Master's Thesis

Validation of DIVDRA for upscaling solute transport

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Abstract

To make an adequate estimation for travel time distribution for the solute transport occurring within the dimensions of the NHI-WQ grid cells, upscaling of the flow and transport processes at this scale is needed. Implementing the DIVDRA (DIVide DRAinage) upscaling concept, developed by Alterra, into MODFLOW could be a solution to solve this problem. This comes down to adjusting the way drainage features in MODFLOW are schematized and parameterized. When done correctly, this would give a proper travel time distribution for large cell sizes as in the NHI model.

This research will focus on the validation of DIVDRA that could be used for implementing DIVDRA (quasi-2D) into MODFLOW to represent the sub grid drainage fluxes. Before DIVDRA can be implemented the behaviour of the analytical concept has to be validated by comparing it with numerical alternatives. DIVDRA will be compared with MODFLOW and MT3DMS reference models to validate the concept. It is also interesting to compare the DIVDRA concept with other upscaling methods, to review the benefits and added value of the DIVDRA approach. The need for validation of DIVDRA is confirmed in Bakker and Schaars review report (Bakker & Schaars, 2015) Their report describes the findings and recommendations for validating the use of the DIVDRA concept within NHI for salt transport modelling. The recommendations on how to perform such a validation are divided into four steps: The first step is analysing the current analytical formula with relevant input of LHM, time depending water balances and time depending TRANSOL/DIVDRA simulations. For the second step a 2D or 3D reference model should be built with a high resolution of 1 meter in horizontal and vertical, with which groundwater flow and solute transport could be calculated with MODFLOW and MT3DMS. As a third step the simulations should be executed with fixed fluxes for the different drainage systems. And the final verification should be done with a simulation of fixed stage for each drainage system in MODFLOW.

Essential problem for upscaling of the NHI-WQ resolution to 250 by 250-meter cell size is that the horizontal discretization changes. Therefore, the travel time distribution of solute transport is changed and also not representative for solute transport. Figure 3 shows the different between a high resolution model and a scaling approach without horizontal discretization within the 250 by 250 meter cell size. This scaling approach of the 2D models gives unrealistic travel time distributions and therefore wrong solute transport representation. During this research different approaches of drainage distance would be compared with the 2D reference model. Important indicators for travel time distribution are the flow lines through the 2D reference model. An overestimation and underestimations due to upscaling, affects the solute transport and therefore the output concentrations.

To improve the scaling concept, the travel time distribution has to be optimised. The travel time depends on the flow lines through the system. To optimize the flow line, the occurrence of sub region under stream. This important process is underestimated in all of the scaling approaches. Therefore, the decay is over or underestimated and the outcomes could not be used for regulation or policy makers. Improving the sub region under stream makes the DIVDRA scaling approach more reliable and to use as a replacement for the high resolution model.

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Definitions

Alterra:	Knowledge institute from UR Wageningen
ANIMO:	Agricultural Nutrient model
BPI	Basic parameter index, homogeneous models
DIVDRA:	Divided drainage fluxes
Hydrus 2D:	Software package for simulating water, heat, and solute movement in two- and three-dimensional variably saturated media
IDF:	Raster files with non-equidistant raster sizes.
iMOD:	Interactive modelling program developed by Deltares.
IPF:	Represent point data that can be displayed in different ways.
IFF:	iMOD Flowpath File, represents line data generated by path line simulation.
MetaSWAP:	Meta model of Soil Water Atmosphere Plant.
MODFLOW:	Three-dimensional (3D) finite-difference groundwater model.
MT3DMS:	Modular 3-Dimensional Transport and Multi Species
NHI-WQ:	Dutch Hydrological instrument water quality (*Dutch: Nederlands Hydrologisch intstrument*).
Python:	Program language to run iMOD modules automatically.
Path line simulations:	Function to compute flow lines In iMODPATH based on budget terms that result from iMODFLOW computations (Vermeulen, van der Linden, & Minnema, 2015).
SPI	sandy parameter index, stratified models.
Sub regional under stream	Flow lines that will stream under need the nearest drain towards the next drain.

List of symbols and units

Table 1 Symbols and units

Description	Symbol	Unit
Time	T	day
Distance horizontal direction (west –east)	x	m
Distance horizontal direction (north-south)	y	m
Distance vertical direction	D	m
Layer depth	Δz	m
Recharge	rch	mm
Velocity	v	m day^{-1}
Porosity	N	$m^3 m^{-3}$
Conductance	Cond	m^2 day^{-1}
Surface level	mv	m
Discharge flux	Q	m^3 day^{-1}
Characteristic length		
characteristic length	Λ	m
horizontal permeability	K	m day^{-1}
depth of aquifer	D	m
vertical resistance	c	day^{-1}
Scaling approaches		
Drainage length	L	m
Drainage system	D_i	*i* drainage segment depth m
Drain discharge	$Q_{drain,i}$	*i* drainage segment flux m^3 day^{-1}
Horizontal discharge flux	$q_{drain,i}$	*i* drainage segment flux m^2 day^{-1}
Area of catchment	A	m^2
Average hydraulic head	$φ_{avg}$	m
Volume per drain	V_i	*i* drainage segment flux m^3 day^{-1}
Primary drainage depth	$D_{primary}$	m
Secondary drainage depth	$D_{secondary}$	m
Depth per layer	d_z	m
Total depth	D_{tot}	m

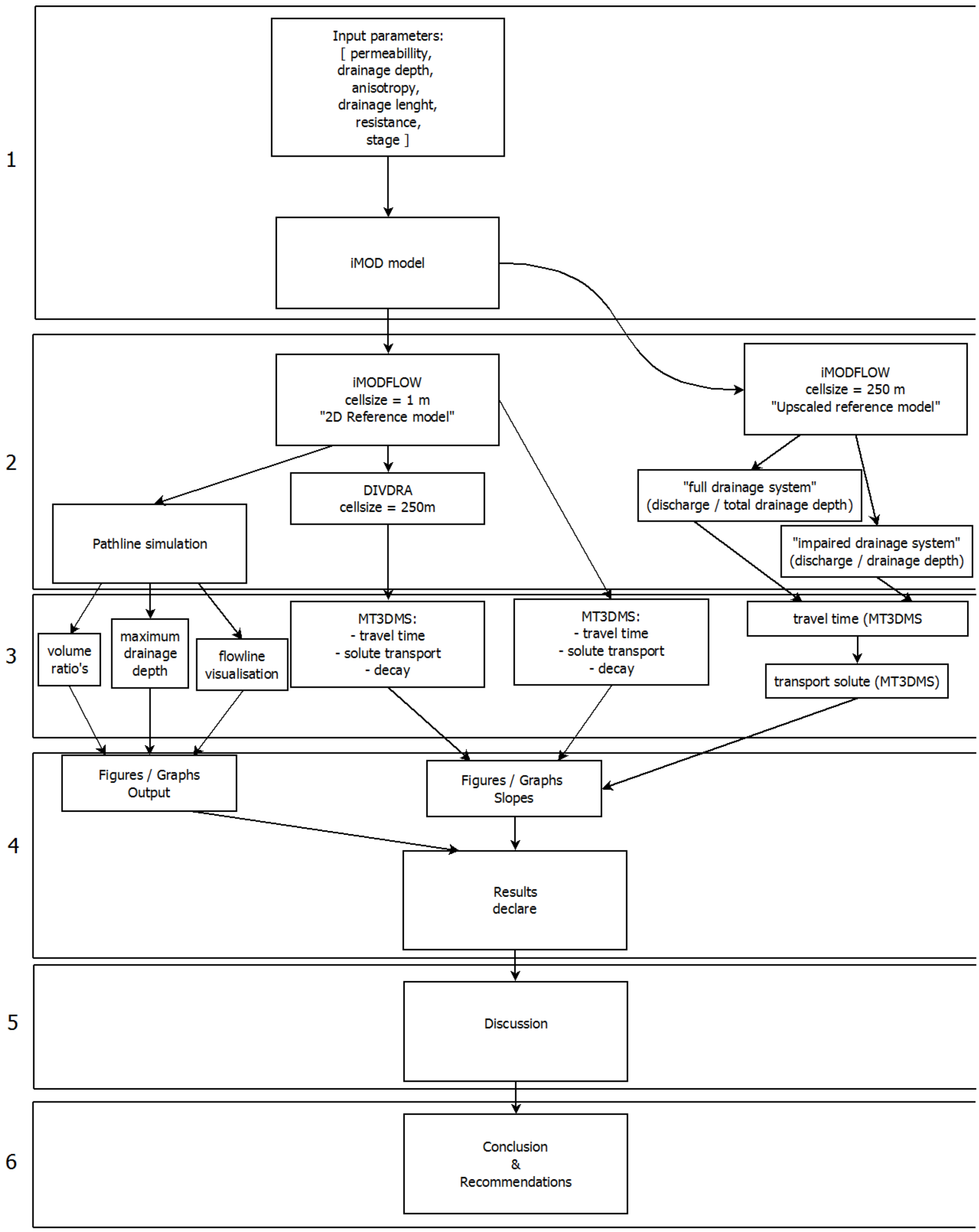


Figure 1 Schematic approach of research.

1. Introduction and research questions

1.1 Problem definition

The National Hydrological Model Instrument – Water Quality, abbreviated as NHI-WQ is a model instrument for calculating groundwater and surface water quality on a national level. It includes the model codes ANIMO (nutrient fate and transport in the unsaturated zone and upper groundwater) and MT3DMS (solute transport in groundwater). The most important reasons to use and couple these two model codes (ANIMO and MT3DMS) for nutrient transport are:

- ANIMO is a state-of-the art process model for transport and conversion of nutrients in the soil and root zone.
- ANIMO cannot be used to model the deeper groundwater fluxes, because it is based on a quasi-2D concept. There cannot be a lateral exchange between model columns, which makes calculation for longer distance not possible. MT3DMS will be used to model these longer distance transport paths.

The NHI model resolution, with a cell size of 250 by 250 meters, is very low for solute transport in the upper groundwater. This keeps the computational time reasonable. However, the drainage pathways often take place on a much finer scale (Figure 2, the red lines). The travel time distributions of these shorter pathways are often dominant for nutrient transport from the soil surface to the surface water. For the NHI model this means that these important transport processes occur within the horizontal dimensions of one model column. Therefore, transport along these shorter paths cannot be resolved numerically, as that requires multiple model cells along the transport routes.

To make an adequate estimation for travel time distribution for the solute transport occurring within the dimensions of the NHI-WQ grid cells, upscaling of the flow and transport processes at this scale is needed. Implementing the DIVDRA (DIVide DRAinage) upscaling concept, developed by Alterra, into MODFLOW could be a solution to solve this problem. This comes down to adjusting the way drainage features in MODFLOW are schematized and parameterized. When done correctly, this would give a proper travel time distribution for large cell sizes as in the NHI model.

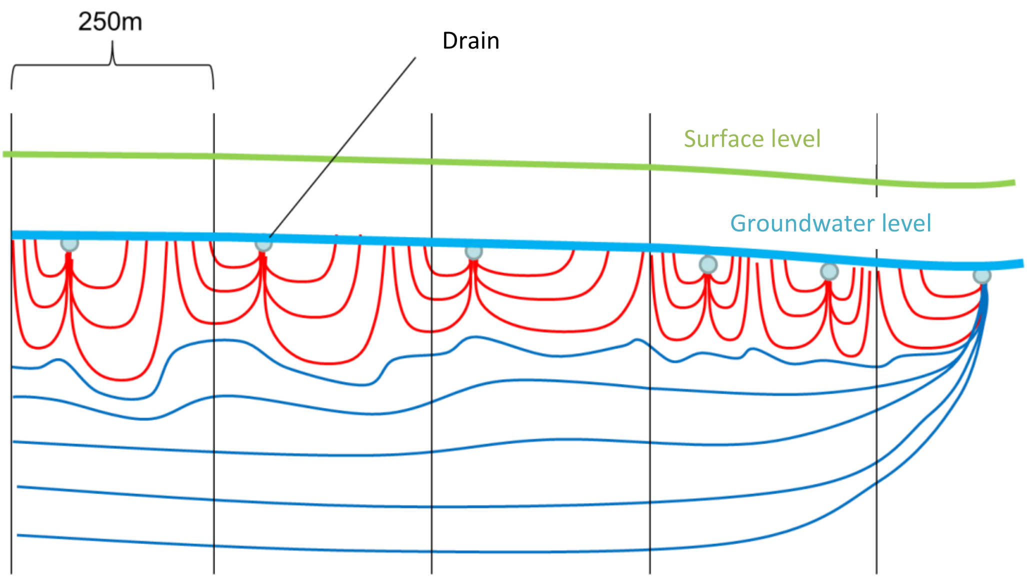


Figure 2 Conceptual representation of the optimal link between ANIMO and MT3DMS. The red flow lines represent the local groundwater flux within the cell boundaries (dimension grid size of 250x250 m). Therefore the groundwater fluxes are calculated with a conceptual quasi-2D model. The solute transport will be modelled with ANIMO. The blue flow lines will cross the cell boundaries (also dimension of 250x250m). These groundwater fluxes are 3 dimensional and solute transport is calculated by MT3DMS.

"DIVDRA in MODFLOW" enables us to compute the local transport processes for coarse model resolutions. The advantage of a successful implementation simplifies the position of the interface between ANIMO (Agricultural-Nutrient-Model) and MT3DMS. Then the interface will situate at the groundwater level, boundary between saturated and unsaturated zone. At the moment it is complicated, because ANIMO (DIVDRA with a quasi-2D drainage concept), and MT3DMS (MODFLOW) is a 3D drainage concept. The interface line at the groundwater table makes it easier to model. The unsaturated zone will be modeled with ANIMO and the saturated zone with MT3DMS. The conceptually groundwater flow actually passes through a quasi-2D to a 3D process. This plane is equally exaggerated. Whereas the current paths no longer drain the model column in 250x250m cell but travel longer distances (see Figure 2). However, the position of this plane in the physical world is unknown. It is also difficult to derive, and moreover variable over time. This makes the definition of the interface plane between ANIMO and MT3DMS unsuitable for practical use. However, if we build the DIVDRA concept in MODFLOW, MODFLOW also has a quasi-2D drainage concept. Concepts on either side of the coupling surface are then equal. With a correct implementation, we can put the coupling surface where we want. As long as it is within the domain in which the drainage process of a quasi-2D process can be proposed. That gives more freedom than the coupling surface on the border between (conceptually) quasi-2D and 3D groundwater flow

Before DIVDRA can be implemented into the NHI-WQ more validation is required. Very little information can be found in the literature on the performance of DIVDRA as an upscaling method. This is remarkable because this method is already widely implemented for regional and nationwide modelling instruments. An exception is Peters and Griffioen (2006), who compared the results of a quasi-2D SWAP/ANIMO model with those of a 2D Hydrus model. The quasi-2D approach is very efficient that is able to model a very high density of drainage network. The adsorption of solute transport in both models is simulated using Langmuir adsorption. For a primary system, only one drain in the cell, the differences are small. Although the differences between Hydrus 2D and ANIMO increases if a second drain is added to the model. Although the quasi-2D model has the best output in general there are limitations. For example the more complex flow and adsorption conditions are added to the model (Peters & Griffioen, 2006). The focus during this research is on the nutrient transport in the saturated and unsatured zone. The errors will theoretically decrease for a quasi-2D approach in the saturated zone. In theory the lateral nutrient flux will become the most dominant flux.

