Norges miljø- og
biovitenskapelige
universitet

Masteroppgave 2023 30 stp
Fakultet for realfag og teknologi

Hydrology of Green Roofs: Inverse Modelling in MODFLOW 6 for Estimating the Saturated Hydraulic Conductivity of a LECA Storage Layer

Grønne taks hydrologi: Invers modellering i MODFLOW 6 for å estimere mettet hydraulisk konduktivitet til et magasinerende LECA-lag

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Acknowledgements

First of all, I would like to express my gratitude to my main supervisor Assoc. Prof. Vegard Nilsen, and co-supervisor Assoc. Prof. Nils-Otto Kitterød for supporting me with the opportunity to work on the interesting and challenging research subject and for discussions and guidance along the way.

Finally, I would like to express my gratitude to my parents and to my lovely wife, Ranie Abu Nima. Thank you for all the help you have given me through all the time of learning and studying. Thank you for lifting me, and for the opportunities ahead. None of the achievements in my life would be possible without your endless love and support.

With gratitude
Noor M. N. Al-khayyat

Abstract

This thesis presents a study on the modelling of green roofs as a stormwater management tool using MODFLOW 6 with the ModelMuse interface. The objective of the research is to evaluate the reliability and capability of MODFLOW 6 as a modelling tool for green roofs and to estimate the hydraulic conductivity of the drainage layer on green roofs. The research work is based on a steady-state experiment conducted on the green roof (4cm of sedum and 15cm of Lightweight Expanded Clay Aggregate; LECA 0-6mm) at the research facility for green roofs at the Norwegian University of Life Sciences (NMBU). The roof was constructed in 2018 and monitored since then, with live data logging from eight water head sensors, and recording of run-off, precipitation, temperature, and several other hydrological parameters.

The use of MODFLOW 6 to simulate the flow in green roofs is not as common as its use as a simulating tool for groundwater flow. In this thesis, the reliability of MODFLOW to model the flow in green roofs under steady-state conditions was successfully evaluated by matching the modelling result with an analytical solution of the flow equations in the drainage layer of the green roof.

In this research work, the model was calibrated for hydraulic conductivity (K) against the observation data from 8 sensors representing the hydraulic head in the green roof. The calibration processes were carried out using both manual calibrations with the Mean Absolute Error (MAE) as the objective function, and inverse modelling with the Parameter ESTimation (PEST) modelling in MODFLOW 6.

The results of this work showed that the model was able to accurately predict the hydraulic conductivity based on the observed hydraulic head in the green roof. Based on the modelling of the steady-state experiment, the hydraulic conductivity of LECA 0-6mm as the drainage layer of the green roof was estimated as $K = 1.5 \cdot 10^{-3}$ $[\mathrm{m/s}]$. This modelled value closely approximates the laboratory-measured value $K_{lab.} = 1.4 \cdot 10^{-3}$ $[\mathrm{m/s}]$. Furthermore, It has been found that the lower values of hydraulic conductivity ($K \leq 1.3 \cdot 10^{-3}$ $[\mathrm{m/s}]$) made the hydraulic head rise higher than the thickness of the drainage layer, while the higher values ($K > 1.6 \cdot 10^{-3}$ $[\mathrm{m/s}]$) made the model dry. Additionally, It was discovered that The calibrated K-value is relatively insensitive to the choice of boundary condition, i.e. the head value at the drain outlet.

MODFLOW 6 proved to be a very robust and powerful physical-based modelling tool that was able to effectively simulate the steady flow in the drainage layer of the green roof in this research work. For the transient flow model which simulates the scenario of time-depending precipitation (unsteady-state conditions), MODFLOW 6 should be evaluated and more research should be conducted.

Contents

1. Introduction

Climate change is expected to have an impact on the Nordic countries in terms of increased temperatures and rainfall. Norway's average annual rainfall has already increased by 20% in the past century. It is expected that heavy rainfall events will continue to occur more frequently throughout the 21st century (Norwegian Ministry Of Climate and Environment, 2013). Moreover, urbanization has led to a greater proportion of ground surfaces being paved over and becoming impervious to rainfall. Thus, the annual mean runoff in east Norway increased by 7.2% (from 1961-1990 to 1991-2020) (Beldring et al., 2022). As a result, more stormwater runs off on the surface instead of infiltrating locally. Therefore, traditional urban stormwater management solutions and strategies are no longer sufficient to address this problem (Andenæs et al., 2018).

In urban areas where stormwater systems are limited, green roofs could be an efficient stormwater management tool (Zheng et al., 2021). Different types of green roofs exist, with variations in the type of drainage layers and vegetation used. The catchment area of the green roof includes not only the roof itself but also vegetation and drainage layers that contribute to the overall water retention capacity (Getter & Rowe, 2006).

In this thesis, the study is performed on an extensive green roof at the facility of green roof research at the Norwegian University of Life Sciences (NMBU). This green roof is a system of vegetated roof that consists of a growth medium (vegetation, 4 cm of Sedum) and a drainage layer (15 cm of Lightweight Expanded Clay Aggregate (LECA) of type 0-6C (≤6 mm)). The benefits of this type of roof are to delay peak runoff, reduce the volume of the runoff, improve surface water quality, and reduce flooding risks in urban areas. (Li & Babcock Jr, 2014).

Optimizing green roofs as a stormwater management tool is based on understanding the flow behaviour in the drainage layer and the effect of the growing medium. In particular, the roof's geometric layout, the nature of the vegetation layer, and the hydraulic conductivity of the drainage layer are critical factors that affect the retention characteristics of green roofs in urban areas where traditional stormwater management is limited (Berndtsson, 2010).

Conceptual modelling of the green roof flow behaviour (i.e. based on the rational method) has been studied using conceptual modelling tools such as SWMM (Burszta-Adamiak &

Mrowiec, 2013; Cipolla et al., 2016), and DDD-urban (Bassøe, 2020). Other studies considered physical-based modelling such as HYDRUS 1-D (Hilten et al., 2008; Palla et al., 2012) and SEEP/W (Eriksson, 2013). This thesis focuses on using physical-based modelling to study the physical behaviour of the flow in the green roof using MODFLOW 6.

Modelling software such as MODFLOW 6 is routinely used for numerical simulation of the groundwater flow in geological porous media. MODFLOW 6 has the possibility to optimize the performance of the finite-difference flow model by experimenting with different scenarios based on field observations and predefined parameters (Langevin et al., 2017). However, the use of MODFLOW 6 for studying green roof behaviour is less common. The flow of water in green roofs is governed by the equations of flow in porous media (Darcy and continuity equations), which are also used to model the flow in geological subsurface systems in MODFLOW 6. This similarity suggests that the finite-difference model in MODFLOW 6 could also be applied to simulate the flow behaviour in green roofs.

In this thesis, a numerical model in MODFLOW 6 as well as an analytical-mathematical solution were performed to examine the flow behaviour on the green roof. The research work was based on a steady-state recharge experiment performed by Bassøe (2020) and Ydse (2021) conducted at NMBU. The model is first built in MODFLOW 6 and manually calibrated by tuning both the hydraulic conductivity of the drainage layer and the boundary conditions in order to minimize the Mean Absolute Error (MAE) between the observed and simulated hydraulic heads. Next, the calibration was conducted by the numerical inverse modelling which was carried out in MODFLOW 6 utilizing the PEST modelling package (Parameter ESTimation).

The purpose of this thesis is to apply MODFLOW 6 to interpret the data from the previous steady-state recharge experiment (Bassøe, 2020; Ydse, 2021), and also gain experience using MODFLOW 6 for calibration and modelling the hydrologic behaviour of green roofs. In particular, this thesis aims to address the following research questions:

1. How can the boundary conditions at the drain be implemented in MODFLOW 6, and how does the variation in boundary conditions at the drain of the roof affect the simulated head?

2. What are the advantages and disadvantages of calibrating the model using the inverse modelling features in MODFLOW 6 (PEST) compared to manual calibration methods?
3. What is the best estimate of the hydraulic conductivity of the green roof at NMBU, and is the hydraulic conductivity uniformly distributed throughout the storage medium?
4. How suitable is MODFLOW 6 as a tool to simulate run-off from green roofs?

2. Methodology

The vegetation of the green roof in this study is 4 cm of Sedum and the substrate layer is 15 cm of Lightweight Expanded Clay Aggregate (LECA) of type 0-6C (≤6 mm). The research work is based on a steady-state flow experiment, thus the vegetation layer was not included in the model since it only has an effect in a transient model with time-dependent precipitation.

This methodology section aims to provide the theoretical background for water flow processes in the green roof, clarify the calibration processes and the implementation method of the numerical model, explain the development of the model and describe how to collect and analyze data from green roofs to develop a green roof water flow model in MODFLOW 6. The methodology of this thesis is described in the flow-chart in Figure 1:

