland flow

2.2.1 Base case

The regional MIKE SHE model built for FPSAR and PSAR SFR² which investigated the hydrology at Forsmark for current conditions (denoted as 2000 AD in the model) is used as the starting point of the investigation. A full documentation of this MIKE SHE model can be found in Werner et al. (2013). Some minor modifications were made to this model before being applied to this study: The

² Model name: PSU_regional2000AD_R85_131213.she

connection to the current SFR was removed and the model area was reduced (Figure 2-2). Unsaturated conditions were also simulated at every position in the grid for the base case whereas the model used for FPSAR and PSAR SFR only examined unsaturated conditions within a subset of cells and then applied the results of these cells to the rest of the model area.

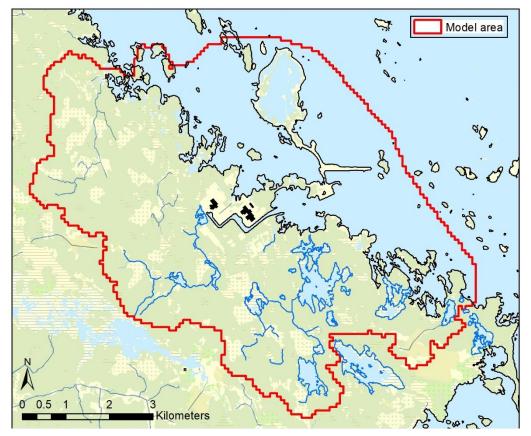


Figure 2-2. Model area

The MIKE SHE model used for the base case uses a daily time step and an 80×80 m horizontal grid resolution. Vertical discretization of the saturated groundwater zone is accomplished using 16 calculation layers: two layers representing the regolith and 14 layers for the bedrock. See section 2.2.3 for more information about MIKE SHE calculation layers. A complete description of the model set-up and parameterization for the base case is presented in Appendix B.

For the base case, individual hydrological processes tend to be modelled using the most computationally intense numerical representations available in MIKE SHE. This study singles out four specific hydrological processes and their numerical representation in the model. These processes are unsaturated flow, overland flow (i.e. surface runoff), and open channel flow. In the base case, unsaturated flow is represented the full Richard's equation (eq. 10.7 in DHI 2022) and both overland flow (surface runoff) and open channel flow are estimated using the St. Venant equations (see Sections 6 and 8, respectively, in DHI 2022). Attaining numerical solutions of both the Richard's and St. Venant equations is computationally intense and can substantially increase model run-times. Most of the calculation cases considered in this study examine alternate methods of representing these three processes.

2.2.2 CC1: Monthly time-steps

The base case hydrological model used daily time-series data of precipitation and potential evapotranspiration in its calculation of surface and subsurface flows. For this calculation case, the meteorological inputs to MIKE SHE was reduced from a daily to a monthly temporal resolution using monthly averages thus significantly reducing the number of time-steps used in the model.

2.2.3 CC2: 10 computational layers

Bulk groundwater transport is simulated in MIKE SHE using finite-difference approximations of the governing flow equation for three-dimensional flow in a saturated porous media (see eq. 12.1 in DHI 2022). This requires that a grid of finite elements is created within the model space.³ In MIKE SHE, these elements are created using a matrix of "columns" (i.e. same dimensions in the horizontal plane) where the top and bottom surfaces of each column coincide with the top and bottom of the geological model as represented in MIKE SHE. Vertical discretization of the columns is accomplished using "calculation layers" which divide the columns into individual finite elements. Vertical discretization of the columns varies; for model areas which are used to simulation more computationally intense processes (e.g. the upper parts of a column where relatively large fluctuations in groundwater flows may be expected) a finer discretization of the columns (i.e. more calculation layers) may be used to improve the accuracy of modelled solutions and reduce issues related to model convergence. However, increasing the resolution of the finite elements used in the hydrogeological modelling in MIKE SHE results in increased model run-times.

In this calculation case the saturated groundwater flow simulations are performed using fewer calculation layers than that used for the base case. The base case used 16 calculation layers for the hydrogeological modelling: 14 calculation layers representing the bedrock and two for the regolith. This calculation case reduces the vertical resolution of the finite elements by using only 10 calculation layers: eight calculation layers representing the bedrock and two for the regolith.

2.2.4 CC2a: 10 computational layers / no MIKE 11

MIKE 11⁴ is a modelling tool used to simulate one-dimensional open-channel flow using the Saint Venant equations (DHI 2017). These equations have several particle applications but are commonly used to examine the profile of the water surface in an open channel, stream discharge and pollutant transport in rivers. Applications of these equations requires information on the channel geometry, topography of the channel bottom and channel slope along the entire length of the channel as well as a parameterization of the channel's "friction" coefficient to solve for the flow-rate and water level in the channel. Dimensioning of the friction coefficient is often done using the Gauckler–Manning roughness coefficients are considered "empirical" in nature as their direct definition is done using strict experimental conditions. For most hydrological applications of the Sant Venant equations, the parameterization of these coefficients is done via model calibration.

MIKE SHE and MIKE 11 are two separate numerical models that are coupled via the overland and groundwater flow components of each model. The models are coupled in a way such that solutions to both numerical models are calculated simultaneously at each time-step (e.g. the amount of groundwater entering or leaving a stream at a given point in the model is dependent on the time- and spatially dependent conditions of each respective model).

When implementing a coupled MIKE SHE / MIKE 11 model, the spatial location of open-channel flow branches (i.e. rivers and streams) are first mapped onto the MIKE SHE model grid using a series of points (known as MIKE 11 "H-points") as shown in Figure 2-3. One-dimensional representations of the open channels interact with the MIKE SHE groundwater model via calculated head-gradients between the water in the open channel and the groundwater table as shown in Figure 2-4.

³ The finite element model for the saturated flow module in MIKE SHE is made up using what are "calculation layers" in MIKE SHE. The hydraulic properties of the calculation layers are taken from the geological model used to build the MIKE SHE conceptual model. The conceptual model uses what MIKE SHE refers to as "geological layers". The discretization of the geological layers and the calculation layers often differs which means that the information from the geological layers (i.e. conceptual model) must be interpolated to the calculation layers (i.e. finite difference grid).

⁴ All current (i.e. after 2015) distributions of MIKE SHE have replaced MIKE 11 with MIKE Hydro River. In spite of this, MIKE 11 was used in this study in order to remain consistent with the hydrological modelling pursued during FPSAR and PSAR SFR.

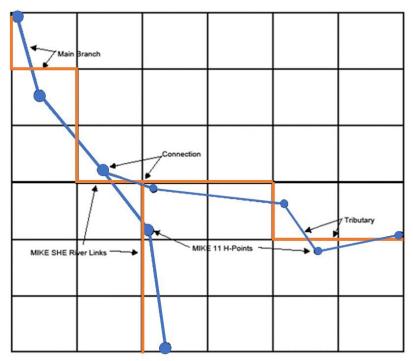


Figure 2-3 Example of MIKE 11 branches (blue) and h-points in a MIKE SHE grid with river links (orange). Figure taken from DHI (2022) (Figure 28.1) with permission from DHI.

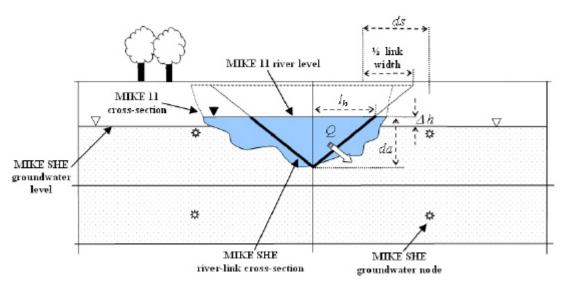


Figure 2-4 A typical simplified MIKE SHE river link cross-section compared to the equivalent MIKE 11 crosssection. Figure taken from DHI (2022) (Figure 28.1) with permission from DHI.

For the hydrological modelling pursued during FPSAR SFR, MIKE 11 was used for the modelling of the flow and water depth in the open channels at Forsmark. When open channels are flowing at a near steady-state (i.e. small changes in the flow entering a channel and leaving a channel over time) solutions to the Saint Venant equations are not computationally intense. However, as flow inputs and outputs begin to change, e.g. during precipitation events, simulations of open channel flow can become more computationally intense thus slowing down modelling times.

Technically, a lake can also be classified as an open channel (assuming the lake has both an inlet and an outlet), however, MIKE 11 is not used to calculate lake levels. Instead, a MIKE 11 channel is simulated between the inlet and outlet of a lake and lake levels are calculated in MIKE SHE by "ponding" in the lake depressions; lake levels change dependent on the water balance of the lake and the lake's bathometry. Flows to/from the lake's inlet/outlet are calculated using MIKE 11 which informs the water balance of the lake (together with evapotranspiration, direct runoff to the lake and recharge/infiltration of groundwater to/from the lake). Water exchange between the MIKE 11

channel in the lake and ponded water in the lake depression simulated in MIKE SHE (via the overland flow module (see Sections 2.2.8 and 2.2.10) is simulated at every time-step.

This calculation case investigated how the removal of MIKE 11, together with CC2, affects model results. In the absence of MIKE 11, all routing of runoff is done using the calculations for overland flow in MIKE SHE using the "finite difference method" which examines a numerical solution of the diffusive wave approximation for the Saint Venant equations to calculate fluxes and water depth on the surface (see Section 2.2.10 for more details).

2.2.5 CC2b: 10 computational layers / no MIKE 11 / internal boundaries in lakes

For the base case, a no-flow boundary condition was used for the saturated groundwater at the model boundaries (i.e. the lateral boundaries and the bottom boundary of the model at -634 m m.a.s.l.) and a prescribed head boundary condition was used to describe the sea-level for the marine portions of the model. Net precipitation, i.e. precipitation minus evapotranspiration⁵, was calculated by MIKE SHE in order to provide the primary boundary for the saturated hydrogeological module in MIKE SHE; it is this volumetric flux of water, i.e. the net precipitation, that drives all of the hydrological and hydraulic processes in the model.

In the base case, lake levels are calculated numerically via a complex water balance which accounts for evaporation, infiltration, lake discharge and direct runoff to the lake. For this calculation case, an "internal" boundary condition is used to describe the water-level of the lakes which uses a prescribed head is to describe the water levels in the lakes. The prescribed head used to describe water levels in the lakes is implemented in a manner similar to how the sea-level is accounted for in the marine portions of the model. By doing this, the numerical calculations of all the hydrological and hydraulic processes that are dependent on the lake levels (i.e. discharge/recharge of groundwater to/from the lake, discharge of surface water via the lake outlet and area-dependent evaporation fluxes) are greatly simplified as they are no longer coupled to the simulated dynamics of the standing water-pressure in the lake. This simplification is hypothesized to reduce simulation times.