This research will focus on the validation of DIVDRA that could be used for implementing DIVDRA (quasi-2D) into MODFLOW to represent the sub grid drainage fluxes. Before DIVDRA can be implemented the behaviour of the analytical concept has to be validated by comparing it with numerical alternatives. DIVDRA will be compared with MODFLOW and MT3DMS reference models to validate the concept. It is also interesting to compare the DIVDRA concept with other upscaling methods, to review the benefits and added value of the DIVDRA approach. The need for validation of DIVDRA is confirmed in Bakker and Schaars review report (Bakker & Schaars, 2015) Their report describes the findings and recommendations for validating the use of the DIVDRA concept within NHI for salt transport modelling. The recommendations on how to perform such a validation are divided into four steps: The first step is analysing the current analytical formula with relevant input of LHM, time depending water balances and time depending TRANSOL/DIVDRA simulations. For the second step a 2D or 3D reference model should be built with a high resolution of 1 meter in horizontal and vertical, with which groundwater flow and solute transport could be calculated with MODFLOW and MT3DMS. As a third step the simulations should be executed with fixed fluxes for the different drainage systems. And the final verification should be done with a simulation of fixed stage for each drainage system in MODFLOW.

Because the research described in this report started before the appearance of Bakker and Schaars (2015), and because the nutrient modelling context in this thesis report differs from the salt transport modelling context in Bakker and Schaars (2015), these recommendations were not followed 100% but our method nevertheless resembles the suggested method for validation as proposed by Bakker and Schaars (2015).

1.2 Objectives

The objective of the current research is …. Before DIVDRA can be implemented it has to validate the behaviour of the analytical concept compared to numerical alternatives. DIVDRA will be compared with MODFLOW and MT3DMS reference models to validate the upscaling concepts.

1.3 Research questions

In order to accomplish the research goal, the following research questions will be answered:

- Is the DIVDRA concept suitable to represent small-scale transport processes in course numerical grids?
- How well does the DIVDRA concept work under various conditions (heterogeneity, drainage complexity, reactivity)?
- How does it compare to other simple scaling routines?

1.4 Reading Guide

In the Theoretical background (chapter 3) the model resolution choices and assumptions for the different scaling approaches are defined. The different upscaling concepts that are used during this research to compare the DIVDRA concept will be introduced and explained. Stratified and homogeneous soil profile implementations of the DIVDRA concept for this research are illustrated. At the List of symbols and units all the symbols and units used in this report are given and explained. This applies for all the equations that are mentioned in this report.

The Method (chapter 3) provides an overview of al tools that are used for the validation of DIVDRA and the input variables. In Figure 1 an overview is given. Also a distinction is made to compare the different upscaling approaches with each other on specific functions (Figure 1, section 3). First the general approach for validation is given for the 2D reference model that is used as a starting point (Figure 1, section 2). Furthermore, all the specific tools are described.

The results of this will be presented in chapter 4. An analysis is made of the 'standard' 2D reference model to validate the outcomes. Therefore, several comparisons are made like, homogenous versus stratified soil profiles (4.1.1), Conservative solute transport versus transport with decay (4.1.2) stationary versus instationary (4.1.3) and the effect of parameters (4.1.4). In the second part of the results the different scaling approaches will be discussed (4.2). These results will also be compared for different stationary scenarios like homogeneous and conservative (4.2.1), stratified and conservative (4.2.2), homogeneous with decay (0) and stratified with decay (4.2.4).

2. Theoretical background

2.1 Scaling problem

Essential problem for upscaling of the NHI-WQ resolution to 250 by 250-meter cell size is that the horizontal discretization changes. Therefore, the travel time distribution of solute transport is changed and also not representative for solute transport. Figure 3 shows the different between a high resolution model and a scaling approach without horizontal discretization within the 250 by 250 meter cell size. This scaling approach of the 2D models gives unrealistic travel time distributions and therefore wrong solute transport representation. During this research different approaches of drainage distance would be compared with the 2D reference model. Important indicators for travel time distribution are the flow lines through the 2D reference model. An overestimation and underestimation due to upscaling, affects the solute transport and therefore the output concentrations.

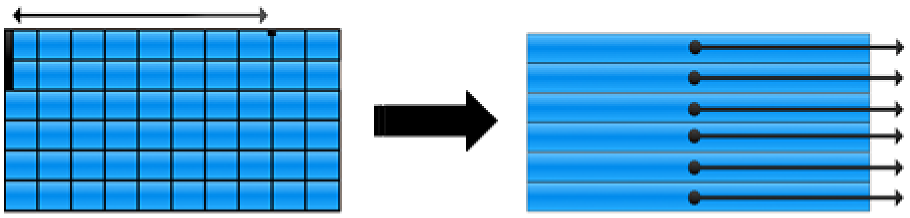


Figure 3 At the left the model with high resolution of horizontal discretization. The drains were represented with the black lines in the cells, primary drain at the left boundary and secondary drain a defined point. The arrow between the primary and secondary drain represents the drainage distance. At the right, a model without horizontal discretization within the 250 by 250 m cell size. This scaling solution will be tested to solve the scaling problem. The nodes in the center of the cells represent the horizontal discharge fluxes.

2.2 Scaling solution

The scaling solutions are divided into several scaling approaches to solve the scaling problem. Each scaling approach has a different solution to divide the horizontal drainage fluxes over the drainage depth. Scaling approach 1 divides the fluxes for primary and secondary drainage systems. Scaling approach 2 divides the total drainage fluxes over the total drainage depth. These different solutions will be compared with the DIVDRA solution. This reveals the advantage of DIVDRA compared to these scaling approaches.

Goal of comparing these different scaling approaches is to review the advantage of the DIVDRA concept. Scaling approach 1 and 2 both divide the discharge fluxes over a certain depth that result in a horizontal flux per layer. These approaches are easier to implement than the DIVDRA concept.

2.2.1 Scaling approach 1

For scaling approach 1 the discharge fluxes are divided over the drainage depth. The $D_{primary}$ refers to the drainage depth of the primary drain and $D_{secondary}$ refers to drainage depth of the secondary drain. This drainage depth is the depth of the drain bottom. The primary drain has a higher depth compared to the secondary drain. The q_i refers to the horizontal drainage flux for each layer. The amount of layer and therefore range of *i* depend on the layer depth (d_z) and depth total depth of the system (D_{tot}). In Figure 3 (right figure) every node represents a horizontal drainage flux, q_i, see equation *0.1*.

$$q_i = \frac{Q_1}{\frac{D_{primary}}{dz}} + \frac{Q_2}{\frac{D_{secondary}}{dz}} \quad (0.1)$$

2.2.2 Scaling approach 2

For scaling approach 2 the discharge fluxes of the primary and secondary drainage system are added and divided by the layers in the z-direction for the total drainage depth as shown in equation *0.2*. The q_i represents the horizontal drainage flux at layer *i*. The number of layers depends on the total depth (D_{tot}) and depth per layer (d_z), *i* is equal to $\frac{D_{tot}}{dz}$. Q_1 represents the primary drainage flux and Q_2 represents the secondary drainage flux.

$$q_i = \frac{Q_1 + Q_2}{\frac{D_{tot}}{dz}} \quad (0.2)$$

2.2.3 DIVDRA

The DIVDRA concept is introduced by Alterra to define the distribution of drainage fluxes with depth. This concept divides the groundwater flux in the subsurface into sub regions that are separated based on the maximum drain distance. A primary drain is also a secondary drain, till $D_{secundary}$. The maximum drain distance is the maximum length between the primary and secondary drains in a 2D field, without repeating itself, see 2.2.3.1. The discharge layers are converted into horizontal discharge layers instead of radial flow patterns, see Figure 11. Every radial flow component will be ignored in the vicinity of line drains. For the NHI water quality project DIVDRA is implemented into the scale of NHI.

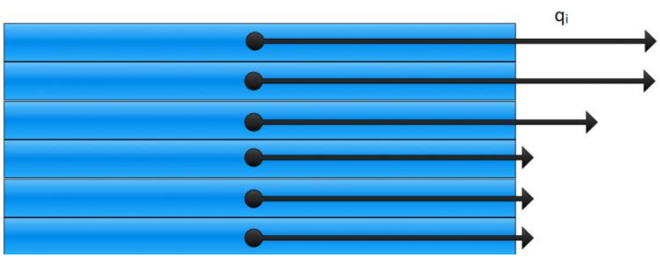


Figure 4 Schematic representation of the DIVDRA approach. The horizontal arrows represent the horizontal drainage fluxes per layer.

2.2.3.1 General concept

An essential assumption that is made is the proportionality of the ratio between V_i, flow volumes per drain order. The flow volume of V_2 is the total volume that the secondary drainage system discharges. Because this is a 2D representation, the ratio of flow volume for a drainage system (V_i) is equal to the discharge flux of the drain (Q_{draini}).

The discharge rates $Q_{drain,\,i}$ (discharge flux per drain order), see equation. *0.3*.

$$\frac{V_i}{V_{i-1}} = \frac{Q_{drain,i}}{Q_{drain,i-1}} \quad (0.3)$$

$$Q_{drain,i} = L_{drain,i}\ q_{drain,i} \quad (0.4)$$

The drainage depth (D_i) is the depth of the drainage volume per drainage order. The flow lines to the 1st order drains only travel through the 1st order drainage depth (D_1), equal for the 2nd order drains. Therefore, by DIVDRA the first order drains will also act as second, third or higher order drains. These drainage depths are based on the assumption that the groundwater volume between the striped lines above D_1 and D_2 in Figure 5 can be neglected (Kroes et al., 2009). This assumption is questionable as mentioned in (Groenendijk & van den Eertwegh, 2004).

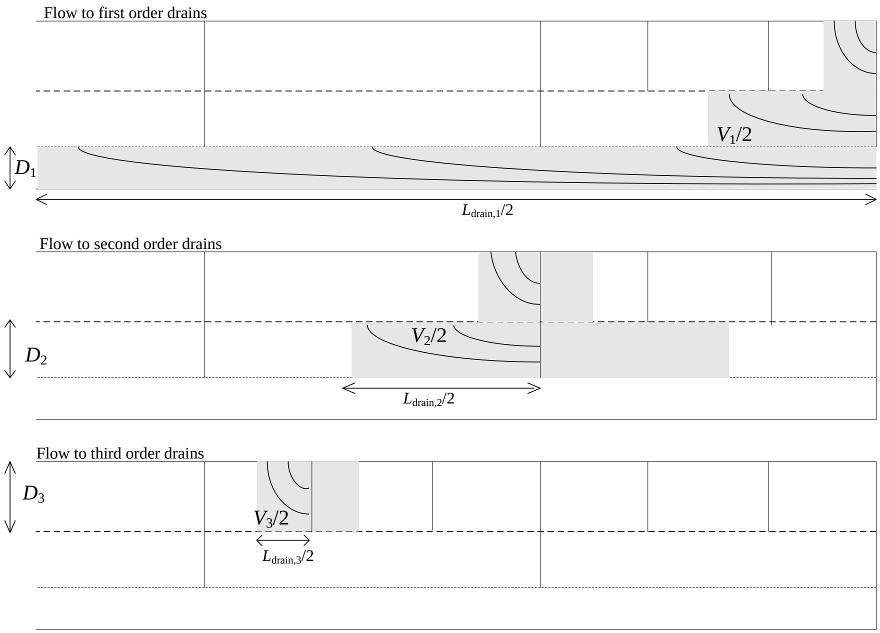


Figure 5 Schematization of regional groundwater flow to drains (Kroes et al., 2009)**.**

In equation *0.5* the 1st order drainage volume is equal to the first, second and third order drain length multiplied by the drainage depth. This is because the assumption is made that every first order drain is also a second, third or higher order drain.

$$V_1 = L_1 D_1 + L_2 D_2 + L_3 D_3 \qquad (0.5)$$

$$V_2 = L_2 D_2 + L_3 D_3 \qquad (0.6)$$

$$V_3 = L_3 D_3 \qquad (0.7)$$

Rewriting the equation of *0.5, 0.6* and *0.7* and substituting *0.2* and *0.3* (Kroes & Dam, 2003):

$$L_1 D_1 : L_2 D_2 : L_3 D_3 = (q_{\text{drain},1} L_{\text{drain},1} - q_{\text{drain},2} L_{\text{drain},2}) : (q_{\text{drain},2} L_{\text{drain},2} - q_{\text{drain},3} L_{\text{drain},3}) : (q_{\text{drain},3} L_{\text{drain},3}) \qquad (0.8)$$

When $q_1 L_1 - q_2 L_2 < 0$, D_1 will be zero and nesting of superposed flow systems on top of the flow region related to D_1 will not occur, therefore D_2 is equal to D_{tot}.

To define analytical formulas for the DIVDRA concept several assumptions are made:

- Steady state during the time increment.
- Constant depth of the drainage systems.

- All streamlines are cylindrical shaped.
- Every radial flow component in these perfect drains will be ignored in the vicinity of line drains.
- Uniform thickness of hydrological profile.