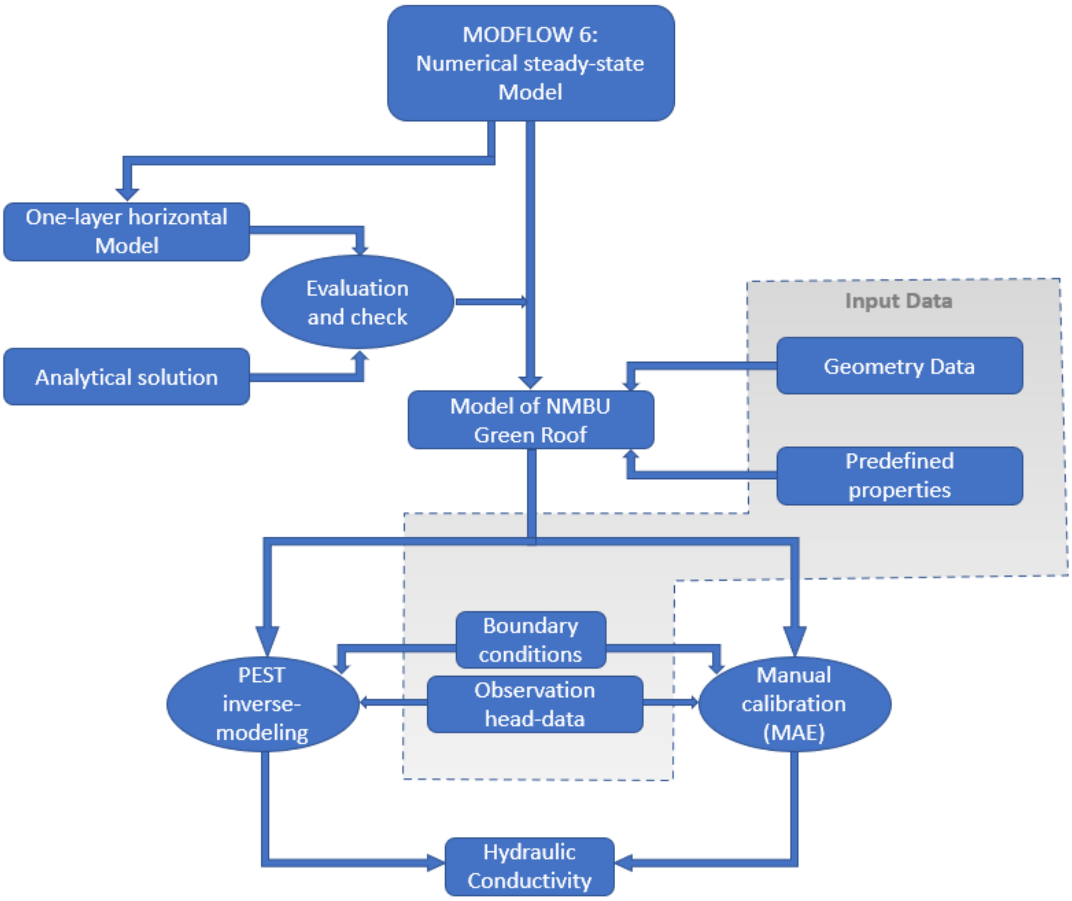

Figure 1: Simplification of the Methodology and the solution approach

2.1. Design and Data Collection of the Green Roof

The work in this thesis is part of an ongoing research project at the Norwegian University of Life Sciences (NMBU) on three roofs with identical surface areas; one black roof without the vegetation and substrate layer, and two green roofs. A weather station was constructed by The Norwegian Water Resources and Energy Directorate (NVE, 2018) to record and log the input and the output data of the green roofs, such as the precipitation, wind speed, each roof run-off, and radiation. (Øyre & Trommald, 2018; Viker-Walsøe & Valle, 2020).

One of the green roofs is instrumented with eight sensors (analogue level transducers) that measure the hydraulic head in the substrate of the green roof. The data from the sensors is collected using a data logger, which records the hydraulic head at a frequency of one minute. The map of sensors is shown in Figure 2 and the coordinates are in Table 1.

The calibration processes in this work are based on the result of the steady-flow experiment conducted by Bassøe (2020) and Ydse (2021). In this experiment, the constant recharge (representing the precipitation) was implemented by feeding water from a perforated tube that was laid in a zig-zag pattern on the top surface of the green roof. It was assumed that the distribution of the recharge water was uniformly over the top surface of the green roof. The water feeding was continuously applied for 10 days. In this thesis, the steady-flow data of this experiment were analysed where the steady recharge rate ($N = 5.48 \cdot 10^{-7}$ $[\mathrm{m/s}]$) was respected. Moreover, the hydraulic heads measured by 8 sensors were extracted and considered as observation data for the calibration processes.

In this research work, a field inspection was conducted at the facility of green roof research at the Norwegian University of Life Sciences (NMBU) to provide field data. The purpose of the inspection work was to ensure the measurement of roof dimensions, sensor locations, dimensions of the drain outlet, and the dimension of the vegetation and the drainage layer of the green roofs.

Based on the fieldwork, The surface area of the green roof is obtained by 9.7 m length and 4.7 m width (the total area is 45.6 m^2). The vegetation layer is 4 cm of sedum. The substrate layer is 15 cm of Lightweight Expanded Clay Aggregate (LECA). The LECA is of type 0-6C (≤6 mm) (Leca Norge AS, 2022). The roof bottom geometry consists of two intersecting planes each having a slope of 24 [mm/m], and a drain box (run-off point) at the corner of the roof (see Figure 2).

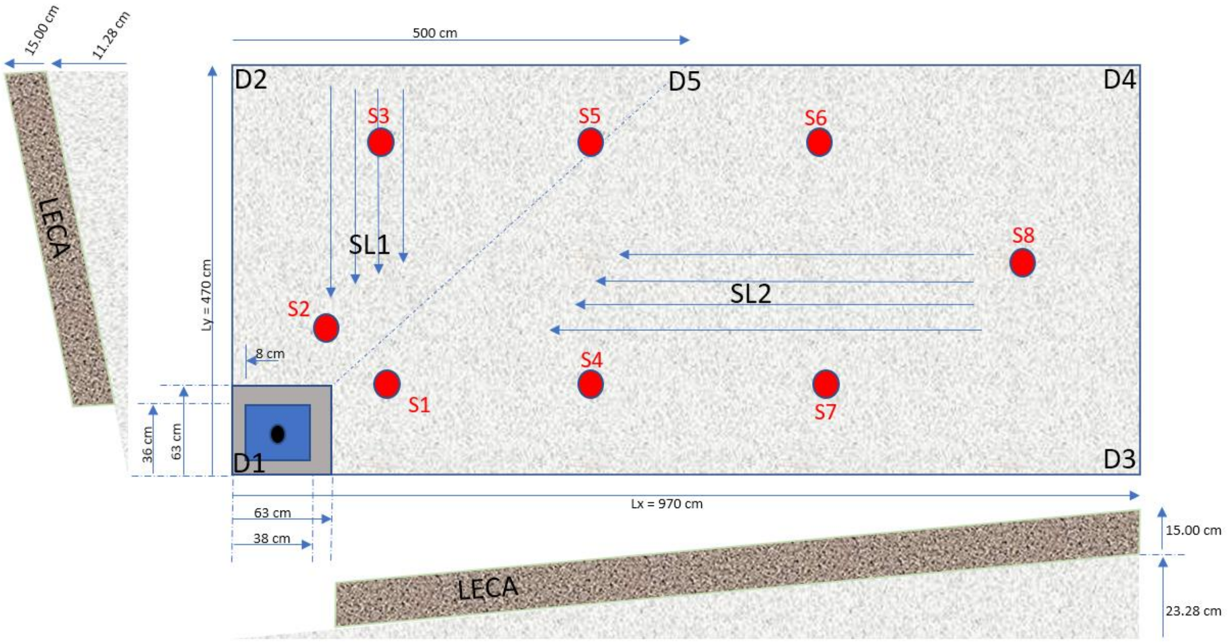

Figure 2: The top and sides-view construction diagram of the green roof with two diagonally crossed surfaces SL1 and SL2. The sensors are marked with S1-S8. The dimensions and the definition of each object are listed in Table 1

Table 1: The name and the coordination of each sensor, the slope of the two surfaces, the measurements of the green roof boundary elevation, and the depth of the LECA layer.

Sensor	Lx [m]	Ly [m]	Object	Length [cm]	Surface	Slope [mm/m]
S1	1.72	0.82	D1 (elevation)	0.00	SL1	24.00
S2	0.99	1.33	D2 (elevation)	11.28	SL2	24.00
S3	1.72	3.46	D3 (elevation)	23.28		
S4	3.36	1.33	D4 (elevation)	23.28		
S5	3.72	3.72	D5 (elevation)	11.28		
S6	6.00	3.52	LECA (depth)	15.00		
S7	5.85	1.22				
S8	8.43	2.46				

2.2. Flow Equations

The substrate layer of the green roof is unconfined, allowing the water table to fluctuate freely as discharge and recharge rates change. In this thesis, an unconfined substrate's hydraulic head equation is calculated using the principles of mass conservation and Darcy's law, which relates hydraulic conductivity, and hydraulic gradient in the subsurface according to the following equation:

Darcy:

$$Q = -K \cdot \nabla h = -\begin{pmatrix} K_{xx} & 0 & 0 \\ 0 & K_{yy} & 0 \\ 0 & 0 & K_{zz} \end{pmatrix} \nabla h \qquad (1)$$

Mass conservation combined with Darcy:

$$\frac{\partial}{\partial_x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial_y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial_z}\left(K_{zz}\frac{\partial h}{\partial z}\right) + Q_s = SS\frac{\partial h}{\partial t} \qquad (2)$$

Here, Q is the Darcy flux, K (K_{xx}, K_{yy}, K_{zz}) is a tensor of the hydraulic conductivity, h is the hydraulic head, ∇h is the gradient of the hydraulic head, SS is the specific storage ($\partial h/\partial t = 0$ at steady-state in this project), t is time, and Q_s is the source/sink term. The hydraulic head h is defined as the potential energy per unit weight of water and is computed from:

$$h = z + \psi \qquad (3)$$

Where z is the elevation and ψ is the pressure head. The source and the derivation of equations (1), (2) and (3) were taken from the following literature: (Harbaugh et al., 2000; Hendriks, 2010; Langevin et al., 2017; Provost et al., 2017).

MODFLOW6 is a software program that models groundwater flow using a numerical approach. It is possible to simulate both transient and steady-state flows with MODFLOW6. Finite-difference numerical methods in MODFLOW 6 could be used to simulate groundwater flow and water flow in porous media in one dimension (single layer) and three dimensions (multiple layers) based on the same equation (1) and (2) (Langevin et al., 2017).

2.3. Model Development

The hydrologic model in this work was developed using MODFLOW 6 and runs through the ModelMuse interface. MODFLOW 6 is a numerical model that simulates the flow of water through porous media using finite-difference numerical methods. ModelMuse is the interface utilized to operate MODFLOW 6. In this thesis, the model was built in MODFLOW 6 using the Node Property Flow (NPF) Package, Time-Variant Specified-Head (CHD), and Recharge (RCH) Package in MODFLOW 6 (Harbaugh, 2005). In this research work, the model was developed to cover and test three scenarios:

- The analytical test of the model: The purpose of this test was to evaluate the reliability of MODFLOW 6 in simulating hydraulic conductivity and hydraulic head on a green roof with a thin layer (15 cm).
- MAE calibrated model: the model was calibrated by minimizing the mean absolute error (MAE) between the observed and simulated hydraulic head in MODFLOW 6. The one-dimension MAE calibration is conducted by tuning the hydraulic conductivity of the green roof drainage layer, while the two-dimension MAE calibration is conducted by tuning the hydraulic conductivity of the green roof drainage layer and the head at the drain outlet
- PEST-calibrated model: this part was conducted by inverse modelling using PEST in MODFLOW 6.

2.3.1. Model Geometry

In this study, it was assumed that the model was isotropic, where the hydraulic conductivity was the same in the x, y, and z directions of the grid. The grid referred to the discretization of the modelled domain into a three-dimensional mesh of cells. Mesh array data was generated based on the dimensions and shape of the green roof layer (Figure 2). The mesh array for the green roof was generated using MatLab as illustrated in Figure 3.