This calculation combined the calculation case CC2 (Section 2.2.4) with a prescribed head boundary condition for all for the lakes Bolundsfjärden, Eckarfjärden and Gällsboträsket (Figure 2-8). A constant head equal to the average observed lake-level for the time-period under consideration (i.e. 2005-2007) was assigned to the model cells within Eckarfjärden (5.22 m), Bolundsfjärden (0.34 m) and Gällsboträsket (1.18 m).

2.2.6 CC3: Represent unsaturated zone with a two-layer water balance

The base case uses the full Richards' equation (Richards 1931) when modelling conditions in the unsaturated zone. The Richards' equation describes the flow of a liquid through a porous medium wherein the portion of the pore-volume available for flow is not full (i.e. the volume is unsaturated). Solutions of the Richards' equation requires a functional relationship between the degree of saturation, the capillary pressure in the pores, and the hydraulic conductivity of the porous media. One of the most commonly used formulations of this relationship was derived by Van Genuchten (1980). While the Richards' equation is hugely applicable within hydrological modelling, there are very few analytical solutions to the equation. Furthermore, the extreme non-linear behaviour of equation means that achieving accurate numerical solutions can require a lot of computational resources. For this reason, MIKE SHE offers other, less computationally intense alternatives to the Richards' equation to help account for water storage in the unsaturated zone. One such alternative is the "two-layer" water balance method.

The two-layer water balance method was originally formulated by Yan and Smith (1994) as a tool to help produce an early example of an integrated groundwater—surface water model. In the two-layer water balance method, an average water content is calculated (assumed to vary linearly with depth) for the entire saturated zone within each grid cell at each time-step. The method assumes that the degree of saturation in the unsaturated zone is dependent on the depth of the groundwater table and can vary between a minimum (commonly assumed to be the field-capacity of the soil) and a maximum (saturation) water content before affecting the level of the groundwater table. As the water content increases beyond the maximum (e.g. due to large precipitation events), all excess water is

⁵ Evapotranspiration is calculated using function of the prescribed potential evapotranspiration

assumed to drain to the water table which will cause the water table to rise; drainage from the unsaturated zone continues until the water content returns to the maximum value. Water content in the unsaturated zone can continue to decrease due to evaportanspiration processes. Volume loss from the unsaturated zone due to evaporation is assumed to continue until the water content in the unsaturated zone reaches its minimum value. Once the water content in the unsaturated zone is at its minimum value, evaporation from the water table is assumed to occur causing the water table to drop; the volume of water evaporating from the water table is dependent on the depth of the water table.

The two-layer water balance method is implemented as a pre-processing portion of infiltration/evapotranspiration calculations in MIKE SHE and does not have an explicit spatial representation in the finite difference grid of the groundwater model. This is to say that the unsaturated zone is not represented within the finite-difference grid cells in the model space but rather as an intermediary step before changes to the water table are calculated. This in stark contrast to the implementation of the Richards' equation in MIKE SHE where a vertically dependent degree of saturation is calculated for each grid cell where unsaturated conditions may exist.

For the base case, the Richards' equation is used to examine water storage in the unsaturated zone. MIKE SHE uses a one-dimensional formulation of the Richards' equation assuming that unsaturated flow occurs primarily in the vertical direction. This simplifies the problem significantly but long runtimes and convergence issues can still arise especially during periods with rapid changes in the degree of soil saturation (e.g. large precipitation events).

For this calculation case, the Richards' equation is replaced with the two-layer water balance method to account for changes in water storage in the unsaturated zone. Three variants of this calculation case are tested with three different parameter sets for the maximum and minimum water contents as well as the saturated hydraulic conductivity (see Table 2-2).

Table 2-2. Water contents (θ) and saturated hydraulic conductivities (K_s) used in subvariants A - C for the twolayer water balance calculation case. " θ saturation" dictates the maximum water content of the soil, " θ field capacity" is the water content at which the soil can freely drain and it is the minimum water content of the soil that is achievable via gravitational forcing (i.e. drainage) and " θ wilting point" is the minimum water content of a soil achievable via root-uptake of water. Direct evaporation from the water table and water-loss due to root uptake occurs for all water contents between θ wilting point and θ field capacity.

Variant	heta saturation	θ field capacity	θ wilting point	<i>K</i> s (m/s)
A	0.3	0.1	0.05	1.0×10 ⁻⁵
В	0.8	0.4	0.2	1.0×10 ⁻³
С	0.1	0.05	0.02	1.0×10 ⁻⁸

2.2.7 CC4: Represent unsaturated zone using gravity flow

Another alternative to the Richards' equation for estimating storage changes in the unsaturated zone (as outlined in Section 2.2.6) is the "Gravity flow" method. This method calculates the total hydraulic head in the unsaturated zone (i.e. the sum of the isostatic, or gravitational head) and the head due to pore-pressure by assuming that the predominant force driving flow in the unsaturated zone is gravity and thus the head due to pore-pressure can be ignored. By making this assumption, volumetric flux can be calculated using Darcy's law using the unsaturated hydraulic conductivity which results in a depth-dependent flow calculation through the unsaturated zone.

This method is implemented in MIKE SHE by assuming a moisture content for the entire unsaturated zone for the initial condition.⁶ Flow through the unsaturated zone is calculated from the top down: The infiltration rate at the top cell boundary is assumed equal to the depth of the overland flow, the infiltration rate then decreases to a value equal to the saturated hydraulic conductivity in the first cell below the surface and the water content of the cell is calculated. If the resulting water content of the first cell, less the water volume lost to evaporation via root extraction, is greater than the field

⁶ This is to say that the moisture content does not vary over the depth of the unsaturated zone. However, the parameterization of the moisture content can vary in the horizontal plane in order to represent soil-specific water contents.

capacity of the soil then a flux calculation to the next cell in the column is calculated. This process is continued for every cell in the unsaturated zone. Any flux leaving the bottom of the unsaturated zone is added to the saturated zone thus raising the water table. This method assumes no direct evaporation losses from the unsaturated zone; all evapotranspiration losses are assumed to occur via root uptake.

While more complicated than the two-layer water balance method discussed in Section 2.2.6 above, the use of Darcy instead of the Richards allows for an explicit solution for the flow equation which is likely to significantly decreases model runtimes.

The base case used the Richards' equation to account for storage changes in the unsaturated zone. For this calculation case, the Richards' equation is replaced with the Gravity flow method to account for changes in storage in the unsaturated zone.

2.2.8 CC5: No overbank spill for surface water bodies

When modelling open channel flow using MIKE 11, it is possible that the calculated water level in the channel may exceed the height of the channel bank. In these instances, one would intuitively expect flooding of the landscape to occur. The "overbank spill" option within MIKE 11 allows for further coupling between MIKE SHE and MIKE 11 by allowing excess flows in an open channel or lake to leave the channel and inundate the grid of the MIKE SHE model as overland flow. Flows from the channel onto the surrounding landscape are calculated using the standard formula for a "broad-crested weir" (see equation 28.8 in DHI 2022). Once leaving the channel, the water is accounted for as overland flow in MIKE SHE. If water levels from overland flow are higher than the water levels in the channel, overland flows are then added to the channel as lateral inflows. If water levels in the channel exceed the ponded water levels outside of the river, excess water from the channel is also added to overland flow within MIKE SHE.

The use of the overbank spill option requires significant parameterization and calibration on behalf of the modeler. Special attention must also be paid to the surface topography which defines the top elevation of the MIKE SHE grid to ensure that floodplain cross-sections are properly represented in the model. Use of the overbank spill option also limits the options the modeler has when solving for overland flow in MIKE SHE. Use of the overbank spill option requires that overland flow calculations are performed using the finite difference method for solving the diffusive wave approximation of the Saint Venant equations (see Section 2.2.10) and the user is prohibited from using a less computationally intense method to solve the numerical approximation of the Saint Venant equations. All of factors combine to result in increased model set-up times and runtimes and can also lead to convergence issues which may not be easily diagnosed.

The base case uses the overbank spill option to account for flood inundation from surface water bodies (rivers/streams and lakes). This calculation case removes the overbank spill option for surface water bodies.

2.2.9 CC5a: No overbank spill for surface water bodies / gravity flow for unsaturated zone

This calculation case is a combination of the calculation cases CC4 and CC5 (Sections 2.2.7 and 2.2.8 respectively) where the overbank spill option is deactivated for surface water bodies and the gravity flow approximation is used to describe storage changes in the unsaturated zone.

2.2.10 CC5b: No overbank spill for surface water bodies / gravity flow for unsaturated zone / subcatchment method for overland flow

The base case uses "finite difference method" to calculate overland flow. This method examines a numerical solution of the diffusive wave approximation for the Saint Venant equations using a twodimensional finite difference grid to represent the surface of the model.⁷ Numerical solutions can

⁷ The Saint Venant equations are also used in MIKE 11 to calculate flow-rates and water depths for openchannel flow (see Section 2.2.4). However, MIKE 11 uses a one-dimensional formulation of the equations while the overland flow module applies the equations in two-dimensions.

either be achieved explicitly (i.e. the "standard" for solving differential equations numerically where both the present and a future time-step are considered) or implicitly using the "successive over relaxation" (SOR) solver in MIKE SHE (Section 25.1.3, DHI 2022) As briefly mentioned in Section 2.2.8, using the explicit solver can increase model runtimes and convergence issues, and the SOR solver can help decrease runtimes but results are less accurate. For these reasons, MIKE SHE provides alternative options for calculating overland flow which can help to decrease runtimes and model complexity. One such option is the "simplified overland flow routing" method.

The simplified overland flow routing method calculates overland flow using the Mannings equation combined with an empirical relationship between flow depth and a surface's detention storage. The method divides the model area into "subcatchments" and assumes that each subcatchment can be represented as a single hill-slope; the hill-slope is representative of the average elevation gradient within the catchment and the length of the hill represents the length of the longest flow-path in the subcatchment. Flow routing is achieved by routing overland flow within a subcatchment directly to a surface water body (where surface water is modelled using MIKE 11 thereafter) and/or by assigning an integer code to each subcatchment which prescribes the order of the subcatchment cascade (e.g. overland flow from subcatchment two flows into subcatchment three and subcatchment two receives overland flow from subcatchment one).

Evapotranspiration and infiltration processes are handled on a cell-by-cell basis even when using the simplified overland flow routing method. An average water depth of overland flow for the entire basin is calculated and used as inputs to calculate cell-specific evapotranspiration and infiltration volumes. Once this is done for every cell within a subcatchment, a new average water depth is calculated for the entire basin.

As previously mentioned, the base case uses the finite difference method for calculating overland flows in the model. For this calculation case, the subcatchment method for overland flow is combined with the calculation cases CC4 and CC5 (Sections 2.2.7 and 2.2.8 respectively) where the overbank spill option is deactivated for surface water bodies and the gravity flow approximation is used to describe storage changes in the unsaturated zone.