2.2.3.2 Homogenous isotropic soil profile

In a homogeneous isotropic soil profile, the permeability is spatially constant and equal in both the horizontal and vertical direction. DIVDRA assumes hydraulic heads and flow rates that are constant in an isotropic situation. Equation *0.9 - 0.20,* shows the derivation of the drainage depths for a situation with two drainage systems (a primary and secondary drainage system).

$$V_2 = L_2 D_2 \qquad (0.9)$$

$$V_1 = L_1 D_1 + L_2 D_2 \qquad (0.10)$$

$$\frac{V_2}{V_1} = \frac{Q_2}{Q_1} \qquad (0.11)$$

$$\frac{L_2 D_2}{L_1 D_1 + L_2 D_2} = \frac{Q_2}{Q_1} \qquad (0.12)$$

$$\frac{L_1 D_1 + L_2 D_2}{L_2 D_2} = \frac{Q_1}{Q_2} \qquad (0.13)$$

$$\frac{L_1}{L_2}\frac{D_{tot} - D_2}{D_2} + \frac{L_2 D_2}{L_2 D_2} = \frac{Q_1}{Q_2} \qquad (0.14)$$

$$\frac{L_1}{L_2}\frac{D_{tot} - D_2}{D_2} + 1 = \frac{Q_1}{Q_2} \qquad (0.15)$$

$$\frac{L_1}{L_2}\frac{D_{tot} - D_2}{D_2} = \frac{Q_1}{Q_2} - 1 \qquad (0.16)$$

$$\frac{D_{tot} - D_2}{D_2} = \frac{L_2}{L_1} * (\frac{Q_1}{Q_2} - 1) \qquad (0.17)$$

$$\frac{D_{tot}}{D_2} = \frac{L_2}{L_1} * (\frac{Q_1}{Q_2} - 1) + 1 \qquad (0.18)$$

$$\frac{1}{D_2} = \frac{\frac{L_2}{L_1} * (\frac{Q_1}{Q_2} - 1) + 1}{D_{tot}} \qquad (0.19)$$

$$D_2 = \frac{1}{\frac{\frac{L_2}{L_1} * (\frac{Q_1}{Q_2} - 1) + 1}{D_{tot}}} \tag{0.20}$$

$$D_1 = D_{tot} - D_2 \tag{0.21}$$

2.2.3.3 Stratified soil profile

For a stratified anisotropic soil profile, the drainage fluxes per layer are different compared to the homogenous soil profile due to the cumulative transmissivity that changes through depth. The main difference for the stratified soil profile is the permeability that is included into the DIVDRA formula. For this research only a primary and secondary drainage system is used for validation, this simplifies also the stratified formula. In equation *0.22* the formula is given, combined with equation *0.23* the unknown parameter is also D_2.

$$K_1 D_1 : K_2 D_2 = \frac{Q_1 - Q_2}{L_1} : \frac{Q_2}{L_2} \tag{0.22}$$

$$D_1 = D_{tot} - D_2 \tag{0.23}$$

Equation *0.24* and *0.25* show the implementation of the horizontal discharge flux into a stratified soil profile. Important is to take the permeability per Δz layer into account for a stratified model. The ratio of k_h per layer is divided by the cumulative k_h for each order. Equation *0.24* is for the horizontal discharge fluxes of the primary discharge system and equation *0.25* for the secondary drainage system.

$$q_{d,1,i} = q_{d,1} \frac{k_{h,i} \Delta z_i}{\sum_{i_{z=\varphi_{avg}}}^{i_{z=-D_1-D_2}} k_{h,i} \Delta z_i} \qquad \text{for} \qquad -D_1 - D_2 < z < \varphi_{avg} \tag{0.24}$$

$$q_{d,2,i} = q_{d,2} \frac{k_{h,i} \Delta z_i}{\sum_{i_{z=\varphi_{avg}}}^{i_{z=-D_2}} k_{h,i} \Delta z_i} \qquad \text{for} \qquad -D_2 < z < \varphi_{avg} \tag{0.25}$$

2.2.3.4 Analytical solution for 3 drainage systems

Equation *0.8* is equal to the ratio of *0.26* that should give a ratio formula for D_3 (tertiary drainage system). To solve this equation, the secondary drainage depth is zero so the system becomes a primary and secondary drainage system.

$$L_1 D_1 : L_2 D_2 : L_3 D_3 \tag{0.26}$$

$$D_{tot} = D_1 + D_2 + D_3 \tag{0.27}$$

If $D_1 = 0$

$$\frac{L_2 D_2}{L_3 D_3} = \frac{q_2 L_2 - q_3 L_3}{q_3 L_3} \tag{0.28}$$

$$\frac{L_2 (D_{tot} - D_3)}{L_3 D_3} = \frac{q_2 L_2 - q_3 L_3}{q_3 L_3} \tag{0.29}$$

$$\frac{D_{tot} - D_3}{D_3} = \frac{q_2 L_2 - q_3 L_3 \frac{L_3}{L_2}}{q_3 L_3} \tag{0.30}$$

$$\frac{D_{tot} - D_3}{D_3} = \frac{q_2 L_2 - q_3 L_3}{q_3 L_2} \tag{0.31}$$

$$\frac{D_{tot}}{D_3} - 1 = \frac{q_2 L_2 - q_3 L_3}{q_3 L_2} \tag{0.32}$$

$$\frac{D_{tot}}{D_3} = \frac{q_2 L_2 - q_3 L_3}{q_3 L_2} + 1 \tag{0.33}$$

$$\frac{1}{D_3} = \frac{q_2 L_2 - q_3 L_3}{q_3 L_2 D_{tot}} + \frac{1}{D_{tot}} \tag{0.34}$$

$$D_3 = \frac{1}{\frac{q_2 L_2 - q_3 L_3}{q_3 L_2 D_{tot}} + \frac{1}{D_{tot}}} \tag{0.35}$$

3. Method

In this chapter the general approach for validation of the DIVDRA concept is explained and the assumptions that are made to establish the output for validation are laid out. An overview of the software that is used during this research is given combined with theoretical background of the software tools. This software is automated with python scripts. These scripts are used to create al the essential input files and processing threads including post processing and graphical output.

3.1 Design for validation

3.1.1 Approach

To validate DIVDRA it should be compared with a 2D reference model. Also the performance of two other, simpler upscaling approaches is tested against the performance of DIVDRA. Besides the MODFLOW model of the 2D reference model and all the upscaling models there will be also validation by MT3D models for travel time, conservative transport and conservative transport with decay. Also for the MT3D models the 2D reference model will be compared with all the different upscaling approaches.

Different scenarios of drainage complexity, heterogeneity and reactivity will be investigated. Hydraulic head, drainage fluxes and breakthrough curves are the main indicators to validate the DIVDRA concept. The concept will be reviewed for the fluxes to the divided drainage systems, maximum depth of drainage system, travel time distribution of solute transport, solute transport with decay and discharge volume ratios.

3.1.2 2D reference model

The 2D reference model is defined as a closed system with multiple drainage systems with fixed depths. The 2D reference model is defined as closed system with no flow boundaries at the bottom and at the sides. All the recharge that enters the system will be discharged through the drainage systems. The model that is used assumes closed boundary at the primary drainage systems at the end, so at x=0 and x=500 meter.

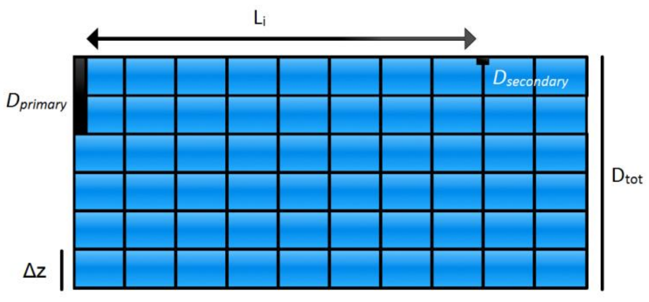


Figure 6 Schematic cross section of 2D reference model

To review the DIVDRA concept several model types are defined: 2D reference, DIVDRA, scaling approach 1 and 2. The 2D reference model is a high resolution model with a 1 m cell size resolution in x and y direction. For the DIVDRA, scaling approach 1 and 2 the x and y resolution is 250 m, because these are 1D models. For this reference model at x=0 the primary drain represents half of total primary drain.

In Table 2 the parameters that are used to define a reference model for this research are given.

Table 3 and Table 4 shows the different model parameters, these river parameters are used to define the model resolution. To compare the different cell sizes and the effects of up or down scaling the parameters of Table 4 is used as starting point. Important boundary conditions are the layer thickness top and bottom is 0 m, closed boundaries and the drains are the only discharge in the model. The parameters are only used to test the model in MODFLOW for the different cell sizes, not to simulate specific realistic scenarios or a specific region. This test is important to be sure that a change in cell size would not affect the outcomes for the 2D groundwater models.

Table 2 Conceptual model parameters to define cell size for reference model.

Model 'Up / down scaling'				
Homogeneous, confined aquifer				
Width (m)	250			
Depth (m)	13			
Grid cells (m)	250 ; 1 ; 0.10 ; 0.05			
Δz	0.05 Top and Bottom has layer with thickness of 0 m			
Drain (left corner)	1 by 1 cell			
Khv (m/day)	10			
Kvv (m/day)	10			
Recharge (mm/day)	1 (increased by factor 100 for testing model)			
Cell size	**250 meter**	**1 meter**	**10 cm**	**5 cm**
Number of columns	1	250	2500	5000
Number of row	1	1	1	1
Number of iterations (outer - inner)	100	1000	1000	1000
Close criteria hydraulic head (m)	$1*10^{-3}$	$1*10^{-3}$	$1*10^{-3}$ (0.1)	0.1
Close criteria mass balance (m^3)	6.25	$1*10^{-4}$	$1*10^{-6}$	$2.5*10^{-5}$
Relaxation factor	0.98	0.98	0.98	0.98

Table 3 "River" model parameters to define cell size for reference model.

'River'	
KHV/KVV	10.0 m/day
Conductance	50.0 m^2/day
Elevation of top level	-1.0 m
Elevation of bottom level	-1.0 m
Infiltration factor	0.0 , no infiltration
Depth (number of layers)	1.0 m (20 layers of 0.05 m)

Table 4 "2 River" model parameters to define cell size for reference model.

'2 Rivers'	
Khv/Kvv	10.0 m/day
Conductance	25.0 m^2/day and 25.0 m^2/day
Elevation of top level	-1.0 m
Elevation of bottom level	-1.0 m
Infiltration factor	0.0 , no infiltration
Depth (number of layers)	1.0 m (20 layers of 0.05m)

3.2 Model resolution

For this research it is important to define a sufficient resolution for the reference model. The characteristic length could give a good indication of the minimal cell size. Characteristic length is an approximation and indication if the stream flux or groundwater flow can be described with chosen cell size, see equation *0.36 - 0.38*. Based on the characteristic length a suitable resolution of the model can be defined. The characteristic length for this model results in a cell size of 5 centimetres. This resolution is required for some parameter combinations and therefore the minimal resolution of the model. Although this high resolution causes numerical problem, the water balance has shown difference more than 5 percent. Due to this numerical problem that effect the mass balance a lower resolution will be compared with the 5 centimetre cell size model. This can give an indication if the model with lower resolution will generate acceptable results for this research. To avoid the numerical problems, the recharge is increased by a factor 100. As a result, all the fluxes will increase by a factor 100. This makes it possible to compare the different resolutions. The comparison is based on average head per layer.

$$\lambda = \sqrt{KDc} \qquad (0.36)$$

$$\lambda = \sqrt{D_{drain} * D_{tot} * c} \qquad (0.37)$$

$$x = \frac{\lambda}{3} \qquad (0.38)$$

In the resolution model the cell size is set on a minimal value for x and y direction in MODFLOW and equal to the model layer thicknesses. Models with a cell size of 5, 10 centimetres and 1 meter are tested and compared to check the output results. Hydraulic head differences between the different cell size models will compare. The scenarios that are given in Table 2 are used to study the influence of model resolution. Therefore several scenarios are calculated for upscaled cell size with 2 rivers (2 drains (MODFLOW river package) at the maximum drain distance). These scenarios are chosen to compare the model outcomes for different cell sizes. Evaluating the hydraulic head for the defined scenarios will give an impression of difference in output related to the cell size. The 5 centimetre cell size model will give the most accurate results.

- Scenario 1 compares the difference between a 5 cm cell size and 10 cm cell size, this to review this effect of upscaled cell size on the averaged hydraulic head.
- Scenario 2 the difference between 1 meter and 5 cm model and the related difference in hydraulic head. This to review the effect of upscaled cell size on the averaged hydraulic head.
- Scenario 3 compares a 10 cm model with 1 m recharge with a 10 cm cell size model with 100 mm recharge (output divided by factor 100). This to review the difference in hydraulic head between 1 mm and 100 mm recharge.

The model is tested with the drain package of MODFLOW. The 5 cm model had some problems to converge due to a very low head difference that results in a minimal flow of groundwater. As a solution the recharge was increased by a factor 100 to increase the head differences and therefore the groundwater flow in the system. At the end all the fluxes had to be divided by a factor 100 per unit length. In Figure 7 are the hydraulic heads plotted on the y-axis and the number of the layer in depth plotted on the x-axis. For each scenario an average hydraulic head for each layer is plotted. The graph shows an almost equal hydraulic head for every layer with the highest difference between the lowest resolution (1 m cell size, 1mm recharge model) and the high resolution model (5 cm cell size, 100 mm recharge).

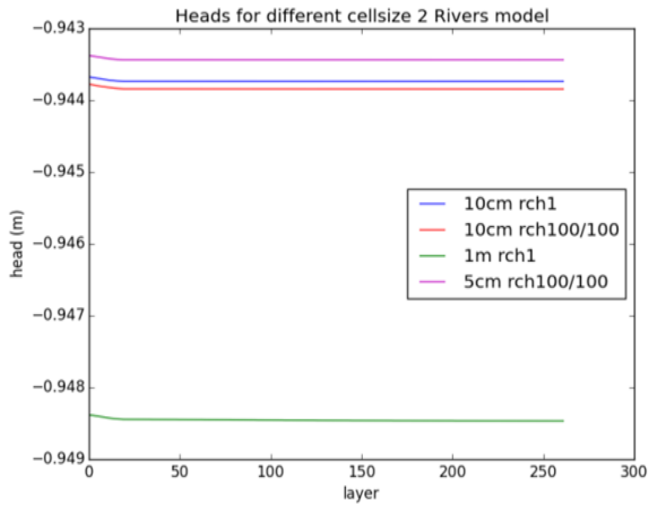


Figure 7 Average head for different model resolution '2 rivers' model.

In Figure 7 an overview of the averaged hydraulic heads for each scenario and specified amount of recharge per day is given. The differences between recharge of 100 mm per day with corrected output by a factor 10 per unit length and a 10 cm model or 1 mm per day is negligible. Also the differences between 5 cm and 10 cm model are within 1 mm difference so therefore very small that it could be neglected. There is a relatively large difference between the 1 m model and 5, 10 cm models.

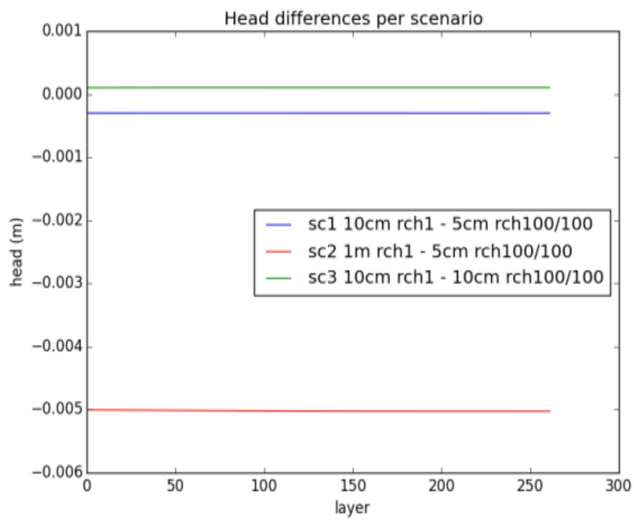


Figure 8 Differences in average head for each model resolution scenario

Figure 8 shows the difference between the 10 cm model and the 5 cm model with a recharge of 100 mm (scenario 1, sc1). Figure 8 gives an overview of input used per scenario and their different value for hydraulic head. The small impact of an increase in cell size to 1 meter on the outcomes of the model's hydraulic head justifies the use of the 1-meter resolution cell size for the reference model.