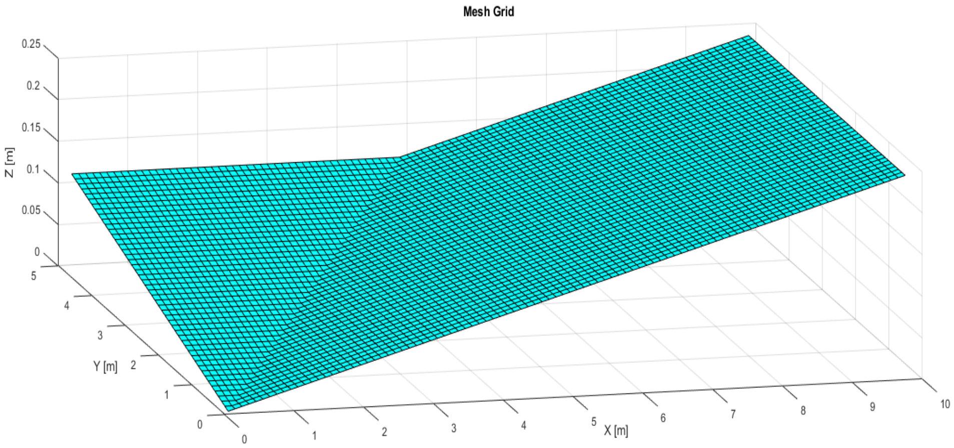

Figure 3: The 3D mesh representing the floor shape of the green roof surface, the x-projection is 9.7[m], and The y-projection is 4.7[m]. The slope along the X side and Y side is 24 [mm/m]. The mesh is an array generated in MatLab.

2.3.2. Model Domain Properties

The NPF Package is a key component of MODFLOW 6 that is used to define the hydraulic properties of the model domain (the drainage layer). The properties of the drainage layer are used to solve the flow equation (equations (1) & (2)) in the finite-difference numerical model in MODFLOW 6. The NPF Package requires input data for the hydraulic properties of the model domain, which can be specified for each cell in the grid. The hydraulic conductivity values should be given in units of length per time (e.g., meters per second) (Provost et al., 2017).

The LECA of type 0-6C was used as the porous media for the green roof in this study. The hydraulic conductivity value for LECA 0-6C was given based on laboratory measurements provided by Leca Norge AS (2022), where it was reported as $K = 1.4 \cdot 10^{-3}\ [\mathrm{m/s}]$. This property is measured in the laboratory under controlled conditions. However, these laboratory measurements may not always reflect the actual range of hydraulic conductivity values that could be found in the field.

In this research work, a range of hydraulic conductivities ($1 \cdot 10^{-3}\ to\ 2.2 \cdot 10^{-3}\ [\mathrm{m/s}]$) was used to simulate and calibrate the model (more details under section 2.4). Where the best estimation of the modelled hydraulic conductivity will be compared to the laboratory-measured value (more under sections 3 and 4).

The incorporation of the hydraulic conductivities as an input value was performed in the model using zone-based properties in MODFLOW 6, where each cell in the grid of the model was defined with the hydraulic conductivity ($K_y = K_z = K_x$; and K_x is an input value). MODFLOW 6's inherent grid generation capabilities were utilized to define the grid for the drainage layer of the roof based on the mesh array data. The model's grid in MODFLOW 6 was designed as a single layer of 97x47 cells. Each cell in the grid was assigned a size of 10 cm x 10 cm x 15 cm to facilitate the accurate modelling of the hydrological behaviour of the green roof. The model in MODFLOW 6 is illustrated in the following figure:

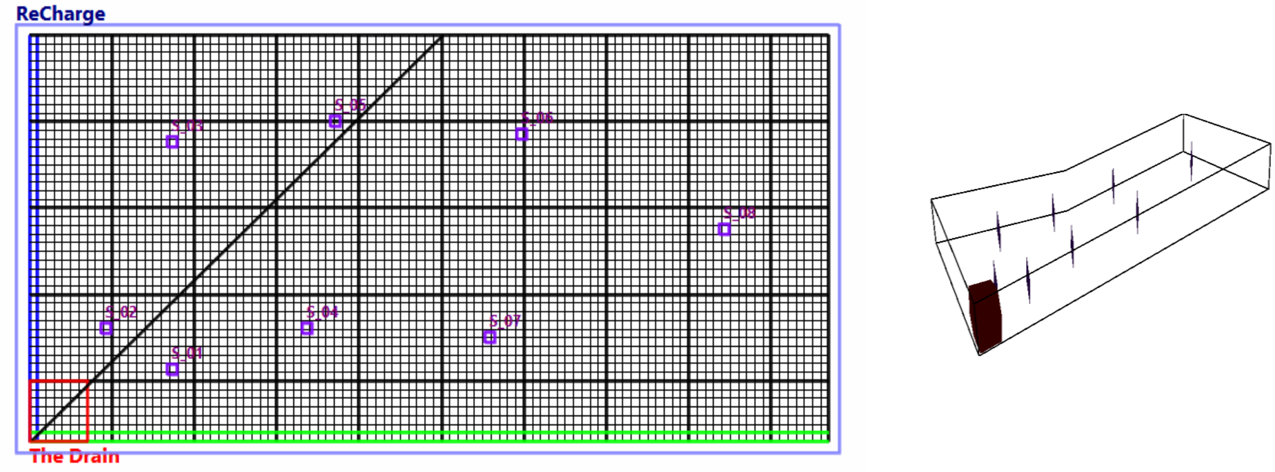

Figure 4: The MODFLOW 6 model in the ModelMuse interface, the right segment shows the top view of the grid with the drain, 8 sensors(S01-S08), and The recharge area. The left segment shows the 3D model.

The Recharge (RCH) package is used to define the specified flux, which represents the precipitation as a recharge rate. The desired distribution of the recharge rate over the model's top must be defined in units of length/time (Langevin et al., 2017). Based on the fieldwork and by analysing the data of the steady-state experiment (Bassøe, 2020), a steady recharge rate $N = 5.48 \cdot 10^{-7}$ $[\mathrm{m/s}]$ was considered to define the flux in the RCH package.

The observations of the hydraulic head were represented by 8 objects referring to 8 sensors. Each object was placed in the grid according to its coordinates on the green roof (see Figure 4 and Table 1). The observation (OBS) package was linked to each object where the heads were defined according to equation (3) in MODFLOW 6.

2.3.3. The Boundary Conditions and the Seepage Face Effect

The Time-Variant Specified-Head (CHD) package was used to define the boundary conditions of the model at the drain of the green roof. The drain implementation of the green roof was carried out through a drain hole located within an open box encompassed by coarse gravel. The LECA layer, representing the porous media of the green roof, was in contact with the coarse gravel. In the design of the green roof model, drain cells were included to represent the roof's drain (Figure 4). In this contrast, the drain of the model was assigned by 7x7 cells defined with the Time-Variant Specified-Head (CHD) package. The graphical illustration of the drain structure can be observed in Figure 2.

Depending on the design of the green roof, a hydraulic head could be generated at the discharge of the model, leading to the appearance of a seepage face effect. The development and behaviour of the seepage face are influenced by the water head at the drain, flow patterns, and the heterogeneity of the layer. Water flow and hydraulic head in the drainage layer are affected by the seepage face behaviour. The seepage face, which represents the boundary where water in a confined or unconfined layer exits to the atmosphere, is a critical element in managing and modelling water flow (Rushton, 2006; Scudeler et al., 2017).

In this thesis based on the fieldwork, it was found that the green roof did not have any sensors to detect the hydraulic head at the drain or at the coarse gravel surrounding the drain. Consequently, it was not clear whether the seepage face effect was sustained at the drain construction in the green roof. This uncertainty could have a significant impact on the modelling of flow in the drainage layer of the roof. Thus, a range of hydraulic heads at the drain ($H = 1 \cdot 10^{-3}\ to\ 20 \cdot 10^{-3}$ [m]) was considered to define the boundary condition in the CHD package. This range of hydraulic heads at the drain was used in the modelling and the calibration process to study the possibility and the effect of seepage face in the green roof.

2.3.4. The Model and the Equation of Analytical Steady Flow

MODFLOW6 is a common flow modelling software that has been applied in various studies to simulate groundwater movement in porous media. However, its reliability in simulating the hydraulic conductivity and hydraulic head in green roofs with small thickness layers has not been extensively evaluated. The analytical model in this thesis presents an evaluation of the reliability of MODFLOW 6 in simulating the hydraulic head in a green roof with a small thickness layer. An isotropic model of a single horizontal layer was developed in MODFLOW 6 to simulate the flow behaviour in the drainage layer of the green roof at the steady-flow condition. The result of this model will be compared to the analytical solution.

The grid of the model was one horizontal layer with a cell resolution of 15 cm x 15 cm, where the depth of the model was 15 cm. The model occupied an area of 9.7 m x 4.7 m. The recharge is on the top of the model and the drain is along the short side of the model as shown in the following figure:

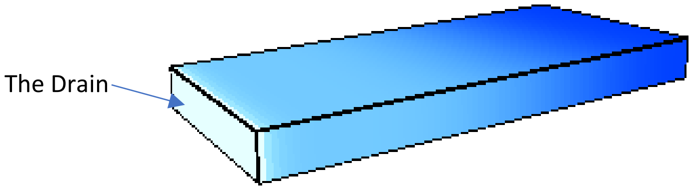

Figure 5: The 3D view of the analytical model of a single horizontal layer in ModelMuse/ MODFLOW6

Reworking of equations (1) & (2) under the steady-flow condition of the green roof when the flow is in the opposite direction of the x-axis (Figure 6), the recharge is represented by the precipitation (N), where the evapotranspiration is negligible, and the substrate is considered homogenous and isotropic (the hydraulic conductivity is independent of direction), the water flow equation of the green roof was derived and represented as:

$$N\,x = K\,h\frac{dh}{dx} \tag{4}$$

Here, N is the recharge (precipitation) $[L/T]$, X is the distance in the x-direction $[L]$, K is the hydraulic conductivity $[L/T]$, h is the head elevation $[L]$, and $\frac{dh}{dx}$ is the hydraulic gradient in the x-direction $[L/L]$.