2.3 Model input data

All of the MIKE SHE models investigated in this study require time-series inputs for potential evapotranspiration (PET) and precipitation in order to define the top boundary condition of the models. A time period of 2005-2007 was chosen for this study. The choice of this time-period was almost entirely arbitrary with the exception of two points of reasoning: 1) only two years of data should be examined in order to limit the time spent on data management and analyses of model results, and 2) the time period should coincide with the time-span examined for the hydrological modelling used for FPSAR and PSAR SFR (Werner et al. 2013) thus providing the possibility of further applying the analyses in this study to any future hydrological modelling endeavors relevant for SFR.

The time-series inputs of PET and precipitation are given below in Figure 2-5 and Figure 2-6 respectively.

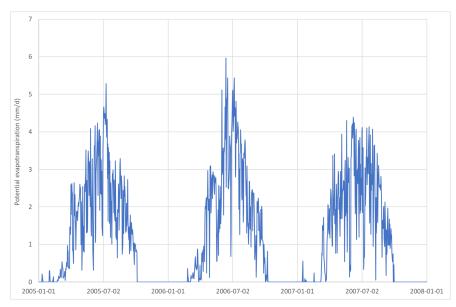


Figure 2-5. Time-series inputs of potential evapotranspiration (PET) for the entire model area in mm/d.

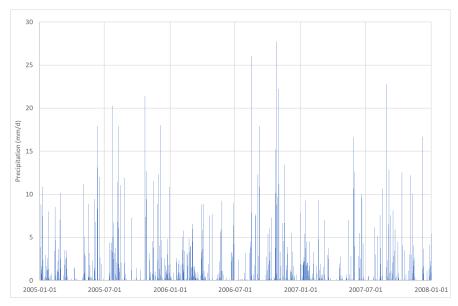


Figure 2-6. Time-series inputs of precipitation for the entire model area in mm/d.

2.4 Performance criteria

Model performance is evaluated against measured data for groundwater levels (in both the bedrock and the regolith), discharge data and water levels in lakes. The names and locations of the ground-water observation wells used to evaluate model performance are presented in Figure 2-7. The names and locations of the discharge points (weirs) and positions where water levels are measured in the lakes are presented in Figure 2-8.

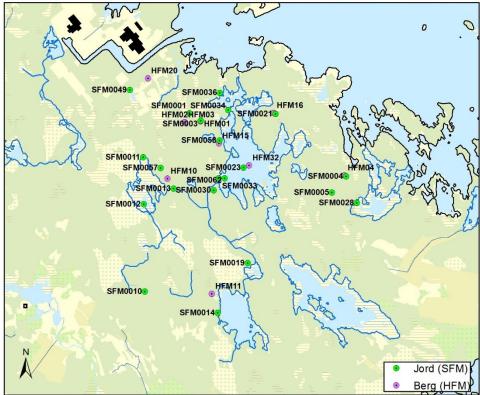


Figure 2-7. Observation points in soil (SFM, "Jord") and bedrock (HFM, "Berg") included in the model analysis.

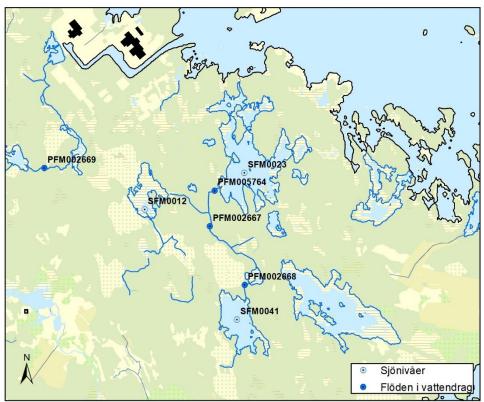


Figure 2-8 Observation points in lakes (SFM, "Sjönivåer") and streams (PFM, "Flöden i vattendrag") included in the model analysis.

The performance of each calculation case is evaluated against the measured time-series data for the groundwater observation wells at the positions presented in Figure 2-7 and the discharge and lake-level data at the positions presented in Figure 2-8. Performance of each calculation case with regards to the modelled groundwater levels and modelled lake levels is assessed using the mean absolute

error (MAE) and the mean error (ME) (the equations used for the MAE and ME are presented in Appendix A. The MAE and ME were also used to evaluate model performance for hydrological modelling conducted during FPSAR and PSAR SFR (Werner et al. 2013). These metrics were therefore used in this study as to be consistent with the hydrological modelling work conducted during FPSAR and PSAR SFR (Werner et al. 2013). Runtimes of each calculation case are also compared to the base case as a ratio of the calculation case's runtime relative that of the base case.

When assessing model performance in regards to the modelled discharge, the ME and MAE are relatively poor measures of performance due to the large variability in the measured and calculated time-series relative those for the groundwater and lake levels. For the discharge predictions, model performance is instead presented in terms of accumulated flow.

3 Results

Model performance criteria and model runtimes for each calculation case are presented in Section 3.1. Model performance is assessed relative observed time-series data for groundwater levels (in both bedrock and regolith boreholes) and water levels in the lakes. For the discharge and lakelevel data, performance criteria are reported for each individual measurement point in this section. For the groundwater levels, performance criteria are reported as the averages across the individual monitoring points, i.e. an average MAE and ME is calculated using the individual MAEs and MEs calculated for each of the bedrock (HFM) and regolith (SFM) groundwater monitoring points (see Figure 2-7).

All calculation cases were not considered when calculating the errors for the modelled discharge. This was due to the unavailability of these type of results for certain calculation cases and to the limited availability of computational and personnel resources during the course of this study. For these reasons, the available resources were focused on only certain calculation cases when calculating the ME and MAE of the modelled discharge; the following calculation cases were omitted from these analyses:

- CC1 and CC2 (Section 2.2.3) are not presented as there was no significant reduction in calculation time relative the base case (Table 3-4) and it was not deemed to be an efficient use of the limited resources available for this study to produce these results.
- CC2a (Section 2.2.4) and CC2b (Section 2.2.5) calculation cases do not include MIKE 11 in the simulation and therefore do not have flow results readily available for presentation.⁸
- For CC3, variants A-C (Section 2.2.6), results are only presented for variant C (Table 2-2) as it is this case that best reproduces the groundwater levels compared to the base case (see results in Table 3-1).

Additional results for selected calculation cases are presented in Section 3.2 in the form of spatial mapping of the ME for the modelled groundwater levels and time-series plots of the modelled flows and accumulated flows at measurement points. For similar reasoning as described above, omission of certain calculation cases from further graphical analyses was necessary to optimize the computational and personnel resources (see Section 3.2).

The calculation cases were carried out using two different computers. The first four calculation cases (CC1 - CC2b, Sections 2.2.2 - 2.2.5) were performed using a modelling computer housed at SKB. A local computer (housed at the DHI offices) was used for the remaining calculation cases (CC3 - CC5b, Sections 2.2.6 - 2.2.10). The base case (Section 2.2.1) was performed using both computers. For this reason, run-times are presented relative those for the base case in this section.

As previously mentioned in Section 2.2, no calibration was performed on the individual calculation cases; each calculation case uses the same parameter set used in the base case. This means that the results can be interpreted as the effects of structural changes in the model in the absence of an iterative calibration step (i.e. changes in the parameter set used in the base case in an attempt to increase the performance of the individual calculation case).

3.1 MAE, ME, error in accumulated flows and relative runtimes for all calculation cases

The performance criteria for the calculation cases, as well as the model runtimes for each calculation case are presented in the tables below. The ME and MAE for the modelled groundwater levels in the regolith (SFM) and bedrock (HFM) for all of the calculation cases are given in Table 3-1. The ME and MAE for the modelled lake levels at Eckarfjärden, Bolundsfjärden and Gällboträsket are given in Table 3-2. The error in accumulated flows over the simulation period, relative the measured data, for the monitoring points downstream of Eckarfjärden, Stocksjön, Gunnarsbosträsket and upstream of

⁸ It is theoretically possible to examine modelled flows at the measurement points via an examination of the overland flow results in these two calculation cases. However, this level of examination of modelling results was deemed outside of the objectives of this study.

Bolundsfjärden are given in Table 3-3. Model runtimes for all of the calculation cases are given in Table 3-4.

When modelling the regolith (SFM) and bedrock groundwater (HFM), the base case generally underestimated groundwater levels (i.e. ME > 0) at the SFM points and overestimated groundwater levels (i.e. ME < 0) at the HFM points (Table 3-1). CC3 (variant C) and CC5 both outperformed the base case with regards to the ME and MAE of the predicted groundwater levels at the SFM and HFM points. The worst performing calculation cases, with regards to the modelled groundwater levels, were CC2a and CC5b; both these calculation cases generally overestimated groundwater levels at both the SFM and HFM observation points.

When modelling the water levels in Eckarfjärden (SFM0041), Bolundsfjärden (SFM0023) and Gällsboträsket (SFM0012), the base case generally underestimated lake levels in all of the lakes (Table 3-2). The worst performing calculation case, with respect to the modelled lake levels, was CC2a. All other calculation cases performed relatively well at capturing the measured levels in the lakes relative to the base case when examining the MAE.

When modelling discharge, the base case did a reasonable job of representing the discharge data with the exception of the discharge upstream of Bolundsfjärden (PFM005764) (Table 3-3). Almost all of the calculation cases examined performed worse than the base case at modelling the discharge at all of the monitoring points with the exception of CC5 which performed better than the base case when modelling discharge downstream of Eckarfjärden (PFM002668) and Gunnarsbosträsket (PFM002669). In general, all other calculation cases overestimated the flows at each of the stations to a greater extent than that predicted by the base case.

The fastest model investigated, relative to the base case, was CC5b; the runtime of this calculation case was 8% of the total runtime of the base case (Table 3-4). All other calculation cases were faster than the base case with total runtimes between 20% and 98% of the total runtime of the base case.

Calculation case	SFM		HFM	
	ME	MAE	ME	MAE
Base case	0.12	0.42	-0.41	0.49
CC1: Monthly time-steps	0.33	0.48	-0.52	0.68
CC2: 10 computational layers	0.13	0.42	-0.52	0.69
CC2a: 10 computational layers / no MIKE 11	-0.44	0.66	-0.40	0.51
CC2b: 10 computational layers / no MIKE 11 / internal boundaries in lakes	0.10	0.41	-0.64	0.67
CC3: Represent unsaturated zone with two-layer water balance: variant A	-0.35	0.55	-0.98	0.98
CC3: Represent unsaturated zone with two-layer water balance: variant B	-0.38	0.57	-0.99	1.00
CC3: Represent unsaturated zone with two-layer water balance: variant C	0.03	0.40	-0.33	0.47
CC4: Represent unsaturated zone using gravity flow	-0.25	0.44	-0.82	0.83
CC5: No overbank spill for surface water bodies	0.12	0.42	-0.38	0.46
CC5a: No overbank spill for water bodies / gravity flow for unsaturated zone	-0.25	0.44	-0.82	0.83
CC5b: No overbank spill for surface water bodies / gravity flow for unsaturated zone / subcatchment method for overland flow	-0.17	0.65	-1.13	1.16

 Table 3-1. Average ME and MAE for the modelled groundwater levels at the regolith (SFM) and bedrock (HFM) groundwater monitoring points for the simulation period of 2005-2007.