Also the water balance of the model changes due to a changing model resolution. The hydraulic head distribution for the 5cm and 10 cm models is very close. A finer mesh will result in a slighter higher hydraulic head compared to the 1 meter model. This would be the result of the transport flux direction through the cells. The reason is that in the 1-meter model a cell with a discharge flux is relatively larger than in a 10 cm model (or 5 cm model). The discharging cell is also larger and therefore it has an increased impact on the hydraulic head. The hydraulic head will be lower compared to models with a smaller cell size. This difference of 5 mm (0.005 m) as shown in Figure 8 is within the tolerable margin, especially for the scale of model that will be used in this model. Therefore the 1-meter cell size in x and y direction is sufficient to use as reference model.

3.2.1 Closing criteria

Changes in cell size affect the closing criteria to be applied in the MODFLOW model. The head closure criteria are related to the units of the problem to be solved. For the water balance closure criteria it is related to the accuracy in the head. Increasing the resolution will also increase the number of inner iterations that is required to solve the PCG (Preconditioned Conjugate Gradient) solver.

The closing criteria of the models are presented in Table 2. There is a closing criteria hydraulic head [m] and mass balance [m^3]. For hydraulic head this value varies between 0.001 [m] and 0.1 [m]. The mass balance is a much critical closing criteria that varies from $2.5*10^{-5}$ [m] to 6.25 [m].

3.2.1.1 Flowpath

The MODPATH function is an implementation of the MODPATH code (Pollock, 2012). MODPATH is a particle tracking post processing model that computes 3D flows path using groundwater flow simulations of MODFLOW (Pollock, 2012).The particle tracking scheme uses analytical expression for particle movement within each finite difference cell. To the MODPATH function is used to determine the drainage depth and the drainage volume. The path line simulation can also produce a visualization of the flow lines. This visualization gives a clear overview of the drainage fluxes to the different drainage systems in the model. This should give an excellent overview of the fluxes in the 2D reference model that could be compared with the volumes of the DIVDRA equivalent.

In Table 5 the input parameters for flow path simulations are given. The solute tracer is released at the top of the top of the model between x= 0 and x=250 meter. The starting points of Table 5 are used to compare the travel time distribution for the different scaling approaches. The input parameters of Table 6 re used to determine the discharge volume distribution. This gives an of the flow lines distribution in the reference model or upscaled models. These starting point are also used to determine the maximum drainage depth for each scaling approach as plotted at chapter 4.2.

Table 5 Horizontal starting points for path line simulation.

Starting points Horizontal	
Xll, xur, yll ,yur	0 – 250 m, 0.0-1.0 m
Radius	1 m
Z direction	0 m (present in top layer)

Table 6 Vertical starting points for path line simulation.

Starting points Vertical	
Xll, xur, yll ,yur	250 m, 0.0-1.0 m
Radius	1.0 m
Z direction	0 t/m -13 m (present in top layer)

3.2.1.2 MODFLOW

MODLOW is used to simulate groundwater flow in the 2D reference model determined in chapter 3.1.2. MODFLOW uses the Darcy equation to solve this numerical problem, see chapter 3.3.1.1. The discharge fluxes of the 2D reference model are used for the all the upscaling approaches. These discharge fluxes are divided over the specified discharge layers, see chapter 2.2. For these scaling approaches the discharge layers are implemented into extraction wells. To solve the numerical iteration in MODFLOW a starting head is required. Therefore, the starting head of the 2D reference model of the bottom layer is used as starting head for the bottom layer of the upscaled models.

3.2.1.3 MT3DMS

To compare the solute transport through the different model approaches MT3D is used, see chapter 3.3.2. For the travel time only the porosity has to be set at the same value for the MT3DMS models. The maximum time of releasing tracer particles is determined at 50 years. The maximum runtime is set at 18250 days (50 years). This to have a mass balance between solute particles that enters the system a

Some minimal dispersion is added to prevent extreme oscillation in the output graphs for solute transport. A pulse with a concentration of 10.0 is released at the end of the 31th and a continuous addition with a concentration of 1.0 at the 334th day of every year. A tracer with decay is determined with the RCT package in MT3DMS, therefore the decay rate is set at a 5 d^{-1}. Every stress period of the MT3DMS needs to be equal to MODFLOW model to succeed the process.

3.2.2 Scaling approach 1

The discharge fluxes are extracted from the 2D reference model and implemented into extraction wells for fixed discharge layers. Implementing scaling approach 1 corresponds with the DIVDRA routine. Input parameters are equal only the horizontal discharge occurs only in the top layers instead divided over the total drainage depth. For the reference model the drainage systems occurs also in the top layers. In Figure 9 scaling approach 1 is schematically presented. The discharge fluxes are situated in the top layers of the model en therefore groundwater fluxes will move in vertical direction for discharge. Important is to realise that these discharge fluxes are directly related to the hydraulic head and drainage resistance of the 2D reference model. These discharge fluxes are fixed due to the outcomes of the 2D reference model with the specified parameters and drainage resistance.

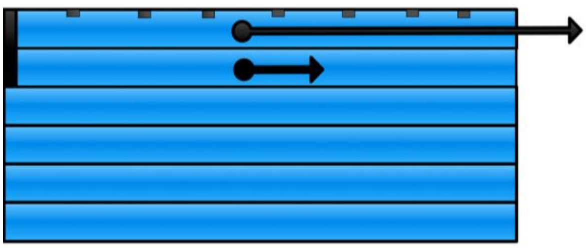


Figure 9 Scaling Approach 1 only horizontal discharge flux

3.2.3 Scaling approach 2

For the scaling approach 1 the model parameters and boundary conditions are equal to the DIVDRA model, but the discharge fluxes of the extraction wells are defined differently. The discharge flux q_i is presented in Figure 10 as a horizontal flux. These fluxes are the results of hydraulic head and drainage resistance in the 2D reference model and implemented into discharge wells. Discharge wells are located in every discharge layer and represent the drains in the upscaled models.

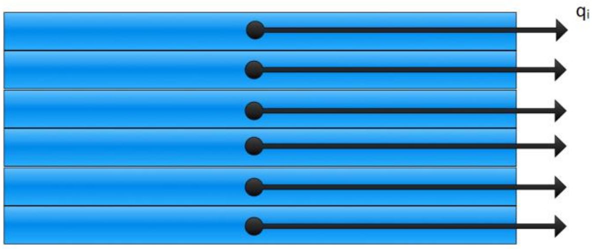


Figure 10 Scaling Approach 2 only horizontal discharge flux

3.2.4 DIVDRA model

For this research only primary and secondary drainage systems are compared with the 2D reference models. The homogenous soil profiles are used to get an impression of the behaviour of the DIVDRA concept. These profiles are defined as basic models BPI (basic parameter index, fixed set of parameters, see Table 10). Stratified models are a more realistic representation of the solute transport through sandy soils. Multiple combinations of parameters are tested but only the interesting outputs will be discussed.

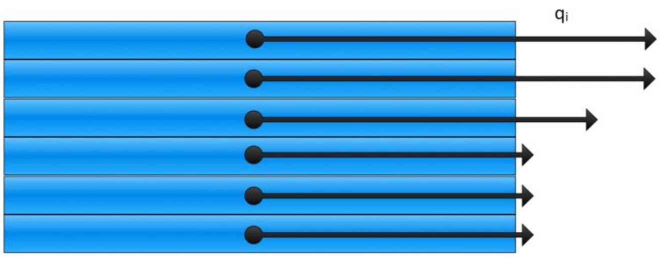


Figure 11 DIVDRA schematically representation of discharge fluxes per layer.

For the DIVDRA model the discharge fluxes of the primary (Q_1) and secondary (Q_2) drainage system are used as input value for the analytical DIVDRA formula. These discharge fluxes are the sum of the discharge fluxes per layer of all drains belonging to a particular system (primary or secondary). Also the drainage distances are given, L_1 is 500 meters and L_2 is 33, 100 or 166 meters. Implemented into

DIVDRA formula (chapter 2.2.3) the drainage depth of the primary and secondary drainage system can be calculated.

The discharge flux per model layer is defined as:

$$q_{1_i} = \frac{Q_1}{\frac{D_{tot}}{dz}} \qquad (0.40)$$

$$q_{2_i} = \frac{Q_2}{\frac{D_2}{dz}} \qquad (0.41)$$

These discharge fluxes are the input values for the extraction wells. The well package uses IPF files to define the input data for the wells. The wells are situated in every model layer, the extraction rate represents the discharge flux per layer. To execute the model a fixed head is required to perform the calculation. This fixed head is set at the bottom layer of the model and is equal to the averaged hydraulic head of the bottom layer of the 2D reference model.

3.2.4.1 Drainage system correction

Due to the fact that the primary drainage system is a half the total primary system a correction is necessary for the discharge fluxes of the system that are used to define the drainage depth for DIVDRA, mentioned in chapter 2.2.3.1.

$$Q_{2DIVDRA} = \left(1 + \frac{1}{2} * \left(\frac{1}{N_2}\right)\right) * Q_{2MODFLOW} \qquad (0.42)$$

$$Q_{1DIVDRA} = Q_{1MODFLOW} - \frac{1}{2} * \left(\frac{1}{N_2}\right) * Q_{2MODFLOW} \qquad (0.43)$$

N_2 = number of secondary drains of the 2D reference MODFLOW model.

Equation *0.42* and *0.43* are implemented into the discharge flux distribution of the DIVDRA MODFLOW models. Equation *0.42* shows that DIVDRA divides the discharge fluxes of the $Q_{2MODFLOW}$ equally. Therefore the $Q_{2DIVDRA}$ depend on the number of secondary drains in the system. The 1 represents the ratio of secondary drains and the ½ represents the ratio of the primary drain. This because every primary drain also represents a secondary drain. The $Q_{1DIVDRA}$ is equal to the $Q_{1MODFLOW}$ minus the primary drain that is presented by the secondary drain ($Q_{2DIVDRA}$.), see equation *0.43*.

3.2.5 Model variations

3.2.5.1 Homogeneous versus stratified

The homogenous models are used as base models to start the comparison between different parameters. These models have a different value for permeability but a fixed drain distance and drainage level. That influence of the permeability for the travel time distribution. The results of the homogeneous soil profile and the stratified soil profile will be presented, see chapter 4.1.1.

3.2.5.2 Conservative versus decay

Travel time distribution gives an indication of the transport through the model. The solute transport is plotted for concentration versus time, see chapter 4.1.2.

$$Cumaltive\ mass\ per\ time = \frac{dM}{dt} \tag{0.44}$$

dM = sink at time (t) – sink at time (t-1)

dt = time (t) – time (t-1)

Comparing tracer with decay to the conservative tracer will give a good indication for the effect of travel times between the different scaling approaches. An increased travel time will increase the time to decay, therefore the solute concentration decreases. This has significant impact on solutes that are sensitive for decay.

3.2.5.3 Stationary and instationary

Stationary model

Input parameters are set for the NHI related scenarios. These parameters value are defined for different areas of the Dutch subsurface. For example, short drain distances and low permeability for the west part and long drainage distances and high permeability for the east part of the Netherlands. Interesting is to review the behaviour of the DIVDRA concept for different scenario in the Dutch subsurface and the different response between the 2D reference model and DIVDRA model. In report of BOFEK2012 (Wösten et al., 2013) parameters for the Dutch subsurface are presented. The conductance's are defined from the drainage resistances as given in "The basics for model concepts" (de Lange, 1997a). In "Use of boundary conditions" (de Lange, 1997b) the use of drainage resistance is preferred instead of the 'feedings resistance'.

The model will be defined as a 'bucket model' there the boundaries will be closed and the only outgoing fluxes are at the drainage systems. This to monitor for optimal monitoring of the output fluxes. These conditions will not be the perfect representation or realistic, but it is the only solutions the check the performance and differences between the models.

Instationary model

For an instationary model the input recharge events differ from the stationary recharge events. The input for this research is from a NHI recharge dataset, Figure 12. The input for this research is from a NHI recharge dataset and therefore reprehensive to use. On the x axis the recharge is plotted. The y-axis plots the decade, this is a time step of 10 days. An instationary model will increase the validity of the models but increases the computational time also. Therefore the instationary models will only be tested after reviewing the stationary models to select specific scenarios to compare the outcomes of different model concepts.

A difference between a stationary system and an instationary system is the recharge event per unit time. For a steady state model the recharge is fixed at one stress period. An instationarty model has recharge events that will changes per stress period and therefore influences the solute transport.

In the runfile there are changes made to create an instationary model, in the second line of the runfile after the number of layers the third column is set at 3 instead of 1. At the end of the runfile the ‘packages for each layer and stress period' and the starting date for the model has to be set at the same amount of recharge in mm per day must be specified between the RCH header and the RIV header in the last column.

The recharge events are extracted from the NHI recharge measurements of 2003. These recharge events could also have a negative recharge that can been interpreted as an evaporation event. Recharge data is extended for 2002 is a copy of the data of 2004 to increase the recharge to more than one year. A leap year has been avoided to prevent problems in MT3DMS.

For the instationary system a storage coefficient is needed to ensure discharge fluxes during events of negative recharge (evaporation). The storage of groundwater will be negative in his case and therefore continue the discharge during drought. A storage coefficient of 0.015 is used to get also discharge fluxes, hydraulic head higher than drainage level. For the instationary models the DRN package in MODFLOW is used instead of the RIV-package to avoid infiltration from the ‘river’ to the saturated groundwater zone. The DRN package only discharge groundwater, infiltration is excluded.