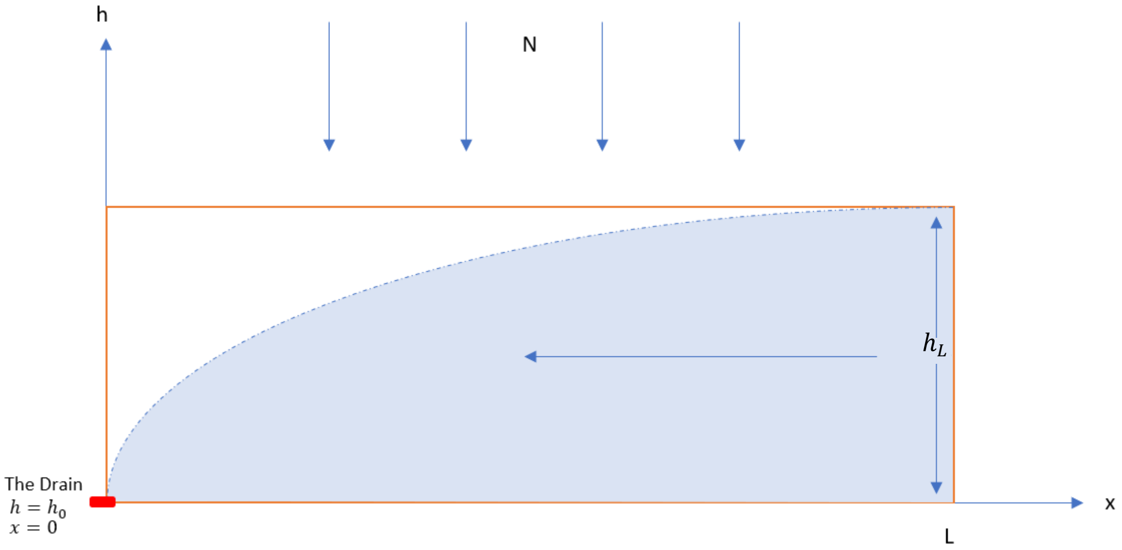

Figure 6: Steady water flow in a recharged (N), unconfined substrate of the green roof. The total length of the roof is L, where the flow is in the direction of the drain point at x = 0. The total depth of the green roof substrate is hL.

The integration and reworking of equation (4) give:

$$h^2 = \frac{N}{K} x^2 + C \qquad (5)$$

By employing the boundary condition of the green roof at a steady water flow (as shown in Figure 6) into equation (5) as follows:

At $x = 0$, and $h = h_0$; then $C = h_0^2$.

At $x = L$, then $h = h_L$. Thus, equation (5) become:

$$h_L^2 = \frac{N}{K} x^2 + h_0^2 \qquad (6)$$

Equation (6) will be used forward in this thesis as the governing equation of the steady-state flow in the single horizontal drainage layer of the green roof. This equation will be used to evaluate the reliability of MODFLOW 6 in simulating the hydraulic conductivity and hydraulic head in a green roof with a small thickness layer. The evaluation is listed under the Results part of this thesis.

2.4. Calibration Methods

It is a significant challenge in the modelling process to calibrate the flow model of the green roof to match observed data. Calibration is a crucial step that ensures the accuracy and reliability of the model. Two calibration methods were conducted in this thesis to ensure Modflow 6's accuracy and performance. The calibration process of the model was first conducted manually by minimizing the Mean Absolute Error (MAE), followed by inverse modelling using the numerical PEST (Parameter Estimation) model in MODFLOW 6.

2.4.1. The Minimum Mean Absolute Error (MAE)

The Minimum Mean Absolute Error (MAE) method is widely used for calibrating numerical models in various fields of science and engineering. The MAE method estimates the discrepancy between observed and simulated values by calculating the absolute differences between them. The MAE equation is expressed as:

$$MAE = n^{-1} \sum_{i=1}^{n} |O_i - P_i| \tag{7}$$

Where n is the number of observations, O is the observed hydraulic head data, and P is the model-simulated hydraulic head data. In comparison to other methods like root mean square error (RMSE), this method (MAE) is less sensitive to extreme values or outliers. A particular advantage of the MAE method is that it is effective when it comes to calibrating models to match a set of observation data (Legates & McCabe Jr, 1999).

In the modelling project, the manual calibration process using the MAE method was performed through two steps; one-dimension MAE (1D-MAE) and two-dimensions MAE (2D-MAE). The calibration of the model by 1D-MAE kept all the input parameters constant except for the hydraulic conductivity. The range of hydraulic conductivity ($1 \cdot 10^{-3}\ to\ 2.2 \cdot 10^{-3}$ [m/s]) was considered to involve laboratory measurements but also considers the potential for variability in the field. The 1D-MAE curve was generated by running the model eight times, once for each hydraulic conductivity value. All the input parameters to the model are listed in Table 2 as follows:

Table 2: the input parameters to the model and the range of the hydraulic conductivities that were used in the 1-D MAE calibration.

Parameter	Value	Hydraulic conductivity	Value [m/s]	Hydraulic conductivity	Value [m/s]
Recharge	5.48E-07 [m/s]	K1	1.0E-03	K4	1.5E-03
Head at Discharge	1E-03[m]	K2	1.2E-03	K5	1.6E-03
		K2	1.3E-03	K6	2.0E-03
		K3	1.4E-03	K8	2.2E-03

The impacts of the seepage face effect and the hydraulic conductivity are calibrated using 2D-MAE to improve the performance of the model. The hydraulic head at the drain (seepage face) was difficult to measure where there were no sensors in the vicinity of the drain of the green roof. To account for this challenge, a range of hydraulic head values at the drain was chosen to ensure the possibility of seepage face existence. At the same time, a range of hydraulic conductivity was fed to the model while the recharge rate was kept constant at $5.48 \cdot 10^{-7}$ $[\mathrm{m/s}]$ (the same value as in 1D-MAE, see Table 2). All the input parameters to the 2D-MAE model are listed in Table 3:

Table 3: the range of the hydraulic conductivities and the range of the constant heads at the drain that was used in the 2-D MAE calibration. It also shows the head at discharge as a per cent of the total thickness of the LECA layer (0.15 m).

Head at Discharge (H)	Value [mm]	% of H to LECA layer thickness	Hydraulic conductivity	Value [mm/s]
H1	1.00	0.7	K1	1.0
H2	2.25	1.5	K2	1.2
H3	5.00	3.3	K2	1.3
H4	10.0	6.7	K3	1.4
H5	15.0	10	K4	1.5
H6	20.0	13.3	K5	1.6
			K6	2.0
			K8	2.2

2.4.2. Parameter Estimation (PEST) through Inverse Modelling

Inverse models are widely used in geology, hydrology, and environmental engineering to estimate and calibrate system properties and characteristics. It involves simulating the behaviour and predicting the outputs of the system using a physical mathematical model. The Inverse modelling process requires two steps; the forward problem and the inverse problem.

The forward problem is a problem in which the state of a model, such as the hydraulic head, is predicted with the help of known inputs (e.g. hydraulic conductivity) and based on the parameterization of the model in advance. The inverse problem is solved by PEST. PEST is solving the inverse problem by applying Darcy's Laws and mass conservation based on equations (1) and (2). The solution in PEST involves the prediction of unknown parameters (hydraulic conductivity) of the model based on observation data (hydraulic Heads) by utilizing the iteration method of the model (Zhou et al., 2014).

The Parameter Estimation (PEST) which is included in MODFLOW 6 allows the difference between the observed and simulated values of selected variables to be minimized through the process of iteration (Doherty, 2010; Doherty & Hunt, 2010). In addition to estimating model parameters, PEST also contributes to the assessment of uncertainty. It is important to select calibration targets and parameters carefully when using PEST, as well as fully understand the optimization algorithms that will be used to adjust the calibration parameters (White & Lavenue, 2023).

In this thesis, the forward model in MODFLOW6 was conducted using predefined hydraulic conductivity as a start value. The start value of the hydraulic conductivity was gained from the result of the MAE-calibrated model. The inverse modelling of the green roof model was accomplished through the utilization of the PEST iteration algorithm in MODFLOW 6 by updating the model with 8 observation wells, each well represents an observation head value. The observation head values were extracted by analysing the data from the online database of NVE (2018) for the steady-state experiment performed by Bassøe (2020) and Ydse (2021), while the coordinates of each head sensor were assessed during the fieldwork. Table 4 shows the observation input data to the PEST inverse modelling.

Table 4: A table of the coordination and the observed hydraulic head based on a steady-state experiment; recharge rate $N = 5.48 \cdot 10^{-7}$ $[\mathrm{m/s}]$, the head at the drain $H = 2.25 \cdot 10^{-3} [\mathrm{m}]$.

Sensor	**x vertic [m]**	**y vertic [m]**	**OBS Normal HEAD [m]**
Sensor 1	1.72	0.82	0.129
Sensor 2	0.99	1.33	0.137
Sensor 3	1.72	3.46	0.192
Sensor 4	3.36	1.33	0.213
Sensor 5	3.72	3.72	0.208
Sensor 6	6.00	3.52	0.243
Sensor 7	5.85	1.22	0.246
Sensor 8	8.43	2.46	0.258

For the inverse modelling of the green roof, The PEST package was enabled in MODFLOW 6. The process of conducting PEST modelling involves the following steps:

1. Defining the adjustable input parameters: One adjustable parameter was defined for the PEST modelling of the green roof. This parameter is representing the hydraulic conductivity K_x of the drainage layer of the model. The range of K_x was defined as a log factor with a range of $1 \; to \; 1 \cdot 10^{-8}$.
2. Defining the observation data: The observation data (OBS Normal HEAD; Table 4) were grouped under OBS-group and connected to the parameter K_x under the parameter properties in the PEST package in MODFLOW 6.
3. Preparation of pilot point data: Pilot points are a pattern of XY points with defined spacing. This pattern is used by PEST to estimate an array of hydraulic conductivities that will be spatially interpolated to all of the active cells within the model domain using the Kriging method (Doherty et al., 2010). A uniform pattern of 1 m spacing was generated and defined for the layer of the green roof model. Figure 7 shows the pattern of pilot points for the model domain as following:.

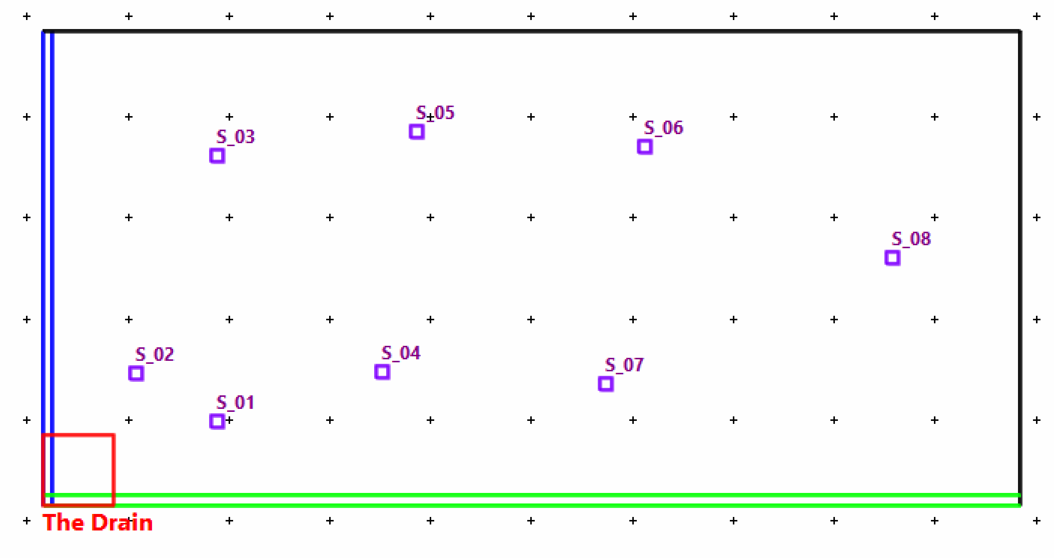

Figure 7: the top view of the model in the ModelMuse interface / MODFLOW 6, A pattern of XY pilot point with 1 m spacing that was applied to the model of the green roof.