Calculation case	SFN	/0041	SFM	/0023	SFM	/0012
	ME	MAE	ME	MAE	ME	MAE
Base case	0.07	0.08	0.01	0.06	0.13	0.14
CC1: Monthly time-steps	0.12	0.12	0.08	0.10	0.20	0.21
CC2: 10 computational layers	0.07	0.08	0.01	0.06	0.13	0.14
CC2a: 10 computational layers / no MIKE 11ª	0.56	0.56	0.31	0.31	1.52	1.52
CC2b: 10 computational layers / no MIKE 11 / internal boundaries in lakes	-	-	-	-	-	-
CC3: Represent unsaturated zone with two-layer water balance: variant A	-0.01	0.06	-0.02	0.05	0.08	0.09
CC3: Represent unsaturated zone with two-layer water balance: variant B	-0.01	0.06	-0.01	0.05	0.06	0.07
CC3: Represent unsaturated zone with two-layer water balance: variant C	-0.09	0.10	-0.09	0.10	0.01	0.13
CC4: Represent unsaturated zone using gravity flow	-0.01	0.06	-0.02	0.06	0.07	0.09
CC5: No overbank spill for surface water bodies	0.07	0.08	0.01	0.06	0.13	0.14
CC5a: No overbank spill for water bodies / gravity flow for unsaturated zone	-0.02	0.07	-0.03	0.06	0.07	0.09
CC5b: No overbank spill for surface water bodies / gravity flow for unsaturated zone / subcatchment method for overland flow	0.05	0.07	0.27	0.27	-0.02	0.09

Table 3-2. MAE and ME for the modelled water levels in Eckarfjärden (SFM0041), Bolundsfjärden (SFM0023) and Gällsboträsket (SFM0012) for the simulation period of 2005-2007. ME and MAE for the calculation case "10 computational layers / no MIKE 11 / internal boundaries in lakes" are not presented as lake levels are given as a boundary condition for this calculation case.

a: Lake levels are interpreted from MIKE SHE instead of MIKE 11; calculation of lake levels in this fashion must account for the topography of the model surface at these areas in order to convert the "ponded" water level given in the MIKE SHE model output to a lake level reported in MASL. Table 3-3. Accumulated flow (acc Q) for the measured data and the percent difference in accumulated flow relative the measured data (diff) for the modelled flows downstream of Ekarfjärden (PFM002668), Stocksjön (PFM002667) and Gunnarbosträsket (PFM002669) and upstream Bolundsfjärden (PFM005764) for the simulation period of 2005-2007.

Calculation case	PFM00- 2668	PFM00- 2667	PFM00- 2669	PFM00- 5764
			aaa O (m3)	· · · · · · · · · · · · · · · · · · ·
	acc Q (m ³)	acc Q (m°)	acc Q (m°)	acc Q (m°)

	diff (%)	diff (%)	diff (%)	diff (%)
Base case	-27%	11%	1%	121%
CC1: Monthly time-steps	-	-	-	-
CC2: 10 computational layers	-	-	-	-
CC2a: 10 computational layers / no MIKE 11	-	-	-	-
CC2b: 10 computational layers / no MIKE 11 / internal boundaries in lakes	-	-	-	-
CC3: Represent unsaturated zone with two- layer water balance: variant A	-	-	-	-
CC3: Represent unsaturated zone with two- layer water balance: variant B	-	-	-	-
CC3: Represent unsaturated zone with two- layer water balance: variant C	82%	154%	152%	421%
CC4: Represent unsaturated zone using gravity flow	12%	65%	48%	223%
CC5: No overbank spill for surface water bodies	3%	41%	-1%	150%
CC5a: No overbank spill for water bodies / gravity flow for unsaturated zone	51%	103%	45%	261%
CC5b: No overbank spill for surface water bodies / gravity flow for unsaturated zone / subcatchment method for overland flow	134%	225%	622%	500%

Table 3-4. Runtimes for all calculation cases.
--

Calculation case	Runtime	
	h	% of Base case
Computer 1 (hosted at SKB)		
Base case	55	
CC1: Monthly time-steps	54	98%
CC2: 10 computational layers	42	78%
CC2a: 10 computational layers / no MIKE 11	18	33%
CC2b: 10 computational layers / no MIKE 11 / internal boundaries in lakes	17	31%
Computer 2 (hosted at DHI)		
Base case	25	
CC3: Represent unsaturated zone with two-layer water balance: variant A	21	84%
CC3: Represent unsaturated zone with two-layer water balance: variant B	21	84%
CC3: Represent unsaturated zone with two-layer water balance: variant C	23	92%
CC4: Represent unsaturated zone using gravity flow	21	84%
CC5: No overbank spill for surface water bodies	10	40%
CC5a: No overbank spill for water bodies / gravity flow for unsaturated zone	5	20%
CC5b: No overbank spill for surface water bodies / gravity flow for unsaturated zone / subcatchment method for overland flow	2	8%

3.2 Graphical presentation of results for selected calculation cases

Due to the large amount of individual data points for which modelling results could be compared against measured data, it was deemed necessary to graphically represent a selection of the modelling results. However, due to time and resource constraints, only a selection of results for selected calculation cases were chosen for further analysis. For this reason, CC2b and CC5a are omitted from further discussion from this point forward. The decision to exclude these cases in the further analyses was the result of a judgement call by the authors in the early stages of the project and should not be interpreted as an indicator of the importance of these calculation cases within the context of this study. Any follow-up work to this study should expand on the model results from CC2b and CC5a.

Figure 3-1 through Figure 3-6 show a spatial representation of the ME of the modelled groundwater levels in the regolith and the bedrock for the base case, CC2a, CC3 (variant C), CC4, CC5 and CC5b. These calculation cases were chosen as they were those that performed the best at capturing the measured groundwater levels relative to the base case. For these calculation cases, results indicate that the models overestimated groundwater levels at most of the bedrock monitoring points (HFM) (Figure 3-1 through Figure 3-6). For the regolith monitoring positions (SFM), errors surrounding the prediction of groundwater levels in the regolith were spatially dependent (Figure 3-1 through Figure 3-6).

Figure 3-7 through Figure 3-9 show the time-series of the model predictions for the lake levels for the base case, CC2a, CC3 (variant C), CC4, CC5 and CC5b. CC2a was chosen to examine via graphical representation due to its exceptional poor performance in capturing the measured lake levels (Table 3-2). CC3 (variant C) was chosen to examine via graphical representation due to its reasonably good performance at capturing the lake levels (Table 3-2) and its high performance in capturing the measured groundwater levels (Table 3-1). CC4 and CC5 were chosen to examine via graphical

representation as these calculation cases performed better than the base case at modelling lake levels (with respect to the MAE). CC5b was chosen to examine via graphical representation as it was the fastest model compared to the base case (Table 3-4).

Figure 3-7 through Figure 3-9 indicate that CC2a was consistently poor at capturing lake levels for all three lakes and generally overpredicted lake levels; this was especially apparent for Eckarfjärden (Figure 3-7) and Gällsboträsket (Figure 3-9). All of the other calculation cases did a reasonable job at capturing the magnitude and variance of the measured data.

Figure 3-10 through Figure 3-17 show the time series of the modelled discharge and accumulated discharge for the base case, CC3 (variant C), CC4, CC5 and CC5b. These calculation cases were chosen primarily based on their performance with the exception of CC5b which was chosen based on it being the fastest of the calculation cases examined (Table 3-4). In general, all of the models overpredicted the discharge over the simulation period (2005-2007); CC5b was the worst performing in this respect.

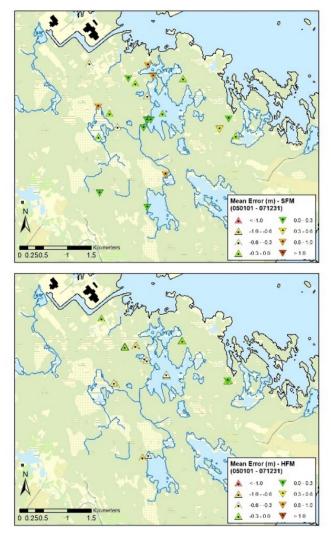


Figure 3-1. Point-specific mean error (ME) for the modelled groundwater levels in the regolith (SFM, top plot) and bedrock (HFM, bottom plot) for the Base case. Upward pointing triangles indicate simulated groundwater levels are generally greater than the observed levels at these points (i.e. a negative ME) and downward pointing triangles indicate that the simulated groundwater levels are generally lower than the measured levels at these points (i.e. a positive ME).

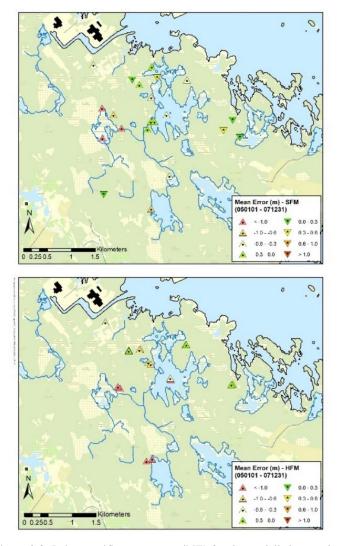


Figure 3-2. Point-specific mean error (ME) for the modelled groundwater levels in the regolith (SFM, top plot) and bedrock (HFM, bottom plot) for CC2a: 10 computational layers / no MIKE 11. Upward pointing triangles indicate simulated groundwater levels are generally greater than the measured levels at these points (i.e. a negative ME) and downward pointing triangles indicate that the simulated groundwater levels are generally lower than the measured levels at these points (i.e. a positive ME).

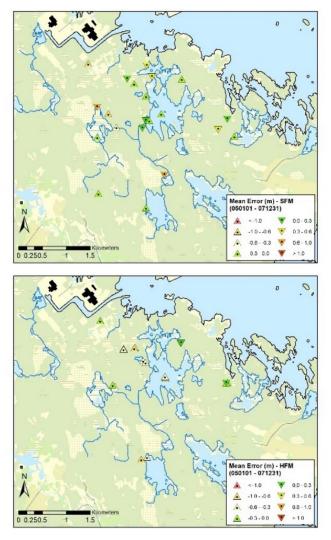


Figure 3-3. Point-specific mean error (ME) for the modelled groundwater levels in the regolith (SFM, top plot) and bedrock (HFM, bottom plot) for CC3: Represent unsaturated zone with a two-layer water balance (variant C). Upward pointing triangles indicate simulated groundwater levels are generally greater than the measured levels at these points (i.e. a negative ME) and downward pointing triangles indicate that the simulated groundwater levels are generally lower than the measured levels at these points (i.e. a positive ME).