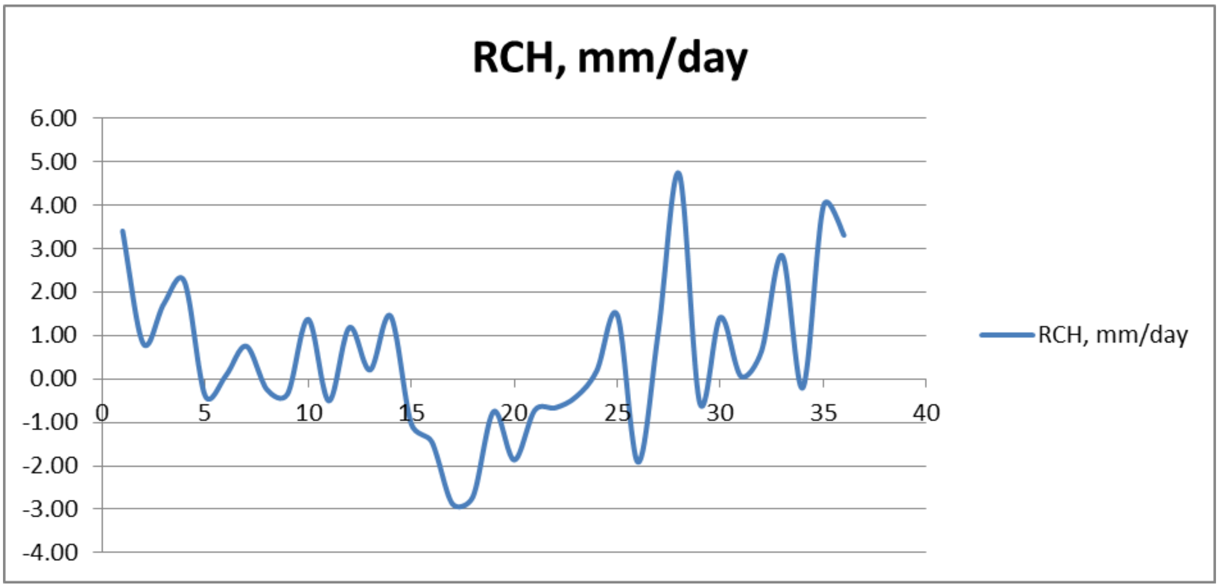


Figure 12 NHI recharge [mm/day] per decade in 2003.

3.2.5.4 Parameter variations

In the review report of the LHM 3.1.1 (Bakker & Schaars, 2015) there is a plan of action defined in four steps that are mentioned in the Introduction. During this research the comparison between the 2D reference model, scaling approach 1, 2 and DIVDRA are tested with a variable amount of parameters. The parameters have a set of variable (Table 7 Variable input parameters) and fixed (Table 8 Fixed input parameters) input parameters. An example of the runfiles for iMODFLOW is given in chapter 17 of the IMOD user manual (Vermeulen et al., 2015).

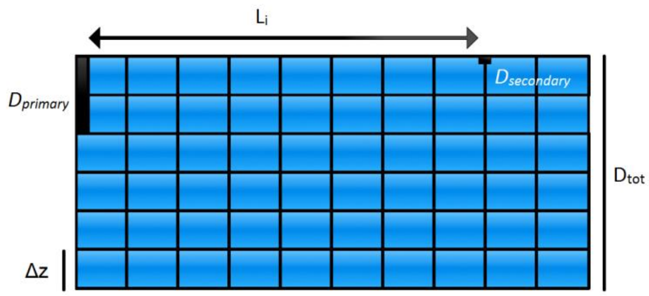


Figure 13 Schematic 2D reference model with drainage length of 166 meter

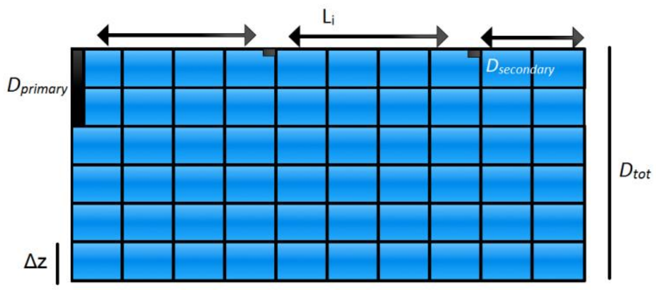


Figure 14 Schematic 2D reference model with drainage length of 100 meter

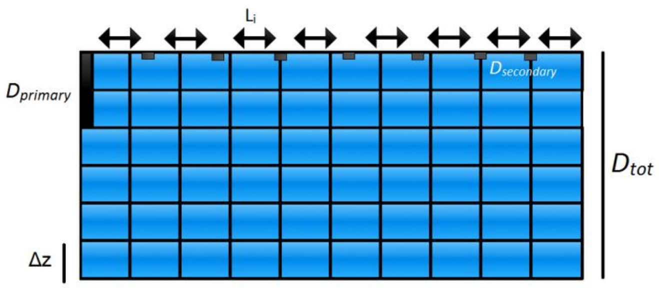


Figure 15 Schematic 2D reference model with drain length of 33 meter

Fixed parameters are the total model thickness, anisotropy, drainage level of primary drainage system and layer depth (thickness in z-direction). The thickness of the model is set at 13 meters, thickness layers z-direction is 0.05 meters, resistance of primary drainage system, resistance of secondary drainage system, anisotropy is 1.0 and the drainage level of primary system is 0.0 meters. The variable parameters are the horizontal permeability, vertical permeability, drain distance to secondary drainage system, drainage level of secondary drainage system and cell size x-y direction. There is also a distinction between homogeneous and stratified models. Homogeneous models have an equal permeability for the total depth. Stratified models have an increased permeability by a factor 3 for the bottom half of the model. This to get an overview of the behaviour of the DIVDRA concept compared to the 2D reference model. An overview of all the model parameters is given in Table 7 and Table 8. The input parameters of MT3DMS runfiles are given in Table 9.

The chosen model parameters will represent the possible scenarios in the Netherlands and therefore the extreme cases in particular. Mostly the lowest and highest possible value for a certain parameter are used. Also a averaged value between these extreme values is added to get a complete overview of possible scenarios in the saturated zone (Wösten et al., 2013). The lowest permeability parameters are matches with the relatively low permeable sandy soils in the Netherlands and the higher permeability parameters with high permeable sandy soils, estuary regions.

Table 7 Variable input parameters

Parameter	Value
Kh_1	2, 5, 10 [m day^{-1}]
Kh_2	6, 15,30 [m day^{-1}]
Drain level secondary system	0.0, 0.25, 0.5, 0.75 [m]
Drain distance	33, 100, 166 [m]

Table 8 Fixed input parameters

Parameters	Value
c_{prim}	1.0 [d] cond: 0.5 [m^2 d^{-1}] per layer(nr of layers= 1/d_z)
c_{sec}	10.0 [d] cond: 0.1[m^2 d^{-1}] per layer (total=0.05/d_z)
Drainage level primary system	0.0
Anisotropy	1.0
Depth (D_{tot})	13.0 [m]
Depth kh_1,kh_2	6.5 , 6.5 [m]

Table 9 Input parameters MT3DMS

Parameters	Value
Porosity	0.30
Maximum simulation time (days)	18250 (50 years), 9125 (25 years), 3650 (10 years)
Flow type	SS, steady state
Additional for solute transport:	-
Input pulse of solute days number	31, 334
Input pulse concentration	10, 1
Additional for decay:	-
Linear adsorption	-
First order decay	
Decay coefficient	0.05 [m d^{-1}]

Al these parameters combinations are simulated and every set of parameters has it specified name, see Table 10 Homogenous model and

Table 11 Stratified model. For the discussion of the outcomes these names are used to refer to a specified parameter set. The stratified models are defined as SPI “sandy soil index” and the homogeneous models are defined as BPI “basic profile index”.

Table 10 Homogenous model parameters and specified name

Kh1 [m / day]	Drain distance [m]	Drain level [m]	Model name
2.0	33	1.0	BPI:1
5.0	33	1.0	BPI:2
10.0	33	1.0	BPI:3
2.0	100	1.0	BPI:4
5.0	100	1.0	BPI:5
10.0	100	1.0	BPI:6
2.0	166	1.0	BPI:7
5.0	166	1.0	BPI:8
10.0	166	1.0	BPI:9

Table 11 Stratified model parameters and specified name

Kh1 [m / day]	Kh2 [m / day]	Drain distance [m / day]	Drain level [m]	Model name
2.0	6.0	33	0.0	SPI:1
2.0	6.0	33	0.25	SPI:2
2.0	6.0	33	0.5	SPI:3
2.0	6.0	33	0.75	SPI:4
5.0	15.0	33	0.0	SPI:5
5.0	15.0	33	0.25	SPI:6
10.0	30.0	33	-0.05	SPI:7
10.0	30.0	33	-0.1	SPI:8
10.0	30.0	33	-0.15	SPI:9
10.0	30.0	33	-0.20	SPI:10
2.0	6.0	100	0.0	SPI:11
2.0	6.0	100	0.25	SPI:12
2.0	6.0	100	0.5	SPI:13
2.0	6.0	100	0.75	SPI:14
5.0	15.0	100	0.0	SPI:15
5.0	15.0	100	0.25	SPI:16
10.0	30.0	100	-0.05	SPI:17
10.0	30.0	100	-0.1	SPI:18
10.0	30.0	100	-0.15	SPI:19
10.0	30.0	100	-0.20	SPI:20
2.0	6.0	166	0.0	SPI:21
2.0	6.0	166	0.25	SPI:22
2.0	6.0	166	0.5	SPI:23
2.0	6.0	166	0.75	SPI:24
5.0	15.0	166	0.0	SPI:25
5.0	15.0	166	0.25	SPI:26
10.0	30.0	166	-0.05	SPI:27
10.0	30.0	166	-0.1	SPI:28
10.0	30.0	166	-0.15	SPI:29
10.0	30.0	100	-0.20	SPI:30

The drainage depth is constant during this research because the change in volume would mainly affect travel time for the tracer particles. An increase drainage depth results in an increased volume that increases the travel time. Therefore, the time scale should have to be increased to reach the maximum concentration of tracer in the model shown in Figure 16. This increase for computational time would not generate better output data. The drainage thickness is therefore set as a fixed input parameter. Increased thickness will decrease the amplitude of the concentration per time unit (see figure below). A higher volume results in a lower impact of one drain cell on the volume discharge cell. In Figure 16 less amplification by increased discharge depth is clearly visible for a model with an increased total depth. More time is needed to fill a volume of 40 m^2 instead of 13m^2. Therefore, the slope of the concentration curve of the model with a 40 m depth is less steep compared to the model with a total depth of 13 meters.

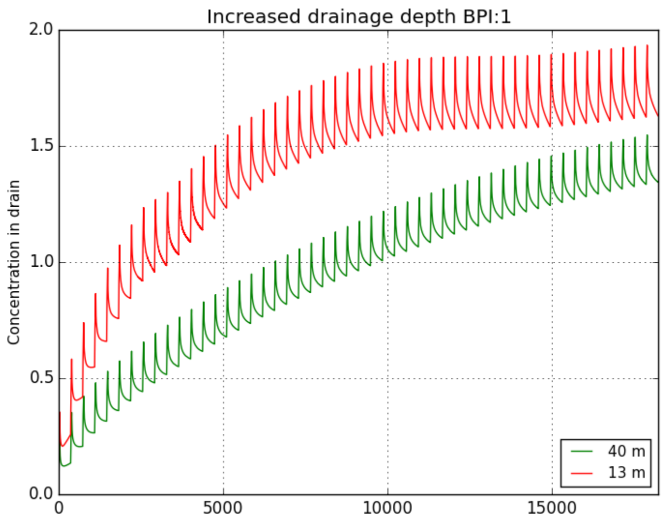


Figure 16 Increased drainage depth for 2D reference model in BPI:1

3.3 Software tools

3.3.1 iMOD

The program iMOD (interactive Modelling) is developed by Deltares. iMOD has a GUI, Guide user interface to control iMODLOW. This is a version of MODFLOW that is adapted for iMOD by Deltares. iMODFLOW works with iMOD input and output files and therefore very useful to compute groundwater models for high spatial areas. iMOD is a viewer and capable to give a rapid overview of model inputs and outputs. For the virtualisation of the MODPATH flow lines the viewer of iMOD is used. iMOD is optimized to work with large data files and is capable to run the models in reasonable timeframes (iMOD User Manual, (Vermeulen et al., 2015)).

3.3.1.1 MODFLOW

MODFLOW is a numerical iteration model that solves groundwater flow equation combined with the Darcy equation. MODFLOW is used to solve the groundwater models during this research. It is also the groundwater flow modelling code of choice in the NHI. For more information about the use and mathematics of MODFLOW see McDonalds and Harbaugh (1999).

3.3.2 MT3DMS

MT3DMS stands for Modular 3-Dimensional Transport and Multi Species, structure for accommodating add-on reaction packages (Zheng & Wang, 1999). MT3DMS is used for solute transport calculations in the model. It will give the best approach to solve transport problems and to compare the 2D solute transport for the numerical model and the DIVDRA model. The fundamentals, solution techniques and numerical implementation of the program are extensively explained in the MT3DMS manual (Zheng and Wang, 1999).

3.4 Implementation into Python

3.4.1 Runfile

The MODFLOW executable gathers the information out of a runfile that is generated in a Python script. To start a groundwater flow model simulation in MODFLOW there is runfile required. This runfile gives the current location of the model, simulation time, grid size, and number of model layers, input file or model parameters and the output variables that needs to be saved. The runfile is easy to reproduce and to change configurations of the entire model. A runfile mainly refers to other input files that contain the model data. Although some constant values or boundary conditions are defined already in the runfile without referring to specific input files. Runfiles are constructed for a region of interest that can be very large, instead of an area of interest that is often smaller.

An important condition for this is maximal overall acceptable error for the water balance below 1% (Vermeulen et al., 2015). If the water balance error margin is below the 1% it is in the acceptable margin. For the increased cell size models, the acceptable error margin is increased to 5%.

In the python subroutine *MT3DMS* several actions take place. First the runfile with all the variables that are required (3.2.5.4 Parameter variations), packages that are used, and the reference to the location of the output of the iMODFLOW model that is used as input for the MT3DMS model has to be defined.