4. Running the PEST check: The PEST check run is a step to indicate the model building errors and check if the input parameters and the solution matrix of the model are working correctly. In case of error indications, the input parameters, including the grouping process of the observation data, should be reviewed and modified.
5. Running the PEST calibration model: The PEST check was conducted with no error where the adjustable parameter (the hydraulic conductivity in the case of this thesis), the observation data (the hydraulic head from the sensors), and the pilot point input file are checked for a successful PEST run.
6. Analyzing the results: The result of the first inverse modelling in PEST is obtained using the last regularization control. This means that the model may be overfitted. However, finding a solution for the model with a minimum error value but less variation in the adjustable parameter (the hydraulic conductivity in the case of this thesis) is more important than obtaining "correct" overfitted parameter values. PHIMLIM is a parameter in the PEST algorithm that sets an upper limit on the acceptable level of misfit between the observed and simulated data. The benefit of PHIMLIM tuning in PEST is to obtain more reasonableness of the model (Doherty et al., 2010; WNC, 2021). The overfitting problem could be adjusted by tuning the regularization control parameter (PHIMLIM) and running the model again (second run of the PEST model). By tuning the PHIMLIM by 5 to 10 per cent lower than the PHIMLIM of the first PEST run, the overfitting problem could be improved (Doherty, 2015).

3. Results

3.1. Analytical Model

The analytical model in this section presents an evaluation of MODFLOW 6. The inputs of the model were the constant hydraulic conductivity and the constant recharge rate (see Table 5). The head at the drain was defined to be a constant value that was a bit larger than zero to avoid numerical error in the simulation (Harbaugh, 2005). The output of the simulation was a model with a head distribution in the domain of the model as in Figure 8. The curve of the simulated hydraulic head as a function of the layer length was executed from the analytical model in MODFLOW 6 and expressed in Figure 9.

Table 5: A table of the parameters used in the analytical and simulated model.

Parameter	**Value**	**Unite**
Recharge (N)	9.26E-09	m/s
Hydraulic conductivity (K)	4.75E-5	m/s
The length of the layer	9.7	m/s
Drain hydraulic head	0.01	m

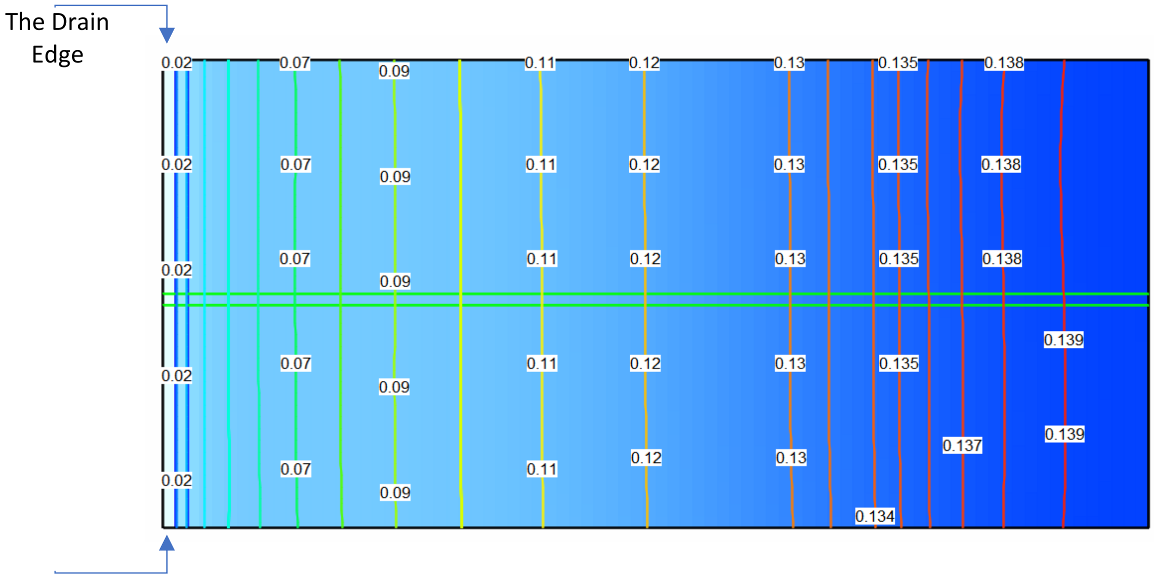

Figure 8: The analytical model in MODFLOW 6/ModelMuse interface. The contour lines refer to the hydraulic head as a function of the layer length of the model based on input parameters listed in Table 5

The input parameters of the model in Table 5 were applied to the analytical solution based on equation (6). The simulated hydraulic head curve from MODFLOW was compared to the analytical hydraulic head and the result is shown in Figure 9. The result of this test showed that the simulated hydraulic head curve was found to be approximately the same as the curve that was analytically calculated and plotted, indicating that the model accurately represents the hydraulic behaviour of the green roof.

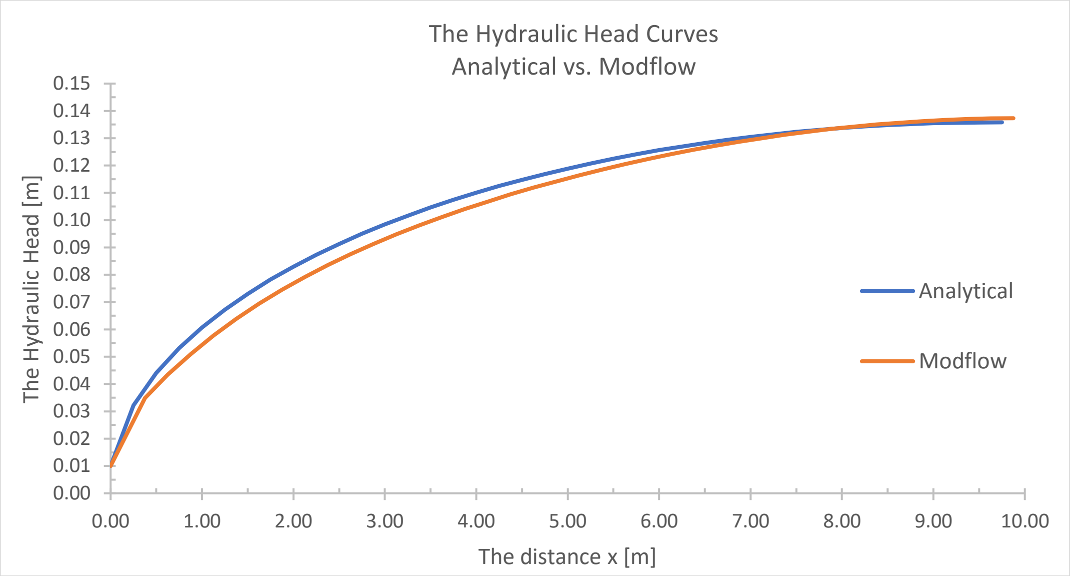

Figure 9: The curve of the steady-state hydraulic heads from the analytical solution and the simulation in MODFLOW, the x-axis is the distance from the discharge, where the discharge is at x = 0 [m], and the y-axis is the hydraulic head [m].

3.2. The Calibration by MAE

3.2.1. One-dimension MAE (1D-MAE)

This calibration was based on one dimensional MAE that kept all the model input parameters constant except for the hydraulic conductivity. All the input parameters to the model are listed in Table 2. In this section, the model was built as explained in section2.3.2 and Figure 4.

The 1D-MAE curve was generated by running the model eight times, once for each hydraulic conductivity value listed in Table 2. The minimum mean absolute error (MAE), between the observed and simulated hydraulic heads, was found to be at its lowest value of 0.015 [m] for the model of the hydraulic conductivity $K = 1.5 \cdot 10^{-3}$ $[\mathrm{m/s}]$. Figure 10 represents the curve obtained from 8 runs of the model, where each run of the model is implemented with one corresponding value of hydraulic conductivity.

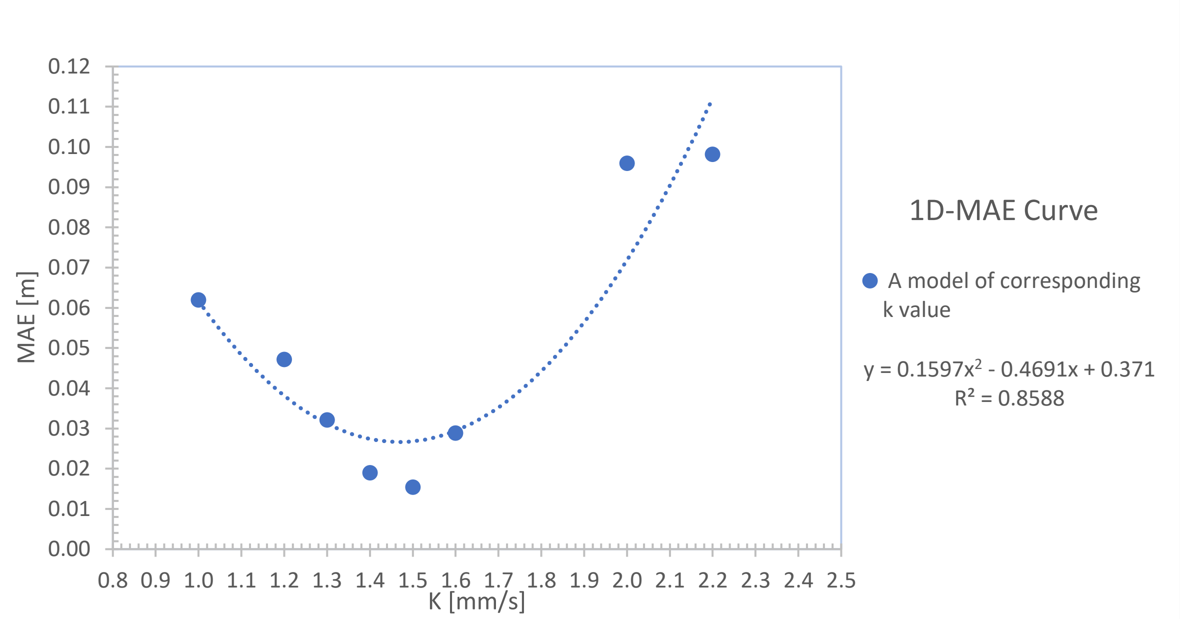

Figure 10: The one-dimension MAE curve of 8 models, each model representing one hydraulic conductivity value as in Table 2. The x-axis is the hydraulic conductivity k in $[mm/s]$, at the y-axis is the value of the minimum absolute error (MAE).