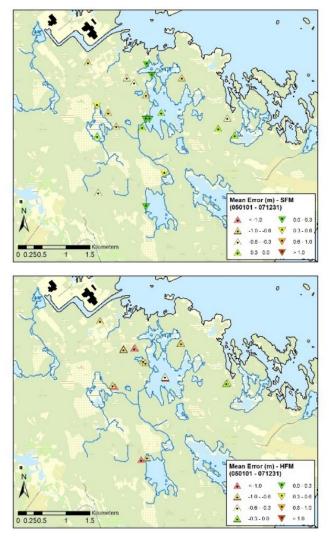


Figure 3-4. Point-specific mean error (ME) for the modelled groundwater levels in the regolith (SFM, top plot) and bedrock (HFM, bottom plot) for CC4: Represent unsaturated zone using gravity flow. Upward pointing triangles indicate simulated groundwater levels are generally greater than the measured levels at these points (i.e. a negative ME) and downward pointing triangles indicate that the simulated groundwater levels are generally lower than the measured levels at these points (i.e. a positive ME).

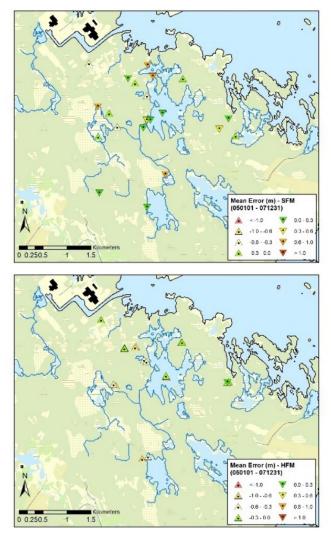


Figure 3-5. Point-specific mean error (ME) for the modelled groundwater levels in the regolith (SFM, top plot) and bedrock (HFM, bottom plot) for CC5: No overbank spill for surface water bodies. Upward pointing triangles indicate simulated groundwater levels are generally greater than the measured levels at these points (i.e. a negative ME) and downward pointing triangles indicate that the simulated groundwater levels are generally lower than the measured levels at these points (i.e. a positive ME).

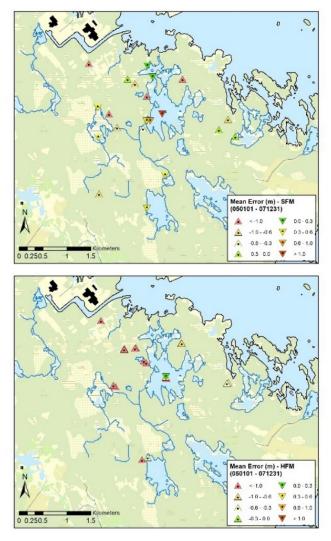


Figure 3-6. Point-specific mean error (ME) for the modelled groundwater levels in the regolith (SFM, top plot) and bedrock (HFM, bottom plot) for CC5b: No overbank spill for surface water bodies / gravity flow unsaturated zone / subcatchment method for overland flow. Upward pointing triangles indicate simulated groundwater levels are generally greater than the measured levels at these points (i.e. a negative ME) and downward pointing triangles indicate that the simulated groundwater levels are generally lower than the measured levels at these points (i.e. a positive ME).

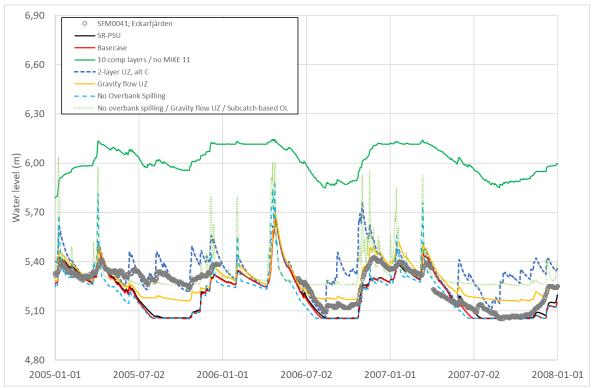


Figure 3-7. Modelled and measured water levels for Eckarfjärden (SFM0041) for selected calculation cases. Modelled lake levels from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

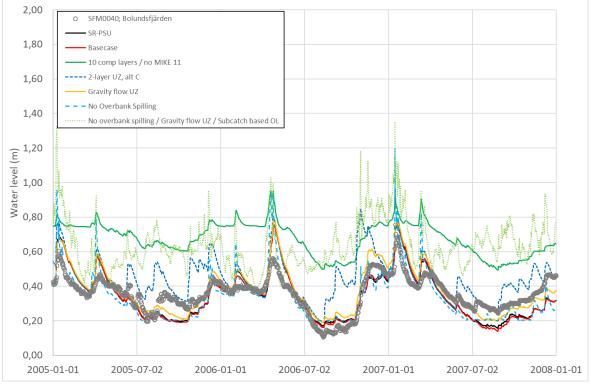


Figure 3-8. Modelled and measured water levels for Bolundsfjärden (SFM0023) for selected calculation cases. Modelled lake levels from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

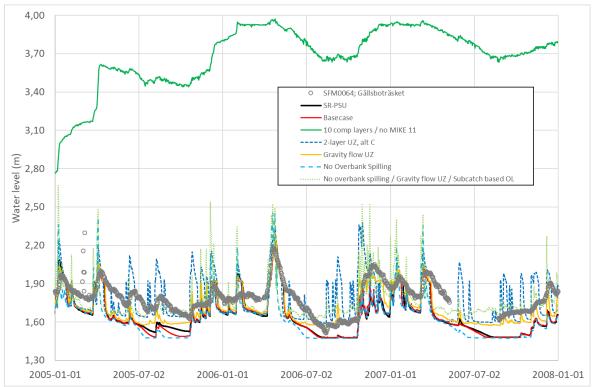


Figure 3-9. Modelled and measured water levels for Gällsboträsket (SFM0012) for selected calculation cases. Modelled lake levels from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

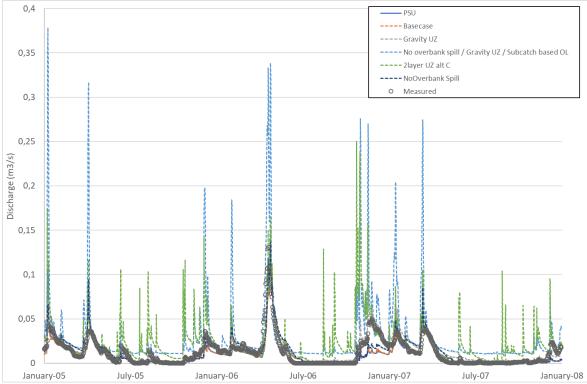


Figure 3-10. Modelled and measured discharge downstream of Stocksjön (PFM002667) for selected calculation cases. Modelled discharge from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

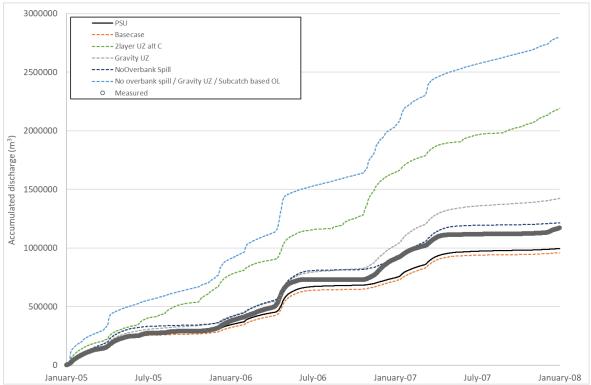


Figure 3-11. Modelled and measured accumulated discharge downstream of Stocksjön (PFM002667) for selected calculation cases. Modelled discharge from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

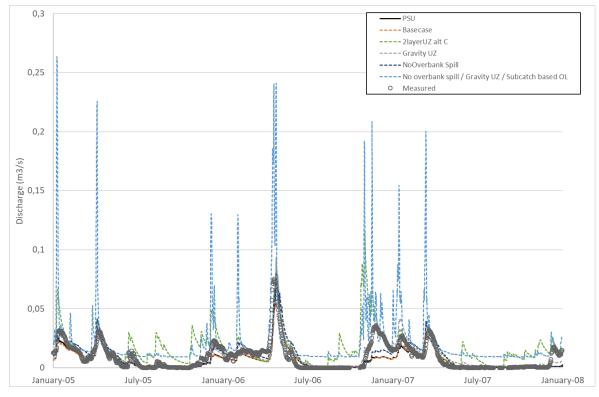


Figure 3-12. Modelled and measured discharge downstream of Eckarfjärden (PFM002668) for selected calculation cases. Modelled discharge from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

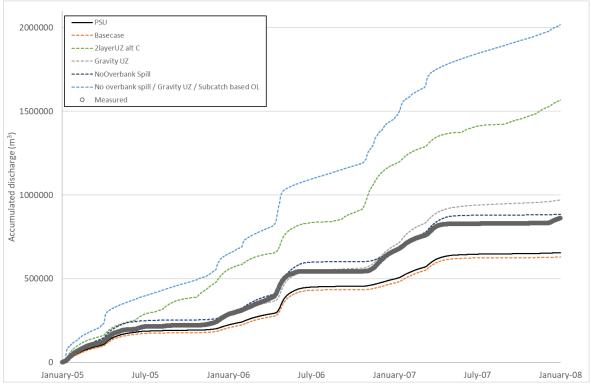


Figure 3-13. Modelled and measured accumulated discharge downstream of Eckarfjärden (PFM002668) for selected calculation cases. Modelled discharge from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

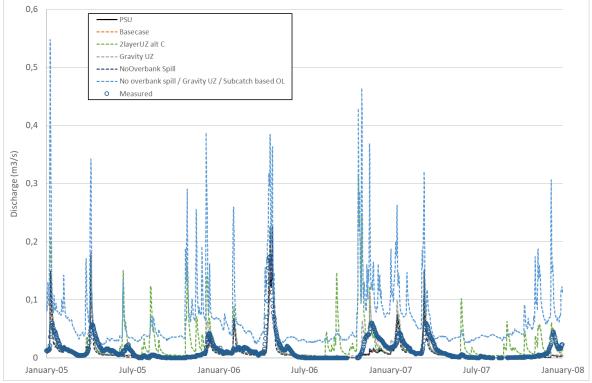


Figure 3-14. Modelled and measured discharge downstream of Gunnarsboträsket (PFM002669) for selected calculation cases. Modelled discharge from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