3.4.2 Stratified soil profile DIVDRA

For implementation into python the conversion of discharge fluxes per horizontal layer has to be defined. In the runfile of MODFLOW every layer will be defined with a fixed discharge flux per layer. Therefore the boundary between D_1 to D_2 results in a decreasing discharge flux. The drainage layers of D_1 have a lower discharge flux compared to the discharge flux of D_1 and D_2 combined. Equation *0.45 – 0.54* shows the DIVDRA implementation for a stratified soil profile that is situated in this research.

$$KD_{tot} = kh_1 * -D_{het} + (kh_2(D_{tot} + D_{het}) \quad (0.45)$$

$$ratio = \frac{\dfrac{q_i * L_i - q_{i+1} * L_{i+1}}{L_i}}{q_{i+1}} \quad (0.46)$$

$$if : q_i * L_i - q_{i+1} * L_{i+1} < 0 \quad (0.47)$$

$$KD_1 = \frac{ratio * KD_{tot}}{ratio + 1} \quad (0.48)$$

$$KD_2 = KD_{tot} - KD_1 \quad (0.49)$$

$$KD_{cum} = sum(KD_{i-1}) + KD_i \quad (0.50)$$

$$if : KD_{cum} = KD_2 \quad (0.51)$$

$$D_2 = i * dz \quad (0.52)$$

$$D_1 = D_{tot} - D_2 \quad (0.53)$$

$$D = [D_2, D_1] \quad (0.54)$$

3.4.3 Use of subroutines

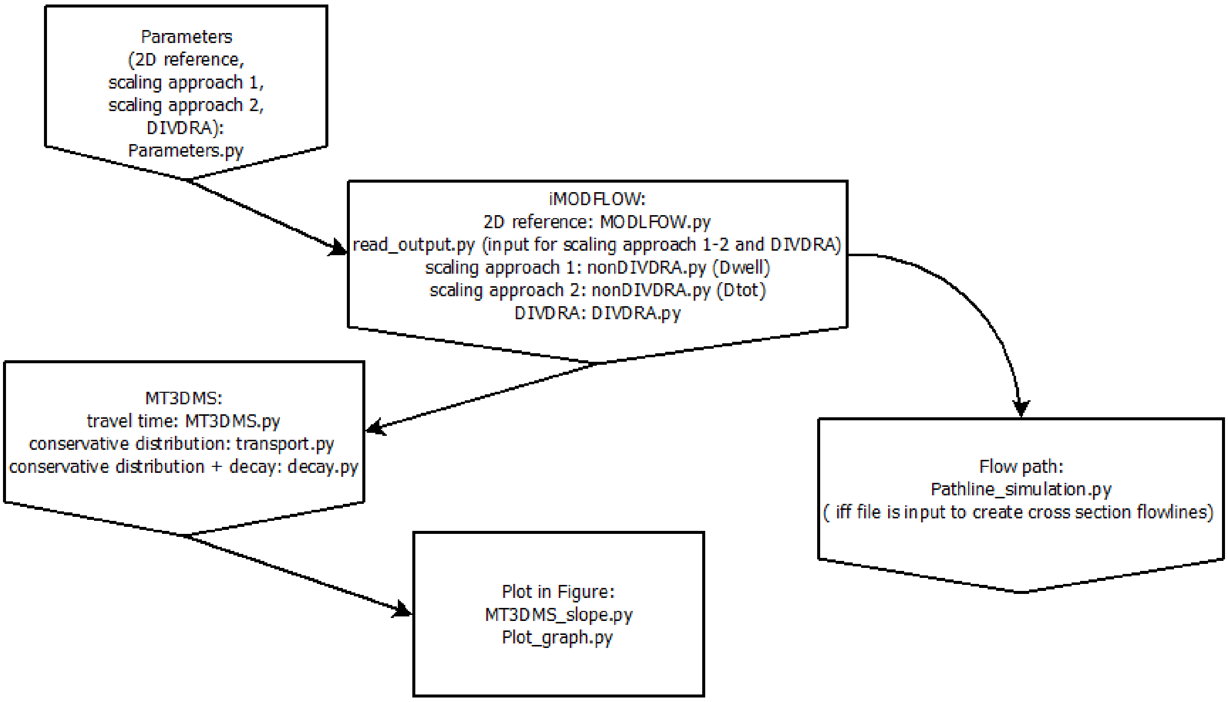


Figure 17 Python scripts used for validation of DIVDRA

In Figure 17 the python scripts that are used for validation are schematically presented. The definitions of the python scripts are defined in Table 12. The input parameters are mentioned in 3.2.5.4 combined with the setting that are described in the method output is generated. The scripts that are mentioned in Figure 17 and shortly introduced in Table 12 are the most important subroutines that are used for this research. Also the post processing is done in python and the graphical outputs are created with the *matplotlib* module of python.

Table 12 Definition of python scripts

Name python script	Definition
Parameters.py	Input parameters for iMODFLOW model and DIVDRA model.
MODFLOW.py	Creates IDF files and ipf file for 250m cell size. - IBOUND,STAGE-'RIV',STAGE-'DRN', INFF, COND. Creates runfiles for iMODFLOW and executes this runfile.
DIVDRA.py	DIVDRA implementation, sum of drainage fluxes and lateral flux partition. Creates runfile + executing
nonDIVDRA.py	Scaling approach 1 and 2 iMODLFOW runfile and executing
MT3DMS.py	Creates runfile for MT3DMS for cell size with 1m and DIVDRA model.
Transport.py	Conservative transport runfile and batch file + executing
Decay.py	Conservative transport with decay runfile and batch file + executing
Pathline_simulation.py	Creates runfile for pathline simulation Creates .ini file for pathline simulation Creates batch file to execute pathline simulation and create an IFF file.
MT3DMS_slope.py	Slope of sink versus time plots Plot of maximum drainage depth, discharge volume ratios.
Plot_graph.py	Plot travel time, conservative transport and differences between scaling approaches. Plot the conservative transport with decay combined with the scaling approaches.

4. Results and discussion

Notable output is reviewed and presented with figures of the results. During the discussion the effects of the assumptions made in DIVDRA will be reviewed. To validate the DIVDRA concept it has been compared based on travel time distribution, conservative transport and transport with decay.

4.1 Analysis of 2D reference model

In Figure 18, Figure 19 and Figure 20 the flow lines for the different drainage distances for the 2D reference model are given. These cross sections show the distribution of the flow lines to the difference drains. In Figure 18 the drain distance of 33 meter (BPI:1) is shown, every 33 meter a secondary drain. The primary drain has the highest discharge volume, most of the flow lines enter the primary drain system. Also in Figure 19 the primary drain has the highest discharge volume. The drain at 100 meter distance from the primary drain is marked with a blue circle. Otherwise it is hardly visible in the cross section. Figure 20 give a cross section of the reference model with a drain distance of 166 meters. This maximum drain distance would have flow lines with the highest residence time and the highest discharge volume compared to the other drain distance scenarios (Figure 18 and Figure 19).

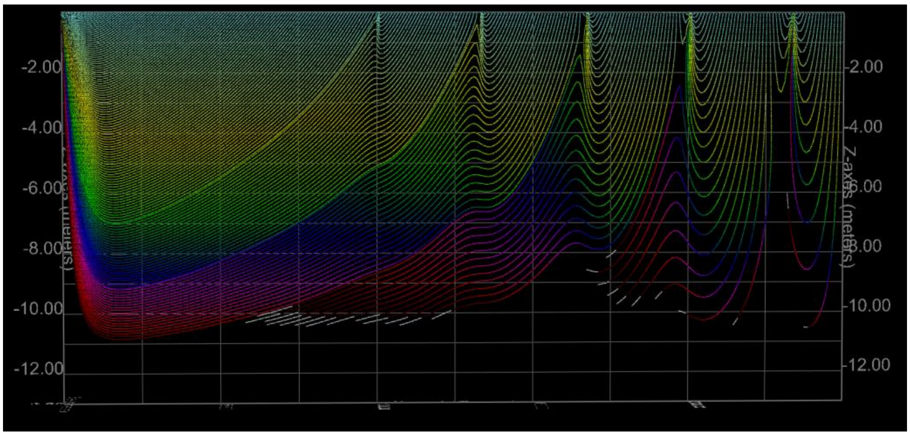


Figure 18 Flow lines for 2D reference model, drain distance of 33 meter (BPI:1).

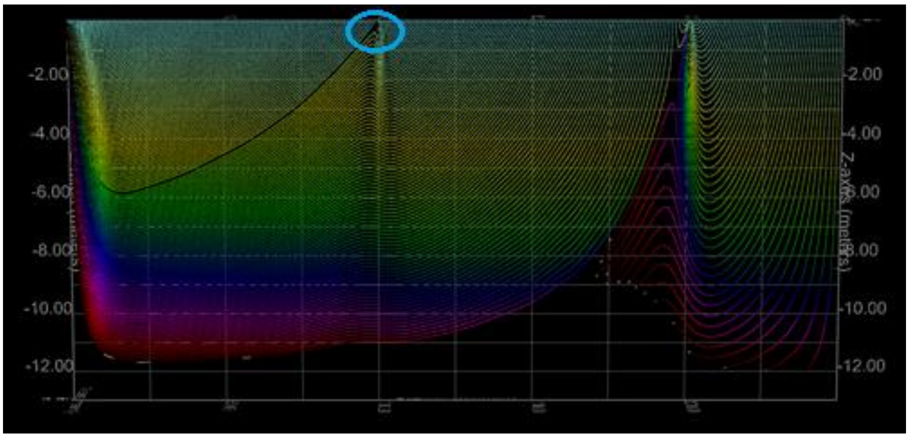


Figure 19 Flow lines for 2D reference mode, drain distance of 100 meter (BPI:4).

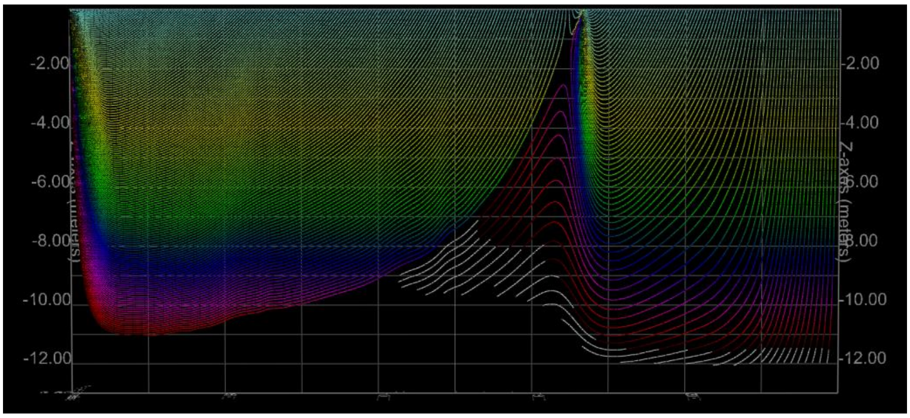


Figure 20 Flow lines for 2D reference model, drain distance of 166 meter (BPI:7).

Figure 21 shows an example with sub regional under stream that increase the transport time for a released particle progressively. The visualization shows the travel time of the particles in years through the system with different colours. Each colour represents a certain travel time value. The scale is defined for cyan (very short travel time), yellow, green, blue, purple, red (longest travel time). This sub regional under stream occurs when the primary drain has a high drain conductance (low drain resistance). This increases the groundwater flux to the drains and therefore the number of flow lines to the primary drain. In Figure 21 this is clearly visible because the flow lines go below the secondary drain to the primary drain.

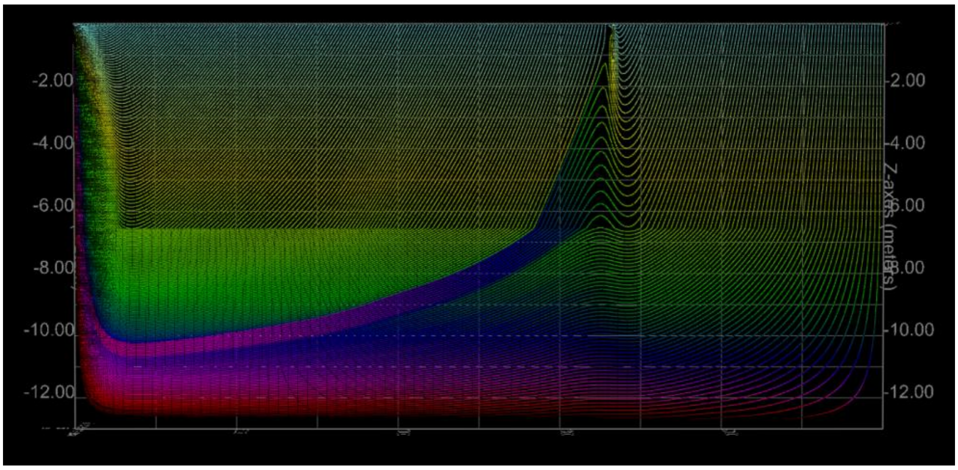


Figure 21 Flow lines to drainage system (drain distance: 166 [m]) with sub regional under stream.

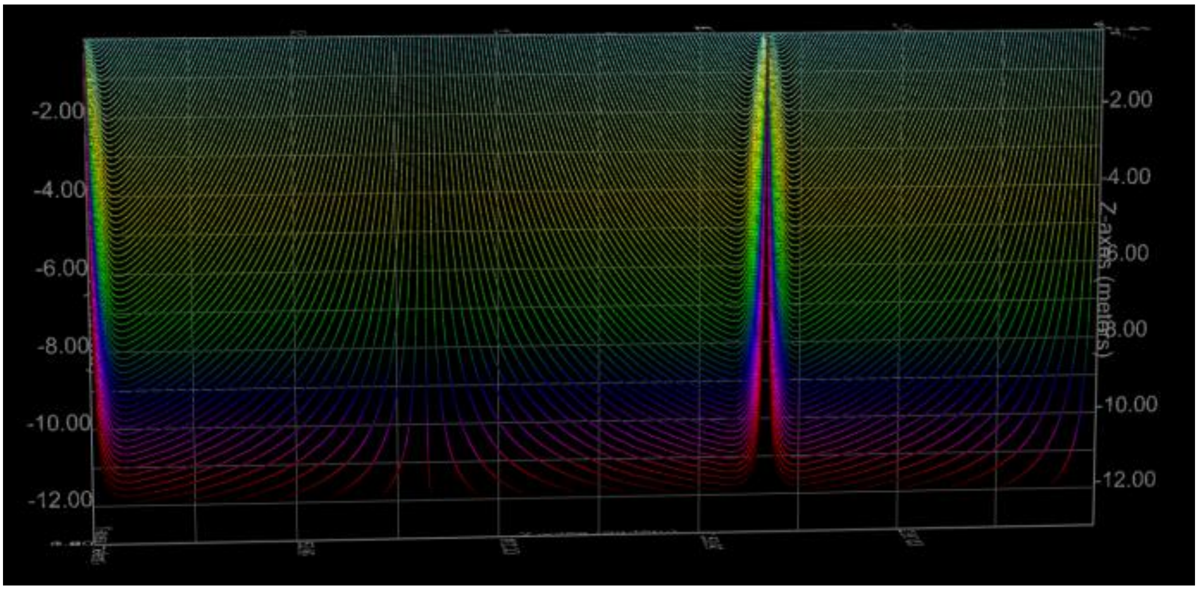


Figure 22 Flow lines to drainage system (drainage distance 166 meter) without sub regional under stream.

In Figure 22 a drainage system without regional under stream is plotted. This model shows also a symmetric distribution of the discharge volume. This flow line example shows similarities with the DIVDRA cross section in Figure 5. This output is without sub regional under stream could occur with a high drainage conductance for the secondary drain. Examples of the reference models shows sub regional under stream, this is not symmetric for every drain. As result of the significantly higher drainage conductance for the primary drain compared to the secondary drains. The ideal representation of DIVDRA (Figure 22) with symmetric flow line distribution will not occur for primary drains (ditches) and secondary drains (line drains) with the correct drain conductance.