The results indicated that the model's optimal range of hydraulic conductivity values lies within $1.3 \cdot 10^{-3}$ $[\mathrm{m/s}]$ to $1.6x1^{-3}$ $[\mathrm{m/s}]$. The model for the hydraulic conductivity of 1.5x10-3 [m/s] resulted in very little deviation between the observed and simulated hydraulic heads. A graphical representation of the observed and simulated hydraulic heads for the model of $K = 1.5 \cdot 10^{-3}[\mathrm{m/s}]$ is plotted in Figure 11.

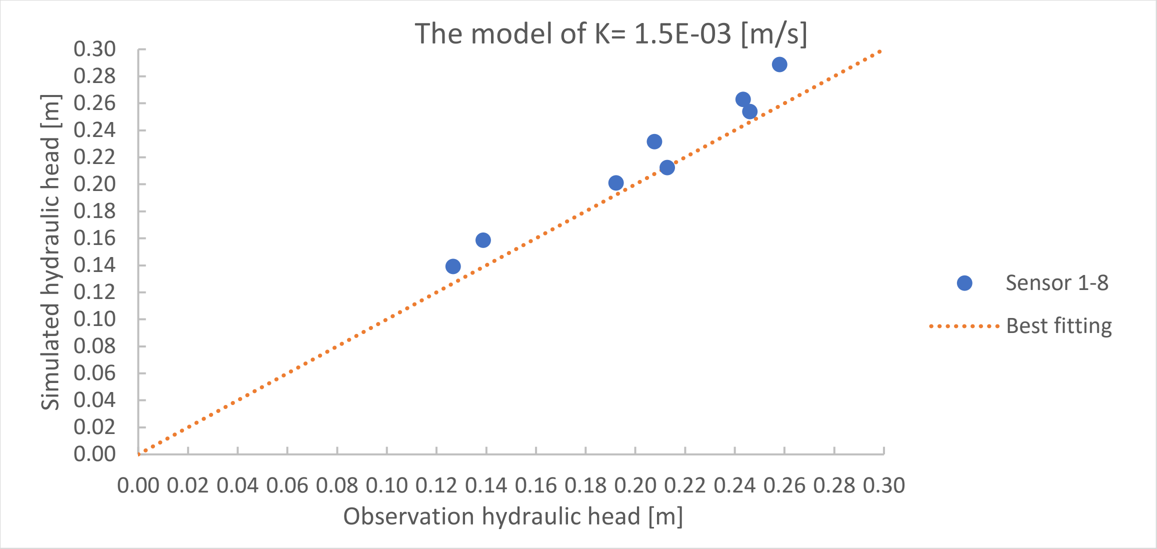

Figure 11: The observed and simulated hydraulic head for the model of hydraulic conductivity $K = 1.5 \cdot 10^{-3}$ $[\mathrm{m/s}]$. the MAE for this model was found to be at its lowest value of 0.015 $[m]$.

It was found that when the hydraulic conductivity exceeded more than $1.6 \cdot 10^{-3}$ $[\mathrm{m/s}]$, the local simulated hydraulic head at the high edge of the model domain was falling at the cell bottom of the domain ($h = 0$ $[\mathrm{m}]$). Indicating that at a higher hydraulic conductivity, the flow in the drainage layer of the model is higher than the recharge rate (the precipitation). Thus, the model of the green roof was drying and the model's performance began to decline.

3.2.2. Two-dimension MAE (2D-MAE)

The green roof in this work has no sensors to detect the hydraulic head at the drain of the roof. To account for this challenge, a range of hydraulic head values at the drain was chosen to ensure the possibility of seepage face existence. At the same time, a range of hydraulic conductivity was fed to the model while the recharge rate was kept constant at $5.48 \cdot 10^{-7}$ $[\mathrm{m/s}]$. All the input parameters to the 2D-MAE model are listed in Table 3. In this section, the model was built as explained in section 2.3.2 and Figure 4.

The model was manually executed 48 times as all combinations of the hydraulic conductivity and the constant head at the drain. A contour plot and a 3D surface plot were generated to represent the result of 2D-MAE calibration, Figure 12 and Figure 13 respectively.

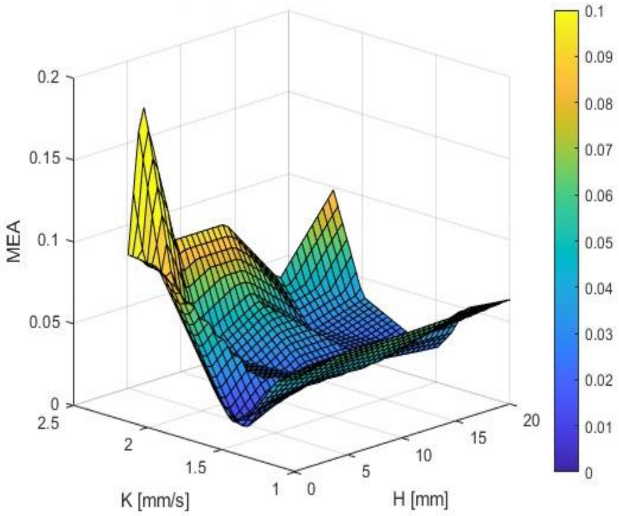

Figure 12: The 3D surface plot of the 2D-MAE calibration of the hydraulic head, at the x-axis is the range of the drain head, the y-axis is the range of the hydraulic conductivities, while the z-axis is the values of the MAE which is also represented in the colour bar.

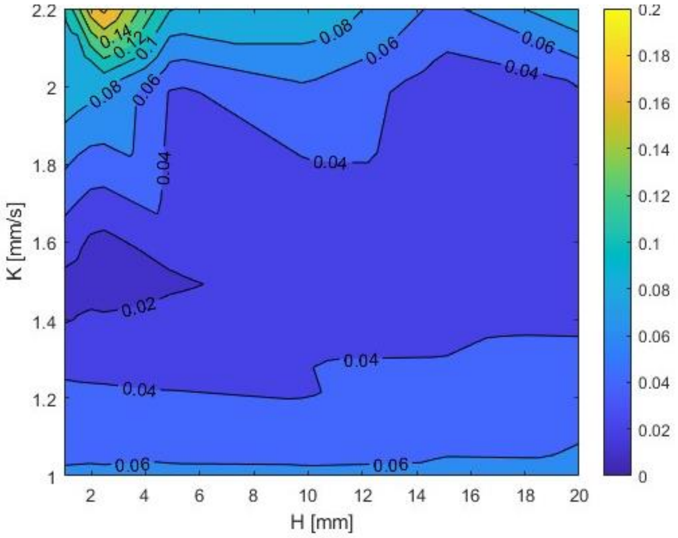

Figure 13: The contour plot of the 2D-MAE calibration of the hydraulic head, at the x-axis is the range of the drain head while the y-axis is the range of the hydraulic conductivities. The colour bar shows the value of the MAE.

The lowest value of MAE (obtained from 46 models-runs in MODFLOW 6) was 0.008 $[\mathrm{m}]$ at the hydraulic conductivity $K = 1.5 \cdot 10^{-3} [\mathrm{m/s}]$ and the drain head $H = 2.25 \cdot 10^{-3}$ $[\mathrm{m}]$. The observed and simulated hydraulic heads of the model at MAE = 0.008 $[\mathrm{m}]$ are represented in Figure 14

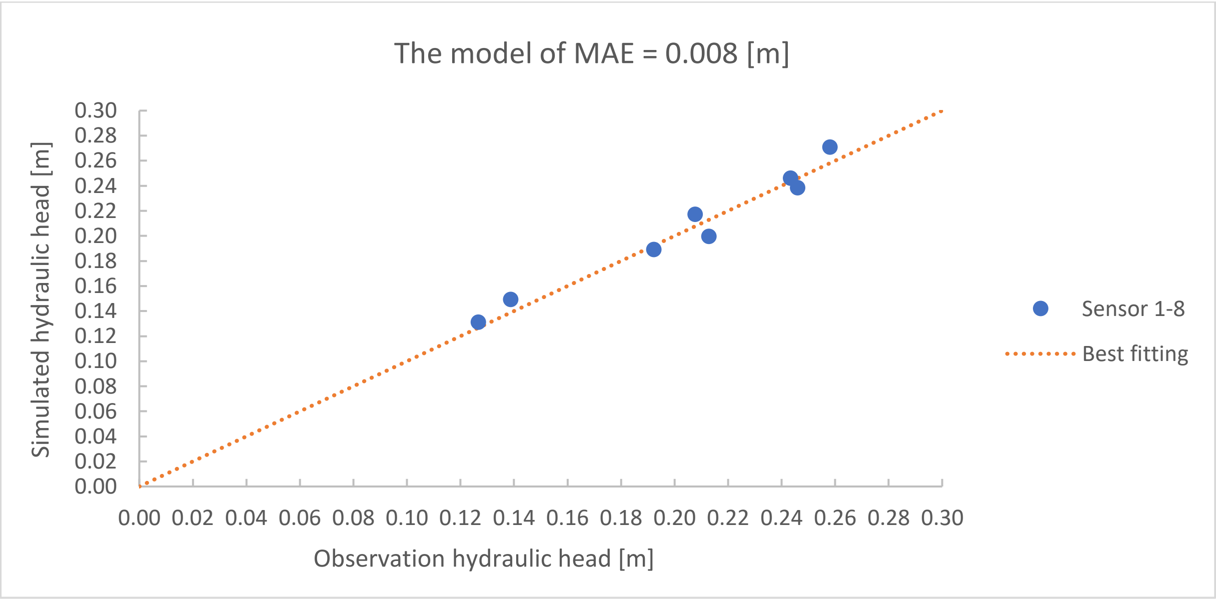

Figure 14: the observed and simulated hydraulic head for the hydraulic conductivity of $1.5 \cdot 10^{-3}$ $[\mathrm{m/s}]$ and constant hydraulic head at the discharge $H = 2.25 \cdot 10 - 3$ $[\mathrm{m}]$.