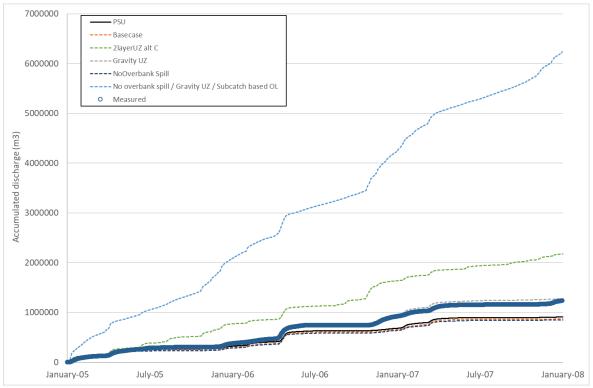


Figure 3-15. Modelled and measured accumulated discharge downstream of Gunnarsboträsket (PFM002669) for selected calculation cases. Modelled discharge from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

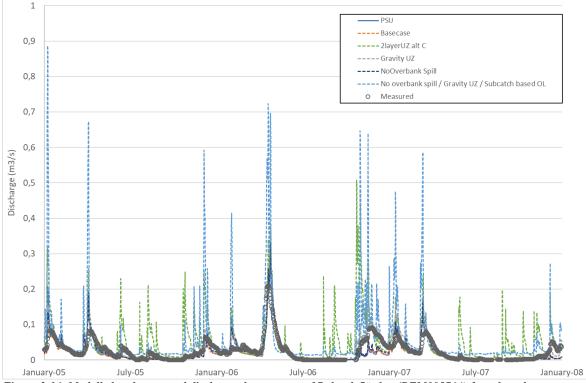


Figure 3-16. Modelled and measured discharge downstream of Bolundsfjärden (PFM005764) for selected calculation cases. Modelled discharge from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

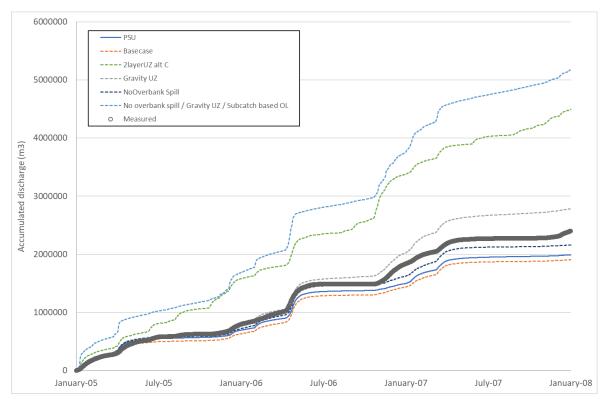


Figure 3-17. Modelled and measured accumulated discharge downstream of Bolundsfjärden (PFM005764) for selected calculation cases. Modelled discharge from the MIKE SHE model produced during the PSU project (FPSAR and PSAR SFR, see Werner et al. 2013) is also presented as a point of comparison.

4 Autocalibration test

The model results presented in Section 3 show the groundwater levels, lake levels and flow-rates calculated by the individual calculation cases presented in Section 2.2. Model parameterizations for all of the calculation cases were primarily based on the model parameterization of the base case (see Appendix B). Of all of the calculation cases considered, CC5b has the shortest runtime of ~2 hours (Table 3-4). It was therefore decided to try and further investigate the potential of this model structure to capture observed hydrological characteristics at Forsmark via model calibration as it is this calculation case that has the largest potential to be used within a Monte-Carlo modelling framework.

Calibration of CC5b is conducted using the "AutoCal" tool available in MIKE SHE. The AutoCal tool is used for performing automatic calibration, parameter optimization, sensitivity analysis and scenario management, and can be used with several the DHI Software tools. It evaluates the model performance for the analyzed parameter sets by calculating a number of comparison statistics between observations and model simulated result. A model simulation in AutoCal can be defined as a sequence of individual model runs where specific parameters are adjusted, performance measures (in this case the RMSE, see eq. A-3) are examined after each simulation and an optimal parameter set is chosen according to which parameter values resulted in the best model performance. Model calibration in this manner is conceptually different than the calibration exercises performed for the hydrological modelling for FPSAR and PSAR SFR wherein model calibration was carried out manually (Werner et al. 2013).

Due to the large list of individual parameters and coupled modules in CC5b, the calibration procedure focused on the overland flow parameters only. This was done for two primary reasons: a) substantial effort was already put into the calibration of the subsurface parameters used in the model during the modelling work pursued under FPSAR and PSAR SFR (Werner et al. 2013) so it is assumed that many of these parameters should represent a realistic parameter set. And b) the overland flow procedures are largely empirical in nature (see Section 2.2.10) where the governing parameters are traditionally attained via calibration procedures.

Time and resource constraints inherent to this study prohibited a comprehensive analysis of the modelling results throughout the calibration exercise. As it was only the overland flow parameters which were included in the calibration exercise, results of the calibration focused only on the modelled overland flow and ignored the modelled groundwater and lake levels. Furthermore, due to these same time and resource constraints, the autocalibration exercise only examined the Gunnarsboträsket watershed (Figure 4-1) as it was here that the "uncalibrated" calculation case performed worst (Figure 3-9, Figure 3-14 and Figure 3-15). It was assumed that any improvements in model performance, pertaining to modelled discharge from Gunnarsboträsket, would be most notable in this watershed.

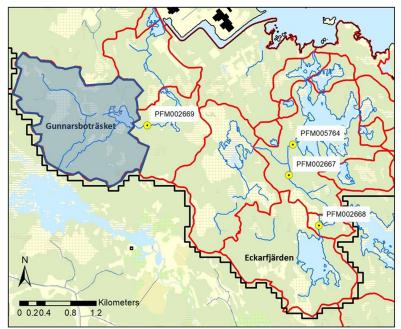


Figure 4-1. Portion of entire MIKE SHE model area with the watershed for Gunnarsboträsket highlighted in blue. Model results for the auto calibration of the "No overbank spill for surface water bodies / gravity flow for unsaturated zone / subcatchment method for overland flow" calculation case are examined relative the measured discharge data at PFM002669.

When using the overland flow module, the entirety of the Gunnarsboträsket watershed is considered as a single hydrological unit and all spatial discretization of the surface properties within the watershed are ignored. This significantly reduces the number of parameters needed to run the overland flow calculations. The subcatcment module has five different parameters that drive the model. These parameters are: slope (-), slope length (m), Manning Number (m^{1/3}/s), detention storage (mm) and initial depth (m).⁹ The calibration exercise examined all of these aforementioned parameters with the exception of the "initial depth" which defines the initial value of the constanthead boundary condition at the outer cells. This parameter is normally set to zero (DHI 2022) which is why this parameter was ignored.

Early attempts to calibrate the model through variation of gave disappointing results which are not shown in this report. Investigations into why results were lacking in expected performance indicated that the "drainage time constant" parameter in the saturated zone module should also be calibrated in order to adjust the amount of ponded water able to reach the saturated zone. The parameter names and the parameter ranges examined in the autocalibration exercise are presented Table 4-1.

Table 4-1. Parameter names and calibration ranges investigated in the autocalibration. The resulting "best
estimates" of the parameter values are also given. The parameters "slope", "slope length", "Manning M" and
"Detention storage" are inherent to the overland flow module in MIKE SHE. The parameter "Drainage time
constant" is inherent to the saturated flow module in MIKE SHE.

Parameter name	Unit	Initial value	Lower bound	Upper bound	Best estimate
Slope	-	0.1	0.0001	10	5.36
Slope length	m	100	10	1000	736
Manning M	m ^{1/3} s ⁻¹	10	1	25	12.6
Detention storage	mm	1	0	2	1.26
Drainage time constant	s ⁻¹	1×10 ⁻⁵	1×10 ⁻⁸	0.001	2.68×10 ⁻⁶

The calibration period used in the autocalibration exercise was March 1st through September 1st, 2006. This period was chosen as it contained both a snow-melting period and a relatively dry period.

⁹ More information on these parameters and their meaning within the context of the subcatchment flow module in MIKE SHE can be found in Chapter 25 in DHI (2022).

Once calibrated, the model was run for a longer period of time (2004-2007) and compared to both the pre-calibrated version of the calculation case and the measured data (2005-2007).

The parameter values which gave the best fit are listed in Table 4-1. Modelled and measured discharge downstream of Gunnarsboträsket is shown in Figure 4-2. Modelled and measured accumulated discharge downstream of Gunnarsboträsket is shown in Figure 4-3. The calibrated model shows a marked improvement in the modelled discharge relative the measured data (Figure 4-2), however, the modelled flows are still consistently higher than those indicated by the measured which, over the two-year period examined, results in an additional 1.5×10^6 m³ of discharge compared to the measured data (Figure 4-3). However, this is a substantial improvement over the uncalibrated model which, over the two-year period examined, produced over 4×10^6 m³ of additional discharge (Figure 4-3). These results indicate that a more comprehensive calibration exercise would likely yield more fruitful results. These results also show that the AutoCal tool in MIKE SHE can be used for future calibration exercises.

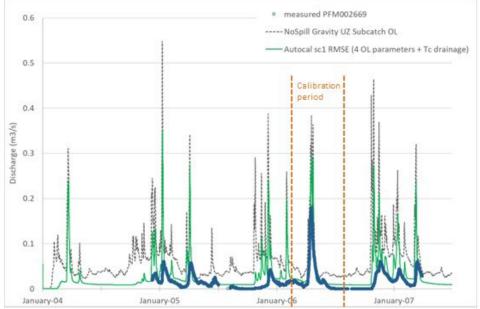


Figure 4-2. Modelled discharge downstream of Gunnarsboträsket for the uncalibrated (grey dotted line) and calibrated model (green line) as well as the measured discharge data at PFM002669 (blue dots) and the calibration period.

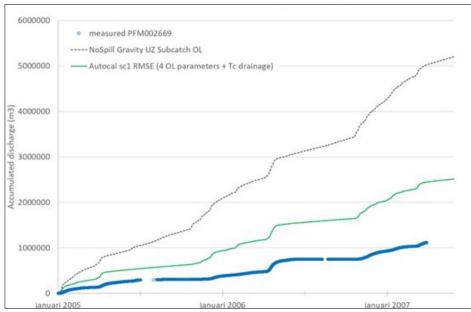


Figure 4-3. Accumulated discharge downstream of Gunnarsboträsket for the uncalibrated (grey dotted line) and calibrated model (green line) as well as the measured accumulated discharge at PFM002669.

5 Suggested future work

This study presented modelling results from 10 different MIKE SHE hydrological model structures and briefly assessed the performance of each against measured groundwater levels, lake levels and streamflow data. The overall purpose of this study was to examine how changes in model structure would affect model runtimes. However, any further perusal of the work presented herein would require a robust analysis of model behaviour and performance before any concrete conclusions can be made which would support a simplification of the model structure represented by the base case in this study. Any future work which intends to continue where this study leaves off should include the following points of analysis:

- An examination of model performance which uses different more robust performance metrics, especially when concerning the performance of the simulated discharge (e.g. Nash-Sutcliffe Efficiency and RMSE).
- An examination of the water-balances for the model area and local water balances for the areas surrounding the lakes. The water balances should be compared to those for the site-descriptive model developed in MIKE SHE.
- Analyses of model sensitivity pertaining to changes in model structure. This should include a sensitivity analysis of the model structure used for the base case as well as sensitivity analyses for the individual model structures considered in the future analyses.