Important for upscaling of the reference model is if this sub regional under stream is the same as in the reference model. These flow lines show a high residence time (purple, red colour lines) compared to the other flow lines. For solute transport this residence time is important parameters for decay. Without these sub regional under stream these flow lines with increased residence time are underestimated. For solute transport with decay the output concentration for the upscaled approaches are overestimated compared to the reference model equivalent.

4.1.1 Homogeneous versus stratified

For a homogenous model the permeability is constant, compared to a stratified model that has an increased permeability at 6½ meter. Higher permeability should increase the horizontal and vertical (anisotropy = 1.0) groundwater flow.

In the Figure 23 concentration of solute tracer at the discharge flux is plotted for a homogenous and stratified soil profile with a conservative tracer. The difference occurs between 0 and 4000 days. For both models the concentration is cumulative over time. The tracer concentration for the homogeneous model is higher compared to the stratified model with equivalent parameters. The stratified model has a higher permeability in vertical and horizontal direction. Therefore, the flow lines enter quicker the drainage system, due to lower residence time. The homogenous model reaches after a shorter time its maximum concentration compared to the stratified model. For the tracer concentration in de drains of Figure 23 this difference is visible between 0 and 4000 days.

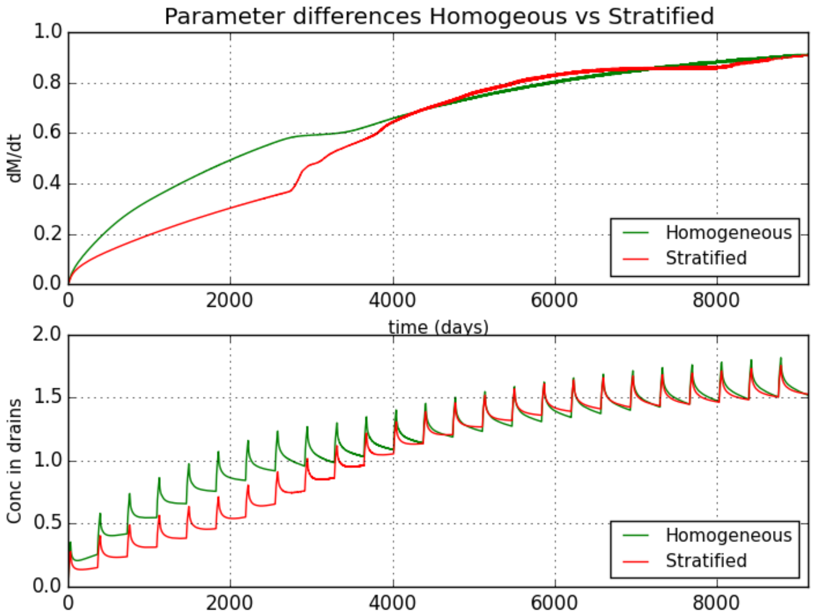


Figure 23 Stratified versus homogenous, cumulative mass difference per unit time and concentration in discharge drains over time.

4.1.2 Conservative versus decay

For conservative transport the concentration in the system becomes the input concentration of the tracer after a certain amount of days. But the model with decay shows a decreased concentration. Due to decay there is a loss of tracer concentration in the system. Therefore less output concentration in the drainage systems is measured (Figure 24). An increased travel time should increase the time of decay and therefore decrease the concentration of tracer. In case of a longer travel time there is more time to decay and therefore less output concentration of the tracer. Therefore, it is also important to check the influence of pollution or fertilizing on the saturated zone. The differences will have an enormous impact on the effects of regulation or predictions for responses of the system. As shown in Figure 24 the output concentration could become 3 times higher for conservative tracer compared to a tracer with decay.

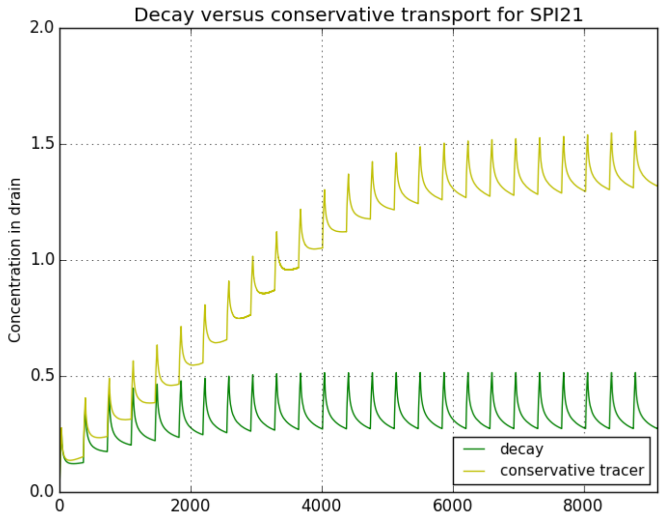


Figure 24 Conservative tracer compared with conservative tracer with decay for SPI:21 ((k_{h1}: 2.0 [m/d], k_{h2}: 6.0 [m/d], drain distance: 166 [m], drain level 0.0 [m]).

4.1.3 Stationary versus instationary

The difference between stationary and instationary is a result of the period with evapotranspiration (negative recharge, see Figure 12). During these drought periods the storage capacity of the system determines the groundwater fluxes in the system. As a result, the flux rate would decrease and travel time increases. Therefore, a solute in an instationary model will have a higher residence time that will the solute more time to decay compared to the same solute and model parameters in a stationary model.

4.1.4 Effects of parameters

The parameters described in Table 10 and

Table 11 are specified in homogenous soil profile models and stratified soil profiles. In this paragraph the differences in drainage level, drainage distance and permeability are compared and explained.

In Figure 25 there is a clear difference between the drainage level of 0.0 meter and 0.25 meter. The drainage level has a direct effect on the discharge volume of the secondary drainage system. This volume increases when the drainage level drops, see the green line of the 0.0 meter drainage level. The period between 3500 and 4500 days when the dM/dt of the green line (drainage level at 0.0 meter) has a higher relative mass over time compared to the red line (drainage level at 0.25m). This has on direct effect of the sub regional under stream that occurs more at the 0.25m model. As a result of the sub regional under stream travel time is higher compared to the model without.

4.1.4.1 Drainage levels secondary drains

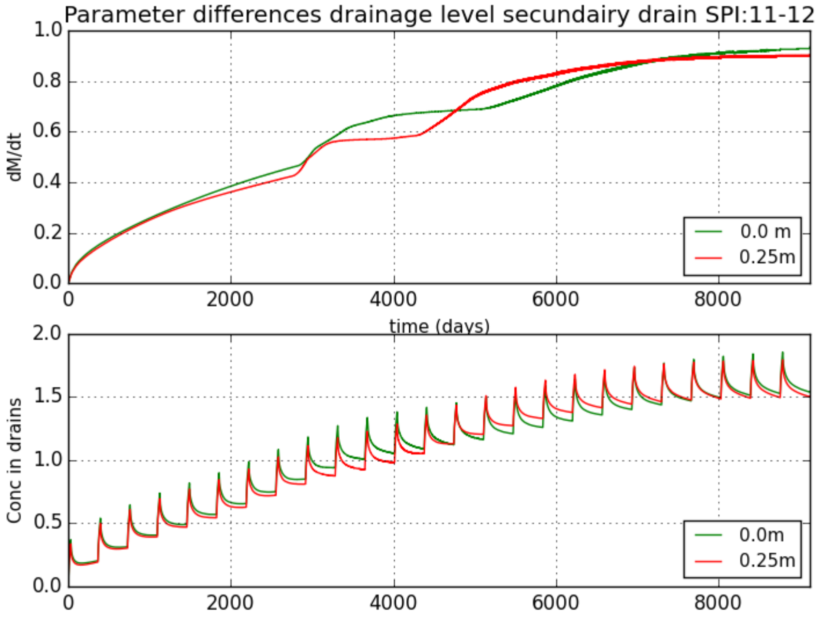


Figure 25 Comparison of drainage levels of SPI:11 (k_{h1}: 2.0 [m/d], k_{h2}: 6.0 [m/d], drain distance: 100 [m], drain level 0.0 [m]) and SPI:12 (k_{h1}: 2.0 [m/d], k_{h2}: 6.0 [m/d], drain distance: 100 [m], drain level 0.25 [m]).

Figure 26 shows the difference between a drainage level of 0.25m and 0.5m for SPI 12 and SPI 13. In Figure 28 a higher amount of flow lines with increase travel time are given due to a higher drainage level. This is also visible in Figure 26 that the curve has an offset in both the models. When the input mass enters a drain the slope becomes horizontal. No cumulative mass increase, so mass in is mass out is a result of the long flow lines that enters the drains. Otherwise the mass in is higher than the mass out and the relative mass increase and therefore the slope. A model with an increased drainage level the system has less drainage relative to the input mass. This results in a slight lower output concentration at the drains due to the slower solute transport.

The solutes enter a drain at a certain time will generate a trend of the dM/dt graph. The more horizontal part represents the very short flow lines in the model, Figure 27 and Figure 28. At these horizontal slopes the flow lines with an increased travel time should also left the system. This equal discharge moment occurs around 3000 days. At this moment the purple, red flow lines of Figure 27 and Figure 28 enters the primary and secondary drains. The input of solute has to build up again to become eventually to a relative dM/dt of 1, fully saturated. This means that the input concentration is equal to the solute concentration at the discharge flux.

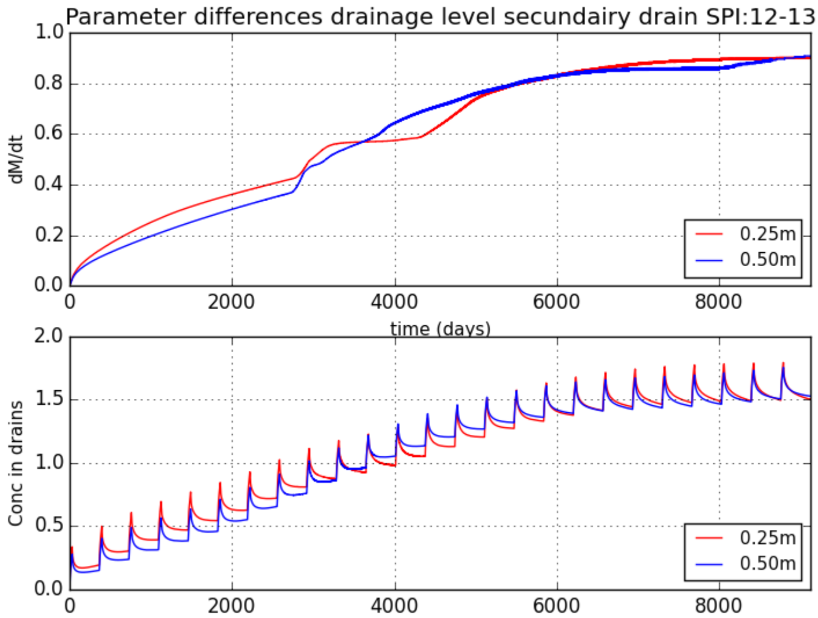


Figure 26 Comparison between drainage levels of SPI:12 (k_{h1}: 2.0 [m/d], k_{h2}: 6.0 [m/d], drain distance: 100 [m], drain level 0.25 [m]) and SPI:13 (k_{h1}: 2.0 [m/d], k_{h2}: 6.0 [m/d], drain distance: 100 [m], drain level 0.5 [m]).

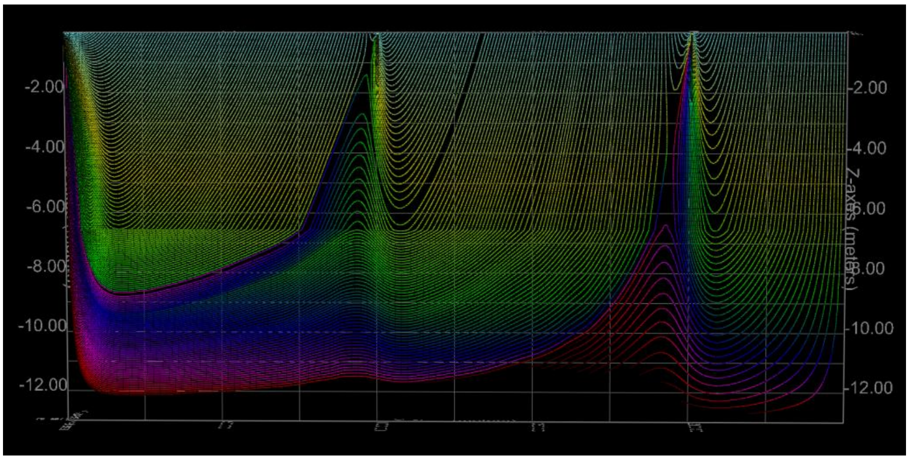


Figure 27 Flow lines of SPI:12 (k_{h1}: 2.0 [m/d], k_{h2}: 6.0 [m/d], drain distance: 100 [m], drain level 0.25 [m]).

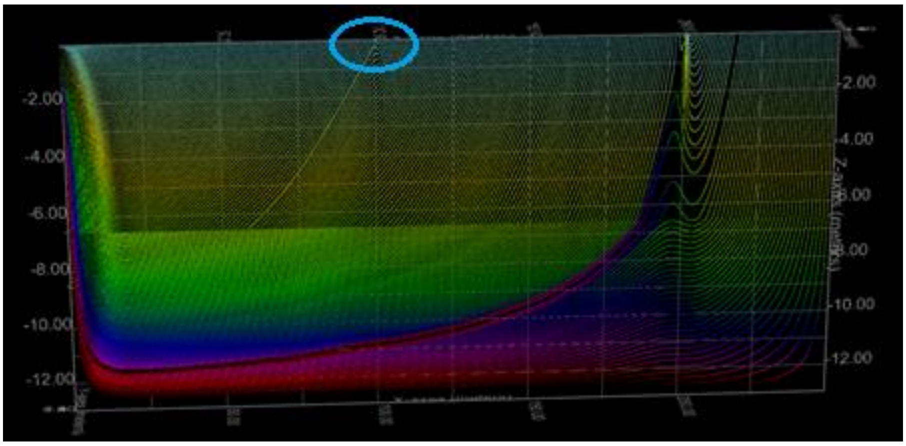


Figure 28 Flow line of SPI 13 (k_{h1}: 2.0 [m/d], k_{h2}: 6.0 [m/d], drain distance: 100 [m], drain level 0.5 [m]).