By analyzing the contour plot of the 2D-MAE calibration (Figure 13), the model was fitted with the observation data of heads ($MAE \leq 0.02\,[\mathrm{m}]$) within a narrow range of hydraulic conductivity values ($K = 1.3 \cdot 10^{-3}\ to\ 1.6 \cdot 10^{-3}\ [\mathrm{m/s}]$). Furthermore, it was observed that at the increase in hydraulic conductivity beyond $1.6 \cdot 10^{-3}[\mathrm{m/s}]$, the local simulated hydraulic head in the drainage layer was falling to the bottom level of the model ($h = 0\ [\mathrm{m}]$), and the model became dry. Consinquesly, the decrease of hydraulic conductivity under $K = 1.3 \cdot 10^{-3}[\mathrm{m/s}]$ in combination with higher values of the head at the drain ($H \geq 10 \cdot 10^{-3}\ [\mathrm{m}]$) results in the local head being raised higher than the thickness of the drainage layer ($MAE \geq 0.06\ [\mathrm{m}]$; total layer thickness = 15 $[\mathrm{cm}]$), and the model became flooded.

However, the optimal K values (Figure 13; $K = 1.3 \cdot 10^{-3}[\mathrm{m/s}]$ to $K = 1.6 \cdot 10^{-3}[\mathrm{m/s}]$; $MAE \leq 0.04\ [\mathrm{m}]$) were nearly independent of the head at the drain (Figure 13; H from 1 to 20 [mm]). Depending on this observation, It could be said that the effect of the seepage face was not generated at the drain of the green roof drainage layer.

3.2.3. The Inverse PEST Modelling

In this section of the thesis, The forward model was built with a drain head $H = 2.25 \cdot 10^{-3}[\mathrm{m}]$ and $K = 1.5 \cdot 10^{-3}[\mathrm{m/s}]$. The building of the model was described in section 2.3 (see also Figure 4). The process of performing PEST modelling was followed (points 1 to 6 in section 2.4.2)

The result of the PEST inverse modelling shows that the best performance of the model was obtained with a narrow distributed range of hydraulic conductivities around $1.5 \cdot 10^{-3}[\mathrm{m/s}]$. This narrow range was applied to the grid of the mode domain and visualized in Figure 15.

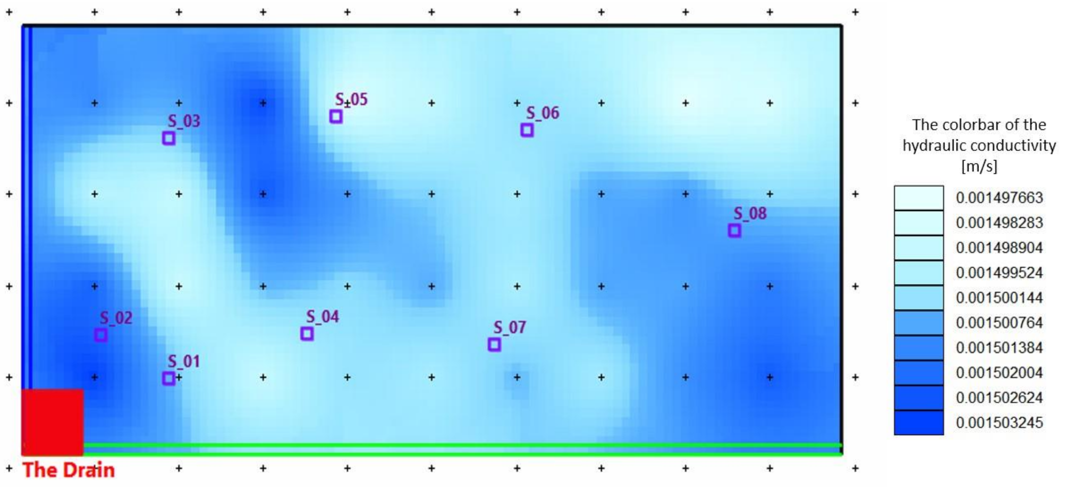

Figure 15: The hydraulic conductivity distribution following the inverse PEST modelling of the green roof model in MODFLOW 6 based on a steady-state experiment where the input parameters are listed in Table 4; the recharge rate is $5.48\text{x}10^{-7}$ [m/s], the head at the drain is $2.25\text{x}10^{-03}$[m] the area of the green roof is obtained by 9.7 [m] length, 4.7 [m] width and the thickness of the layer is 0.15 [m].

A second PEST run was conducted on the model of the green roof based on the result of the first run to overcome the overfitting problem. The regulation parameter PHIMLIM in PEST was set 10 per cent lower than the first PEST run (first run regulation parameter PHIMLIM was 0.008; second run is 0.0072). The second run gave a less-than-perfect fit between the observed data and the simulated data where the hydraulic conductivity $K = 1.5 \cdot 10^{-3}[\mathrm{m/s}]$ for all cells in the drainage layer of the model. Thus, no variation in hydraulic conductivity (see Figure 16). This result is because the variation of K in the first run was not high. If the first run of PEST modelling gives a high variation in the adjusted parameter (K in the case of this research work), the second run of PEST modelling could reduce the overfitting but it is difficult to approach no variation with an acceptable fit between the observed and simulated data (Doherty, 2015).

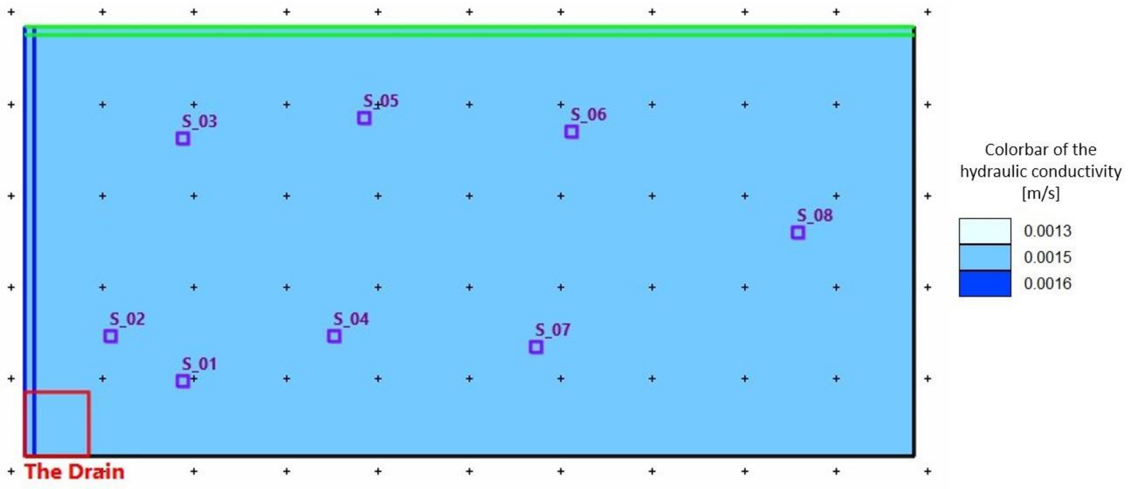

Figure 16: The hydraulic conductivity of each cell in the domain obtained by the regulated second PEST-run (10% lower PHIMLIM). This model in MODFLOW 6 was based on the input parameters listed in Table 4, the recharge rate is $5.48 \cdot 10^{-7}$ $[\mathrm{m/s}]$, the head at the drain is $2.25 \cdot 10^{-3} [\mathrm{m}]$, the area of the green roof is obtained by 9.7 $[\mathrm{m}]$ length, 4.7 $[\mathrm{m}]$ width and the thickness of the layer is 0.15 $[\mathrm{m}]$.

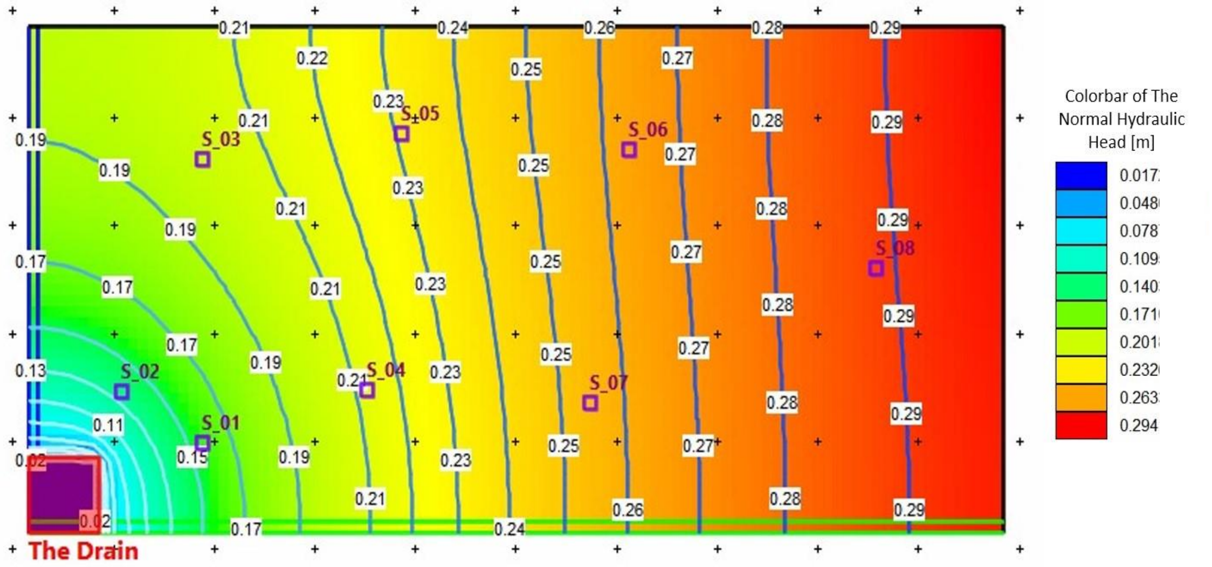

Figure 17: The hydraulic head distribution following the second inverse PEST in MODFLOW 6 based on a steady-state experiment; the recharge rate is $5.48 \cdot 10^{-7}$ $[\mathrm{m/s}]$, the head at the drain is $2.25 \cdot 10^{-3}$ $[\mathrm{m}]$, the area of the green roof is obtained by 9.7 $[m]$ length, 4.7 $[m]$ width and the thickness of the layer is 0.15 $[\mathrm{m}]$.