References

SKB's (Svensk Kärnbränslehantering AB) publications can be found at www.skb.com/publications.

Bosson E, Sassner M, Sabel U, Gustafsson L-G, 2010. Modelling of present and future hydrology and solute transport at Forsmark - SR-Site Biosphere. SKB R-10-02, Svensk Kärnbränslehantering AB.

DHI, 2022. MIKE SHE – User Guide and Reference Manual. Dansk Hydraulisk Institut. Hørsholm, Denmark.

DHI, 2017. MIKE 11 – User Guide. Dansk Hydraulisk Institut. Hørsholm, Denmark.

Graham D, Butts M, 2005. Flexible, integrated watershed modelling with MIKE SHE. In Singh V P, Frevert D K (eds). Watershed Models. Boca Raton FL: CRC Press, 245–272.

Richards L A, 1931. Capillary conduction of liquids through porous mediums. Physics, 1(5), 318–333.

Sassner M, Liakka J, Mayotte J-M, 2022. Effects of a warmer climate on near-surface water balances of biosphere objects examined in the post-closure safety assessments for SFR. Simulations with MIKE SHE SR-PSU 5000 AD model. SKB P-22-05, Svensk Kärnbränslehantering AB.

SKB, 2011. Long-term safety for the final repository for spent nuclear fuel at Forsmark – Main report of the SR-Site project – Volume III. SKB TR-11-01, Svensk Kärnbränslehantering AB.

SSM, 2018. Strålsäkerhet efter slutförvarets förslutning. SSM 2018:07, Strålsäkerhetsmyndigheten, Sweden.

Van Genuchten M T, 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil science society of America journal, 44(5), 892–898.

Werner K, Sassner M, Johansson E, 2013. Hydrology and near-surface hydrogeology at Forsmark - synthesis for the SR-PSU project – SR-PSU Biosphere. SKB R-13-19, Svensk Kärnbränslehantering AB.

Yan J, Smith K R, (1994). Simulation of integrated surface water and ground water systems-model formulation 1. Journal of the American Water Resources Association, 30(5), 879–890.

Appendix A

Equations for mean absolute error (MAE) and mean error (ME)

The mean error (ME) is defined as

$$ME = \frac{1}{n} \sum_{t} (x_{t} - y_{t})$$
 (A-1)

Where y_t is the modelled data-point at time t, x_t is the observed data-point at time t and n is the total number of data points.

The mean absolute error (MAE) is defined as

$$MAE = \frac{1}{n} \sum_{t} |(x_{t} - y_{t})|$$
(A-2)

The root-mean squared error (RMSE) is defined as

$$RMSE = \sqrt[\pm]{\sum_{t} \frac{(x_t - y_t)^2}{n}}$$
(A-3)

Appendix B

 Table B-1. Model name, calculation parameters, model area file name and topographical input file name for the base case

Name of model : PSU_regional2000AD_R85_131213.she

Name	Values	Unit
Time step control		
Time Steps		
Initial basic time step	1	hrs
Max allowed OL time step	1	hrs
Max allowed UZ time step	1	hrs
Max allowed SZ time step	3	hrs
Increment of reduced time step length		
Increment rate (0-1)	0,05	-
Parameters for Precipitation-dependent time step control		
Max precipitation depth per time step	3	mm
Max infiltration amount per time step	1,00E+06	
Input precipitation rate requiring its own time step		mm/hr
OL Computational Control Parameters		
Solver type and solver-specific parameters		
Explicit; Max Courant number (0.1 - 0.9)	0,75	
Common stability parameters		
Treshold water depth for overland depth	0,001	m
Threshold gradient for applying low-gradient flow reduction	0,001	
Overland-river exchange calculation		
Weir formula: Threshold head difference for applying low-gradient flow reduction	0.1	m
	-,-	
UZ Computational Control Parameters		
UZ-SZ coupling control		
Max profile water balance error	0,001	m
Richards equation parameters		
Max no of iterations	50	
Iteration stop criteria (fraction of psi)	0,002	
Max water balance error in one node (fraction)	0,03	
	_,	
SZ Computational Control Parameters		
Solver type		
PCG, transient		
Iteration control		
Max no of iterations	80	
Max head change per iteration	0,05	m
Max residual error	0,005	m/d
Sink de-activation in drying cells		
Saturated thickness threshold	0,05	m
Advanced settings		
Gradual drain-activation	active	
Horizontal Conductance averagins between iterations	active	
No under-relaxation	active	
Maximum exhange från river during one time step		
Max fraction of H-point volume	0,9	
F	-/-	

Model area file name Topography file name PSU_regional.dfs2 fm_dem_110428_extent_SRsite_flatsea2000AD.dfs2

 \Box

	File / value	Unit
Precipiation rate	Precipitation_Högmasten_extrapol_030512-101231.dfs0	
Reference Evapotranspiration	on PET_SICADA2SHE_030514-101231_red15proc.dfs0	
Air temperate	Temperature_Högmasten_030512-101231.dfs0	
Snow Melt		
Melting temperatute	0,5	degC
Degree-day coefficient	1,5	mm/C/d
Min snow storage	0	mm/C/d
Max Wet Snow Fraction	0,1	
Initial Total Snow Storage	0	mm/C/d
Initial Wer Snow Fraction	0	

Table B-2. Climate input file-names (precipitation, PET and temperature) and the snow-melt parameters used in the base case.

 Table B-3. MIKE 11 filename, vegetation data layers and parameters used for the overland flow calculations for the base case.

	File / value	Unit
River		
MIKE 11 file name	SRPSU regional_R85_131213.sim11	
Land use		
Vegetation file	vegetation_lakecharacterisation.dfs2	
	(8 classes for vegetation)	
Vegetation property file	Rotdjup_1m_kc1_Barr_Snow.ETV	
Overland flow		
Manning number (M)	5	m ^{1/3} s ⁻¹
Detention storage	2	mm
Initial depth	OLdepth_070315_noOLinit.dfs2	

Table B-4. Soil profile data layers, vertical discretization of calculation layers and unsaturated soil property files for the unsaturated zone in the base case.

	File / value
Soil profile definitions	UZ_soil_profile_definition_QD2000_Eckfj.dfs2
	(21 different soil classes in file for soil profile definitions)
Vertical discretization (all classes)	0.1 m (10); 0.5 m (8); 1 m (5); 2 m (5)
Unsaturated soil property files	
	Calle ODM UZ deservations and
All except Eckarfjärden	Soils_SDM_UZ_description.uzs
Within Eckarfjärden	Soils_SDM_UZ_description_Eckarfj.uzs
Specified classification	UZ_codes_drainDiv5.dfs2

	Lover level (m.a.s.l)	Kh (m/s)	Kv (m/s)	Specific yield (-)	Specific storage (m ⁻¹)	
<i>Geological layers</i> zla	TOPO_PP_minus03inselections_ext.dfs2	KhZ1_originalKvalues_SeaandLakes_drGäll:		Density 71, succeeded 1, coordon		
					Porosity_Z1a_extended_korr090407_SRsite.df: Ss_Z1a_extended_korr090407_SRsite.dfs2 Porosity_Z1_extended_korr090407_SRsite.dfs: Ss_Z1_extended_korr090407_SRsite.dfs2	
1	z1_IL_v2_ext.dfs2	KhZ1_originalKvalues_SeaandLakes_drGäll:				
2	z2_ll_v2_ext.dfs2	3,00E-07	3,00E-07	0,05	0,005	
3o	z3o_ll_v2_ext.dfs2	0,00015	0,00015	0,2	0,35	
3a	z3a_IL_v2_ext.dfs2	0,00015	0,00015	0,2	0,004	
:4a	z4a_ll_v2_ext.dfs2	3,00E-07	3,00E-07	0,03	0,006	
4Ь	z4b_ll_v2_ext.dfs2	Kxy_Z4b_div30lakes_ejL3_korr1e-8.dfs2	Kv_Z4b_div30lakes_ejL3_korr1e-8.dfs2	0,03	0,006	
ЗЬ	z3b_ll_v2_ext.dfs2	0.00015	0.00015	0.2	0.35	
5	z5_ll_v2_ext.dfs2	Kxy_Z5_Eckarfj_SRsite.dfs2	Kv_Z5_SRsite.dfs2	Porosity_Z5_SRsite.dfs2	0.001	
6	z6_lLv12_ext.dfs2	1,50E-06	1,50E-06	0.15	0,0001	
, tberg	Lowerlevel_Ytberg.dfs2	kh_ytberg.dfs2	kz_ytberg.dfs2	Porosity_Z5_SRsite.dfs2	0,0001	
iedrock+22m	22	kh_ll22m.dfs2	kz_JI22m.dfs2	por_ll22m.dfs2	5,00E-09	
edrock+6m	6	kh_ll6m.dfs2	kz_ll6m.dfs2	por_ll6m.dfs2	5,00E-09	
edrock-10m	-10	kh_ll-10m.dfs2	kz_II-10m.dfs2	por_II-10m.dfs2	5,00E-09	
ledrock-26m	-26	kh_ll-26m.dfs2	kz_II-26m. dfs2	por_II-26m.dfs2	5,00E-09	
ledrock-42m	-42	kh_ll-42m.dfs2	kz_II-42m.dfs2	por_II-42m.dfs2	5,00E-09	
edrock-58m	-58	kh_ll-58m.dfs2	kz_II-58m.dfs2	por_II-58m.dfs2	5,00E-09	
edrock-74m	-74	kh_ll-74m.dfs2	kz_II-74m.dfs2	por_II-74m.dfs2	5,00E-09	
edrock-90m	-90	kh_ll-90m.dfs2	kz_II-90m.dfs2	por_II-90m.dfs2	5,00E-09	
edrock-106m	-106	kh_ll-106m.dfs2	kz_ll=106m.dfs2	por_II-106m.dfs2	5,00E-09	
edrock-100m iedrock-122m	-100	kh_ll=100m.arsz kh_ll=122m.dfs2	kz_li-100m.arsz kz_li-122m.dfs2		5,00E-09	
				por_II-122m.dfs2		
Bedrock-138m	-138	kh_ll-138m.dfs2	kz_II-138m.dfs2	por_II-138m.dfs2	5,00E-09	
Bedrock-154m	-154	kh_ll-154m.dfs2	kz_II-154m.dfs2	por_11-154m.dfs2	5,00E-09	
ledrock-170m	-170	kh_ll-170m.dfs2	kz_II-170m.dfs2	por_11-170m.dfs2	5,00E-09	
iedrock-186m	-186	kxy178m_minvalue.dfs2	kz178m_minvalue.dfs2	por178m_just.dfs2	5,00E-09	
ledrock-202m	-202	kxy194m_minvalue.dfs2	kz194m_minvalue.dfs2	por194m_just.dfs2	5,00E-09	
iedrock-218m	-218	kxy210m_minvalue.dfs2	kz210m_minvalue.dfs2	por210m_just.dfs2	5.00E-09	
ledrock-234m	-234	kxy226m_minvalue.dfs2	kz226m_minvalue.dfs2	por226m_just.dfs2	5.00E-09	
edrock-262m	-262				5,00E-03	
		kxy242m_minvalue.dfs2	kz242m_minvalue.dfs2	por242m_just.dfs2		
edrock-314m	-314	kxy282m_minvalue.dfs2	kz282m_minvalue.dfs2	por282m_just.dfs2	5,00E-09	
ledrock-378m	-378	kxy346m_minvalue.dfs2	kz346m_minvalue.dfs2	por346m_just.dfs2	5,00E-09	
Bedrock-442m	-442	kxy410m_minvalue.dfs2	kz410m_minvalue.dfs2	por410m_just.dfs2	5,00E-09	
Bedrock-506m	-506	kxy474m_minvalue.dfs2	kz474m_minvalue.dfs2	por474m_just.dfs2	5,00E-09	
Bedrock-570m	-570	kxy538m_minvalue.dfs2	kz538m_minvalue.dfs2	por538m_just.dfs2	5.00E-09	
Bedrock-634m	-634	kxy602m_minvalue.dfs2	kz602m_minvalue.dfs2	por602m_just.dfs2	5,00E-09	
				port open classifier	0,002 00	
Geological lenses		0.0001	0.0001		0.8925	
lav		0,0001	0,0001	0,2	0,0025	
lorisontal extent	Sea2000AD_demlt-068_shoreline_rev-pir.df	s2				
Jpper level	-0,68					
.owerlevel	fm_dem_110428_extent_SRsite.dfs2					
	Lower level	Initial head	Outer boundary conditions	Inner boundary conditions		
Computational layer.						
lego1	fm_dem_110428_extent_SRsite_minus_thick		Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030		Fixed head: hav-surfacewater-head_PFM10038_030501-10	
Rego2	z6_ll_v12_ext.dfs2	SZhead_L2_070315.dfs2	Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030			
ledrock-10m	-10	SZhead_L3_070315.dfs2	Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030	0501-101 -		
edrock-26m	-26	SZhead_L4_070315.dfs2	Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030			
edrock-42m	-42	SZhead_L5_070315.dfs2	Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030			
edrock-58m	-58	SZhead_L6_070315.dfs2	Land: Zero-flux; Sea: hav-surfacewater-head_PFM10036_030			
edrock-30m edrock-74m	-50		Land: Zero-flux; Sea: hav-surfacewater-head_PFM10036_030 Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030			
		SZhead_L7_070315.dfs2				
edrock-90m	-90	SZhead_L8_070315.dfs2	Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030			
edrock-90m edrock-106m	-90 -106	SZhead_L9_070315.dfs2	Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030	D501-101 -		
edrock-90m edrock-106m	-90 -106 -138			D501-101 -		
edrock-90m edrock-106m edrock-138m	-90 -106	SZhead_L9_070315.dfs2	Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030	0501-101 - 0501-101 -		
edrock-90m edrock-106m edrock-138m edrock-170m	-90 -106 -138	SZhead_L9_070315.dfs2 SZhead_L10_070315.dfs2 SZhead_L11_070315.dfs2	Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030 Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030 Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030	D501-101 - D501-101 - D501-101 -		
edrock-90m edrock-106m edrock-138m edrock-170m edrock-202m	-90 -106 -138 -170 -202	SZhead_L9_070315.dfs2 SZhead_L10_070315.dfs2 SZhead_L11_070315.dfs2 SZhead_L12_070315.dfs2	Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030 Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_033 Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030 Land: Zero-flux; Sea: hav-surfacewater-head_PFM10038_030	D501-101 - D501-101 - D501-101 - D501-101 - D501-101 -		
edrock-90m edrock-106m edrock-138m edrock-170m edrock-202m edrock-204m	-30 -106 -138 -170 -202 -234	SZhead_L9_070315.dfs2 SZhead_L10_070315.dfs2 SZhead_L11_070315.dfs2 SZhead_L12_070315.dfs2 SZhead_L13_070315.dfs2	Land Zero-flux; Sea: hav-surfacev ater-head_PFM10038_033 Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_033 Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_033 Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_033	D501-101 - D501-101 - D501-101 - D501-101 - D501-101 -		
edrock-90m edrock-106m edrock-138m edrock-170m edrock-202m edrock-234m edrock-314m	-90 -106 -138 -770 -202 -234 -314	SZhead_L9_070315.dfs2 SZhead_L10_070315.dfs2 SZhead_L11_070315.dfs2 SZhead_L12_070315.dfs2 SZhead_L13_070315.dfs2 SZhead_L14_070315.dfs2	Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_030 Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_030 Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_030 Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_030 Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_030	3501-101 - 3501-101 - 3501-101 - 3501-101 - 3501-101 - 3501-101 -		
Sedrock- /4m Bedrock-300m Bedrock-130m Bedrock-130m Bedrock-202m Bedrock-202m Bedrock-234m Bedrock-314m Bedrock-314m Bedrock-634m	-30 -106 -138 -170 -202 -234	SZhead_L9_070315.dfs2 SZhead_L10_070315.dfs2 SZhead_L11_070315.dfs2 SZhead_L12_070315.dfs2 SZhead_L13_070315.dfs2	Land Zero-flux; Sea: hav-surfacev ater-head_PFM10038_033 Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_033 Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_033 Land: Zero-flux; Sea: hav-surfacev ater-head_PFM10038_033	9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 -		
Bedrock-90m Bedrock-106m Bedrock-138m Bedrock-202m Bedrock-202m Bedrock-234m Bedrock-314m Bedrock-314m	-90 -106 -138 -170 -202 -234 -314 -442 -634	S2head_L9_070315.dfs2 S2head_L10_070315.dfs2 S2head_L10_070315.dfs2 S2head_L12_070315.dfs2 S2head_L12_070315.dfs2 S2head_L13_070315.dfs2 S2head_L14_070315.dfs2	Land Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031	9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 -		
Bedrock-90m Bedrock-106m Bedrock-138m Bedrock-170m Bedrock-202m Bedrock-234m Bedrock-234m Bedrock-634m Drainage	-90 -106 -139 -170 -202 -234 -314 -442 -634 File / value	S2head_L9_070315.dfs2 S2head_L10_070315.dfs2 S2head_L10_070315.dfs2 S2head_L12_070315.dfs2 S2head_L12_070315.dfs2 S2head_L13_070315.dfs2 S2head_L14_070315.dfs2	Land Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031	9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 -		
iedrock-90m iedrock-106m iedrock-108m iedrock-170m iedrock-202m iedrock-234m iedrock-234m iedrock-314m iedrock-634m Wainage	-90 -106 -139 -170 -202 -234 -314 -442 -634 File / value	S2head_L9_070315.dfs2 S2head_L10_070315.dfs2 S2head_L10_070315.dfs2 S2head_L12_070315.dfs2 S2head_L12_070315.dfs2 S2head_L13_070315.dfs2 S2head_L14_070315.dfs2	Land Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031	9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 -		
iedrock-90m iedrock-138m iedrock-138m iedrock-170m iedrock-234m iedrock-234m iedrock-42m iedrock-42m iedrock-634m	-90 -106 -139 -170 -202 -234 -314 -442 -634 File / value	S2head_L9_070315.dfs2 S2head_L10_070315.dfs2 S2head_L10_070315.dfs2 S2head_L12_070315.dfs2 S2head_L12_070315.dfs2 S2head_L13_070315.dfs2 S2head_L14_070315.dfs2	Land Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031	9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 -		
Bedrock-90m Bedrock-106m Bedrock-108m Bedrock-170m Bedrock-202m Bedrock-234m Bedrock-234m Bedrock-422m Bedrock-422m Bedrock-634m Drain-sgr Distributed drainage opti- Level	-90 -106 -138 -770 -202 -234 -314 -442 -634 -634 -634 -634 -634 -634 -635 -026 -026 -026 -026 -026 -026 -026 -026	S2head_L9_070315.dfs2 S2head_L10_070315.dfs2 S2head_L10_070315.dfs2 S2head_L12_070315.dfs2 S2head_L12_070315.dfs2 S2head_L13_070315.dfs2 S2head_L14_070315.dfs2	Land Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031	9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 -		
Sedrock-90m Sedrock-138m Sedrock-138m Sedrock-238m Sedrock-222m Sedrock-234m Sedrock-314m Sedrock-534m Deatrock-634m Deatrock-634m Deatrock-634m Deatrock-634m Deatrock-634m	-30 -706 -738 -770 -202 -234 -314 -442 -534 File <i>i</i> value DrialLevels_revEckar(; dfs2 TC_SRPSU_noneg_121017_revGailsbo.dfs2	S2head_L9_070315.dfs2 S2head_L10_070315.dfs2 S2head_L10_070315.dfs2 S2head_L12_070315.dfs2 S2head_L12_070315.dfs2 S2head_L13_070315.dfs2 S2head_L14_070315.dfs2	Land Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031	9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 -		
Bedrack-90m Bedrack-106m Bedrack-106m Bedrack-106m Bedrack-202m Bedrack-202m Bedrack-234m Bedrack-42m Bedrack-442m Bedrack-634m Drainage Distributed drainage opti- evel Ime constant Drain codes	-90 -006 -138 -170 -234 -314 -442 -634 File / value Drain_evels_revEckarf;dfs2 TC_SRPSU_none_121017_revGailsbo.dfs2 Drain_codes_eckarf;dfs2	S2head_L9_070315.dfs2 S2head_L10_070315.dfs2 S2head_L10_070315.dfs2 S2head_L12_070315.dfs2 S2head_L12_070315.dfs2 S2head_L13_070315.dfs2 S2head_L14_070315.dfs2	Land Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031	9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 -		
edrock-30m edrock-136m edrock-136m edrock-170m edrock-202m edrock-234m edrock-442m edrock-442m edrock-634m kain.ege istributed drain.age opti- evel me constant	-30 -706 -738 -770 -202 -234 -314 -442 -534 File <i>i</i> value DrialLevels_revEckar(; dfs2 TC_SRPSU_noneg_121017_revGailsbo.dfs2	S2head_L9_070315.dfs2 S2head_L10_070315.dfs2 S2head_L10_070315.dfs2 S2head_L12_070315.dfs2 S2head_L12_070315.dfs2 S2head_L13_070315.dfs2 S2head_L14_070315.dfs2	Land Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_030 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031 Land: Zero-Hux; Sex hav-surfacevater-head_PFM10038_031	9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 - 9501-101 -		

Table B-5. Input files, parameterization, discretization of calculation layers and files listing initial conditions for the saturated zone in the base case.