As shown in Figure 17, the hydraulic head distribution is obtained by applying the second PEST-calibrated hydraulic conductivity ($K = 1.5 \cdot 10^{-3} [\mathrm{m}/s]$) into the domain of the model. For this model, the observed and simulated hydraulic heads of the model at each sensor in the green roof model are shown in Figure 18.

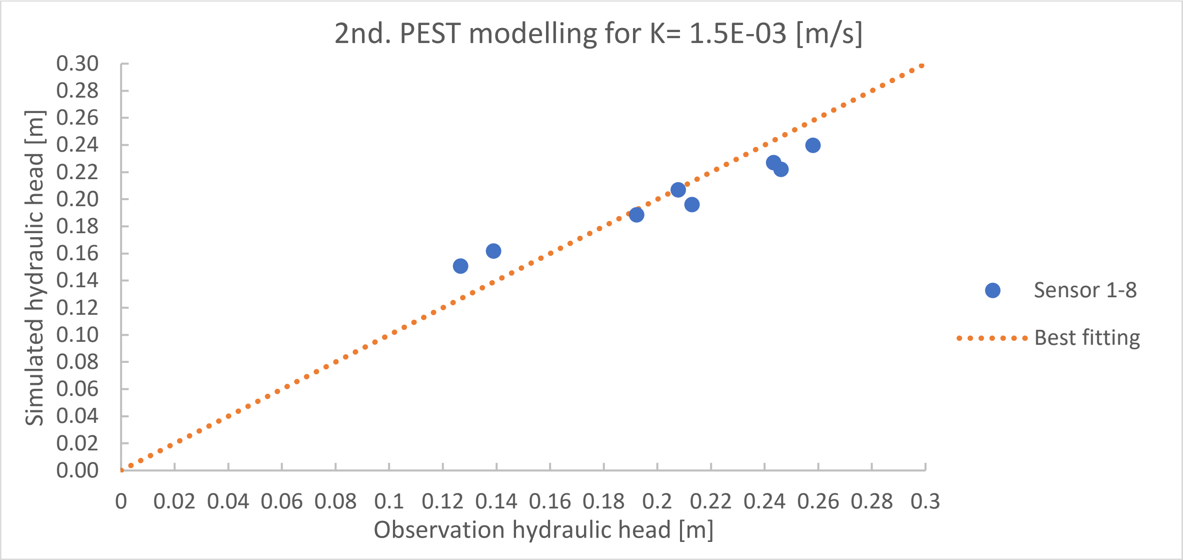

Figure 18: The observed and simulated hydraulic head for the second PEST run (10% lower PHIMLIM) in MODFLOW 6 based on a steady-state experiment; the recharge rate is $5.48 \cdot 10^{-7}$ $[\mathrm{m/s}]$, the Discharge head at the drain is $2.25 \cdot 10^{-3} [\mathrm{m}]$.

4. Discussion

The discussion in this section of the thesis focuses on evaluating the potential of using MODFLOW 6 as a tool to simulate water flow in green roofs, comparing different calibration processes, and investigating the best estimation of the hydraulic conductivity and its distribution, as well as the effect of the boundary condition on the distribution of the hydraulic head in the drainage layer of the green roof. The following discussions based on key observations were made:

The boundary condition plays an important role in controlling the water head in the layer. It was discovered that The calibrated K-value is relatively insensitive to the choice of boundary condition, i.e. the head value at the drain outlet. With the increase in hydraulic conductivity beyond $1.6 \cdot 10^{-3}$ $[\mathrm{m/s}]$, the local simulated hydraulic head in the drainage layer was falling to the bottom level of the model ($h = 0$ $[\mathrm{m}]$), and the model became dry. In the same manner, the decrease of hydraulic conductivity under $1.3 \cdot 10^{-3}$ $[\mathrm{m/s}]$ in combination with higher values of the head at the drain ($H \geq 10 \cdot 10^{-3}$ $[\mathrm{m}]$) results in the local head being raised higher than the thickness of the drainage layer (MAE ≥ 0.06 $[\mathrm{m}]$; total layer thickness = 15 $[\mathrm{cm}]$), consequently the model became flooded. These findings highlight the importance of carefully considering boundary conditions and the distribution of hydraulic conductivity in green roof modelling, helping the engineers to better design the green roof as a stormwater management tool in urban areas.

The use of MODFLOW 6 for studying green roof behaviour is less common than its use as a groundwater modelling tool. Thus, the steady-state modelling of water flow in the drainage layer of the green roof using MODFLOW 6 was evaluated by matching the curve of the simulated hydraulic head to the analytical solution based on equation (6). The results show reasonable agreement between the analytical solution and the simulated model (Figure 9). The propagation of the hydraulic head as a function of layer length was nearly similar to the simulated head in the steady-state model in MODFLOW 6. The result of this evaluation indicates that MODFLOW 6 used in this study is capable of simulating the steady flow in the thin drainage layer of the green roof. This finding validates the use of MODFLOW 6 for the research field of this thesis

By studying the results of the calibration processes, it reveals that manually tuning the model in MODFLOW 6 to minimize the mean absolute error (MAE) between the simulated and observed hydraulic heads gave an acceptable level of fitting; the MAE was 0.015 $[\mathrm{m}]$ based on 1D-MAE and 0.008 based on 2D-MAE, both MAE values at $K = 1.5 \cdot 10^{-3}$ [m/s] (Figure 11 and Figure 14 respectively). Meanwhile, the MAE calibration methods provided insight into the green roof flow behaviour, these methods were resource-intensive and time-consuming (the model was built and executed 56 times in MODFLOW 6). This highlights the practical challenges of using manual calibration methods, especially for complex models. In contrast, the use of PEST inverse modelling in MODFLOW 6 proves to be less time- and resource-consuming even if it requires a good understanding of the PEST algorithm. The PEST inverse modelling forced the model to be over-fitted (Figure 15). However, the overfitting problem was adjusted by changing the regularization control parameter (PHIMLIM increased by 10%) to achieve a less-than-perfect fit between the observed data and the simulated data, resulting in an acceptable model.

In this research work, the modelled hydraulic conductivity for the drainage layer (LECA 0-6C) of the green roof was $1.5 \cdot 10^{-3} [\mathrm{m/s}]$. The modelling result of the hydraulic conductivity is obtained from the three calibration methods utilized in MODFLOW 6 based on field observation. The modelled value ($K = 1.5 \cdot 10^{-3}$ $[\mathrm{m}/s]$) is near the laboratory-measured hydraulic conductivity ($1.4 \cdot 10^{-3}$ $[\mathrm{m}/s]$ by Leca Norge AS (2022)). The modelling value of hydraulic conductivity in this thesis may be acceptable taking into consideration the uncertainties and the weakness of the field measuring sensors and the uncertainty of the homogeneity of the LECA layer raised during the construction of the drainage layer of the green roofs. The modelled hydraulic conductivity of $1.5 \cdot 10^{-3}$ $[\mathrm{m}/s]$ (at steady flow recharge of $N = 5.48 \cdot 10^{-7}$ $[\mathrm{m}/s]$) was almost uniformly distributed (Figure 16), and the Hydraulic head distribution was reasonable (Figure 17).

The use of MODFLOW 6 to model steady flow in the drainage layer of the green roof was an interesting and challenging experience. MODFLOW 6 is an open-source software that is widely used for groundwater flow modelling. The software has different packages covering different physical purposes of the model and different boundary conditions of the targeted model. While MODFLOW 6 is primarily used for modelling groundwater flow, it can also be used to simulate flow in other porous media, including green roofs. There are several different interface software available for running MODFLOW 6, and each has its strengths and weaknesses. In this study, the ModelMuse interface was used for modelling the green roof to take advantage of the model visualization feature. One of the challenges encountered during the research work was the difficulty in finding related studies that simulate the flow in the green roofs using MODFLOW 6. Modelling the flow behaviour in MODFLOW 6 requires a solid understanding of flow physics in porous media, geology, and hydrology. Despite these challenges, MODFLOW 6 proved to be a very robust and powerful physical-based modelling tool that was able to effectively simulate the steady flow in the drainage layer of the green roof in this research work. For the transient flow model which simulates the scenario of time-depending precipitation (unsteady-state conditions), MODFLOW 6 should be evaluated and more research should be conducted. Furthermore, field measurements of the porosity and the specific storage of the LECA are required to build and test the transient model in MODFLOW 6. Generally, the evaluation findings based on steady-state conditions in this thesis support the reliability of the forward unsteady flow model and the modelling of the transient scenario in MODFLOW 6.

5. Conclusion

In conclusion, the research questions posed in the introduction have been investigated, discussed and answered in this thesis, and the work provided useful insights into the modelling of water flow in the unconfined drainage layer of one green roof at NMBU in Ås.

The key observations listed under the discussion part demonstrate that the modelling software (MODFLOW 6, ModelMuse interface) used in this study was positively evaluated. The modelling process was analyzed to reveal the advantages and limitations of utilizing two different calibration methods; manually using the Mean Absolute Error (MAE), and the inverse modelling approach using PEST in MODFLOW6. PEST inverse modelling is a resource- and time-effective calibration method. A careful definition of the parameter range and the regularization control factor is required to avoid model over-fitting in PEST modelling. On the other hand, the MAE calibration methods are work- and time-consuming but provided insight into the green roof flow behaviour.

The modelling result of the hydraulic conductivity for the green roof at NMBU in ÅS is found, based on three calibration methods, to be near the laboratory-measured hydraulic conductivity. The modelling result of hydraulic conductivity $K = 1.5 \cdot 10^{-3}$ $[\mathrm{m/s}]$, while the laboratory-measured $K = 1.4 \cdot 10^{-3}$ $[\mathrm{m/s}]$ by Leca Norge AS (2022). The modelled hydraulic conductivity $K = 1.5 \cdot 10^{-3}$ $[\mathrm{m/s}]$ was almost uniformly distributed in the green roof drainage layer of LECA 0-6C.

The research finding in this study suggests that using MODFLOW 6 as a modelling tool may be useful and effective to understand the green roof water flow behaviour. Furthermore, the investigation into the drainage layer hydraulic conductivity distribution and the effects of boundary conditions (the head at the drain) on the water hydraulic head reveals the importance of wisely considering these factors in green roof design and modelling studies.

This thesis increases the knowledge in the field of green roof water flow modelling and provides a basis for further research using MODFLOW 6. To consider MODFLOW 6 as a truly useful tool for green roof design and optimization, this software must be able to simulate transient situations that cover the following fields; building discharge-recharge models (precipitation-runoff transient model), testing the effect of the evapotranspiration by including the vegetation layer of the roof to the model, and testing different types and thicknesses of the drainage layer of the green roofs.

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