In Figure 28 it looks likes it has only one secondary drain but the blue circle shows the second secondary drain in the model. The flow lines with the highest residence time have to cross 250 meters. This increases the travel time of the tracer particles. Depending on the drainage level the amount of sub region under stream will increase or decrease. Lowering the drainage level limits, the amount of sub regional sub stream and a higher drainage level gives the opposite

4.1.4.2 Drainage distance

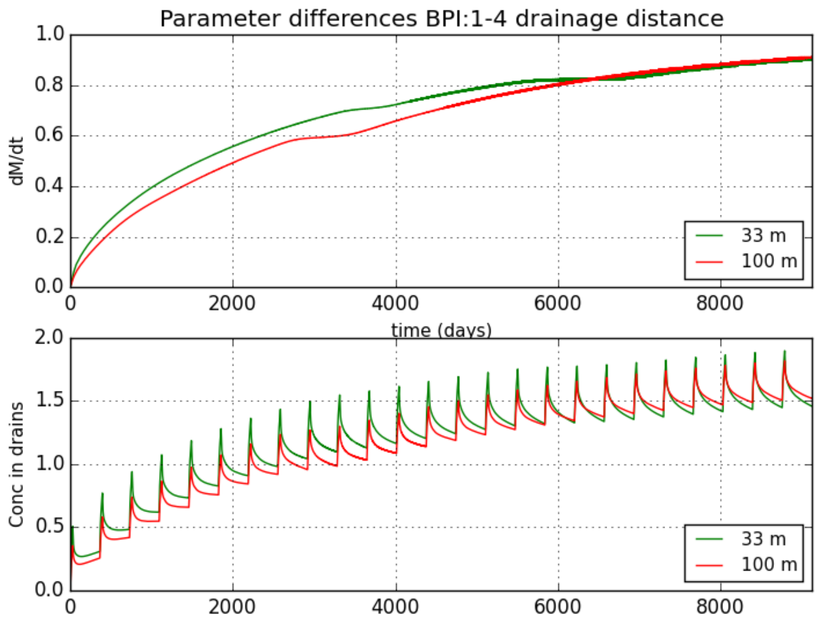


Figure 29 Comparison drainage distance of BPI:1 ((k_{h1}: 2.0 [m/d], drain distance: 33 [m], drain level 1.0 [m]) and BPI:4 (k_{h1}: 2.0 [m/d], drain distance: 100 [m], drain level 1.0 [m]).

The difference between the basis model BPI1 and BPI 2 is very small as shown in Figure 29. The decreased drainage distance increases the amount of short flow lines as shown in Figure 30. Increasing the drainage length increases the flow line length and wherefore the travel time increases. In Figure 30 the longest flow lines occur at 250 meter to the primary drain at x is 0 meter.

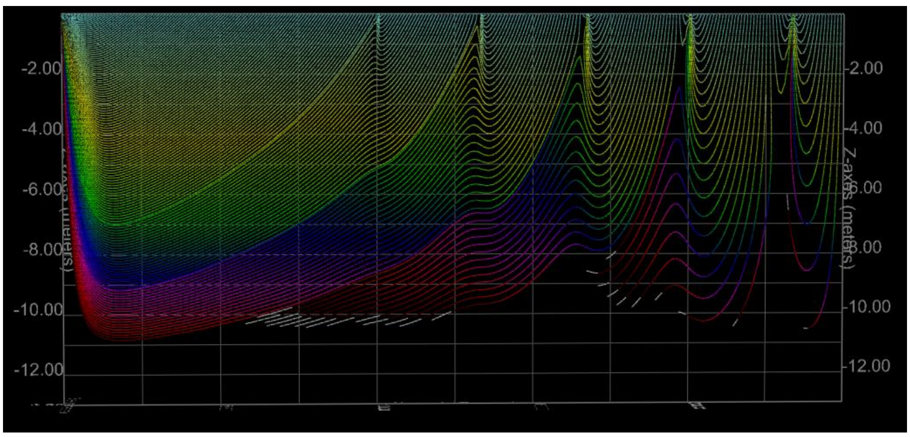


Figure 30 Flow lines for 2D reference model BPI1 (k_{h1}: 2.0 [m/d], drain distance: 33 [m], drain level 1.0 [m]).

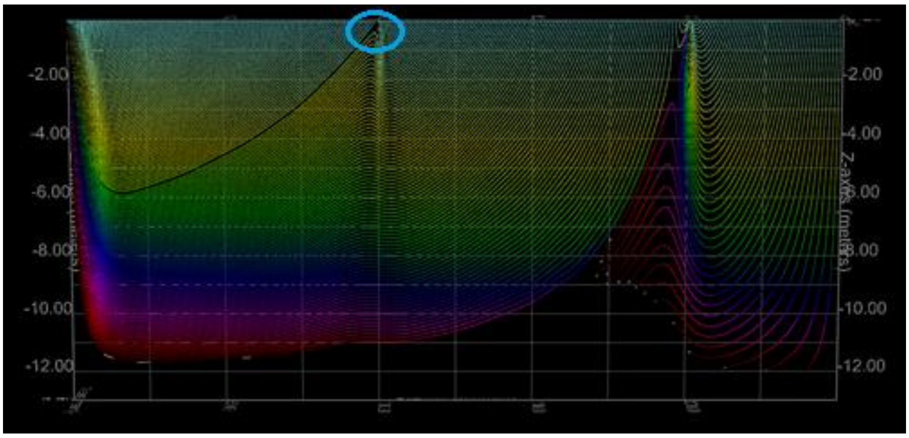


Figure 31 Flow lines for 2D reference model BPI4 (k_{h1}: 2.0 [m/d], drain distance: 100 [m], drain level 1.0 [m]).

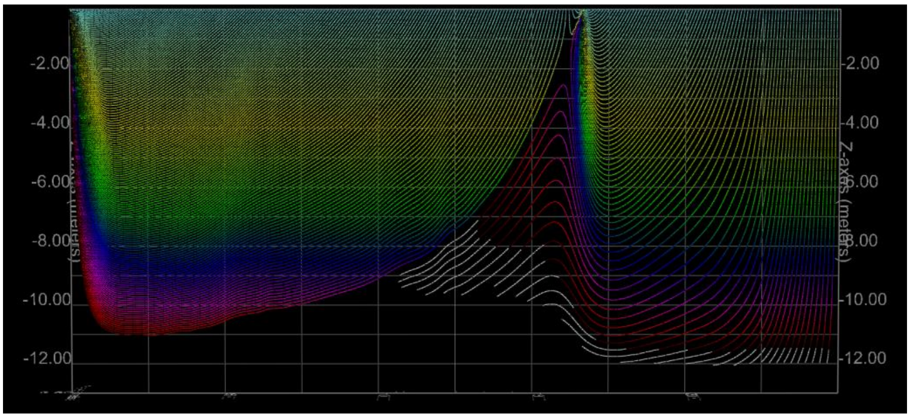


Figure 32 Flow lines for 2D reference model BPI7 (k_{h1}: 2.0 [m/d], drain distance: 166 [m], drain level 1.0 [m]).

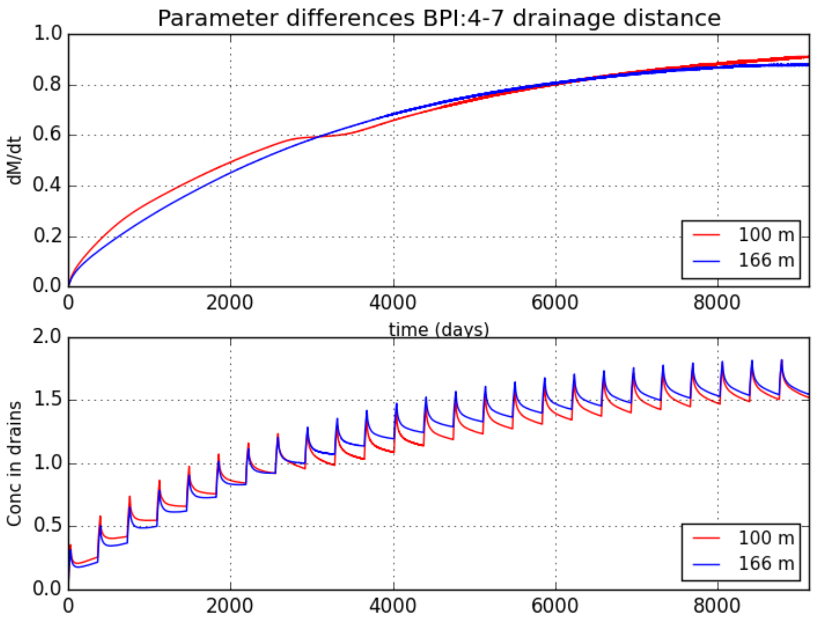


Figure 33 Comparison between drainage distance BPI:4 (k_{h1}: 2.0 [m/d], drain distance: 100 [m], drain level 1.0 [m]) and BPI:7 (k_{h1}: 2.0 [m/d], drain distance: 166 [m], drain level 1.0 [m]).

The small difference between the drainage distance of 100m or 166 m in Figure 33 is also clearly visible in Figure 31 and Figure 32. The shorter flow lines for the 100m drainage distance model include also lower travel time. The small offset of the 100m model is a result of the extra drain in the system that discharges solute a slightly faster until it enters the drains. Increasing the amount of secondary drains, decrease of drainage length, reduces the travel time of particles with a constant total drainage depth D_{tot}. Overall the difference between these two drain distances for these homogeneous soil profile models is minimal.

4.1.4.3 Permeability

For the permeability difference of the soil profile the output concentration at the drains are equal as shows in Figure 34. The offset in the dM/dt curve are directly related to the boundary between the top and bottom part of the soil profile. At the bottom the soil profile has a permeability that is increased by a factor 3 as shown in Table 11. When the solute enters this higher permeable soil it should travel faster and enters the drainage systems shows lower travel times distributions compared to homogeneous soil profile models. The increase in permeability results in a decrease of travel time., see Figure 34.

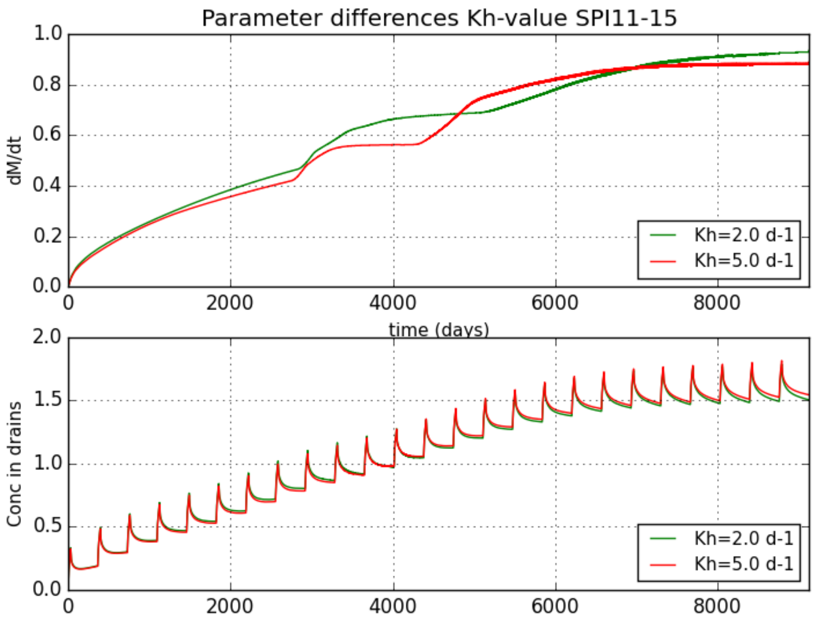


Figure 34 Comparison of permeability between SPI:11 (k_{h1}: 2.0 [m/d], k_{h2}: 6.0 [m/d], drain distance: 100 [m], drain level 0.0 [m]) and SPI:15 (k_{h1}: 5.0 [m/d], k_{h2}: 15.0 [m/d], drain distance: 100 [m], drain level 0.0 [m]).

The difference in permeability shown in Figure 35 for SPI:15 and SPI:17 show an equal trend of the output concentration in the drains. Also the dM/dt offset is very similar only the travel time will be reduced. The effect for solute transport and conservative tracer is negligible for this set of parameters. The small difference could indicate that the permeability is not the limiting factor. For this example, the discharge of solute could be limited by the drainage resistance and therefore the conductance of the drains, considering the minimal difference of the output concentration at the drains.

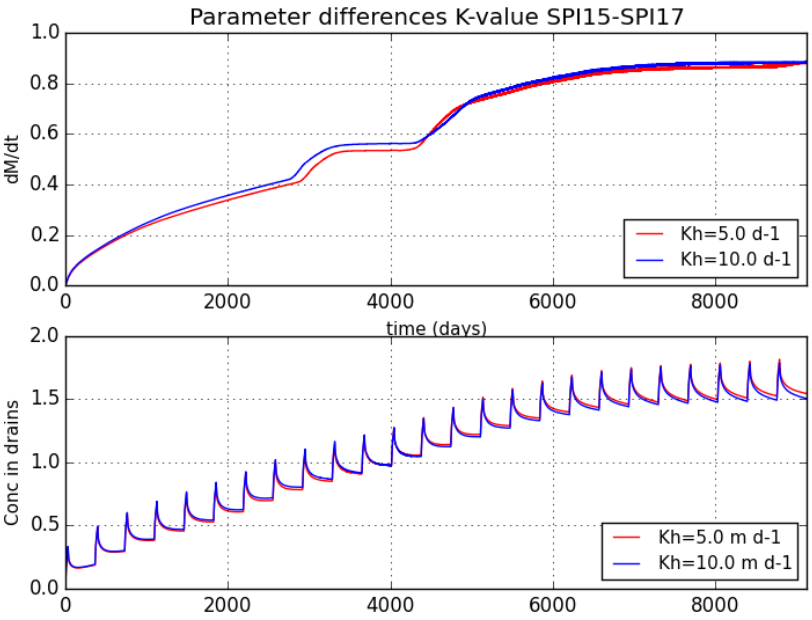


Figure 35 Comparison between permeability of SPI:15 (k_{h1}: 5.0 [m/d], k_{h2}: 15.0 [m/d], drain distance: 100 [m], drain level 0.0 [m]) and SPI:17 (k_{h1}: 10.0 [m/d], k_{h2}: 30.0 [m/d], drain distance: 100 [m], drain level -0.05 [m]).

4.2 Comparison of scaling method

4.2.1 Stationary, homogeneous and conservative

The influence of the second drainage system will increase due to an increase in conductance (decrease of drainage resistance) the difference for slope will increase. First there is an overestimation of the total sinks in the system, horizontal fluxes are too high. Over time the overestimation become an underestimation due to horizontal flux that is to low compared to the numerical model, as shown in Figure 36. The travel time distributions give a good indication how the solute transport migrate through the model.

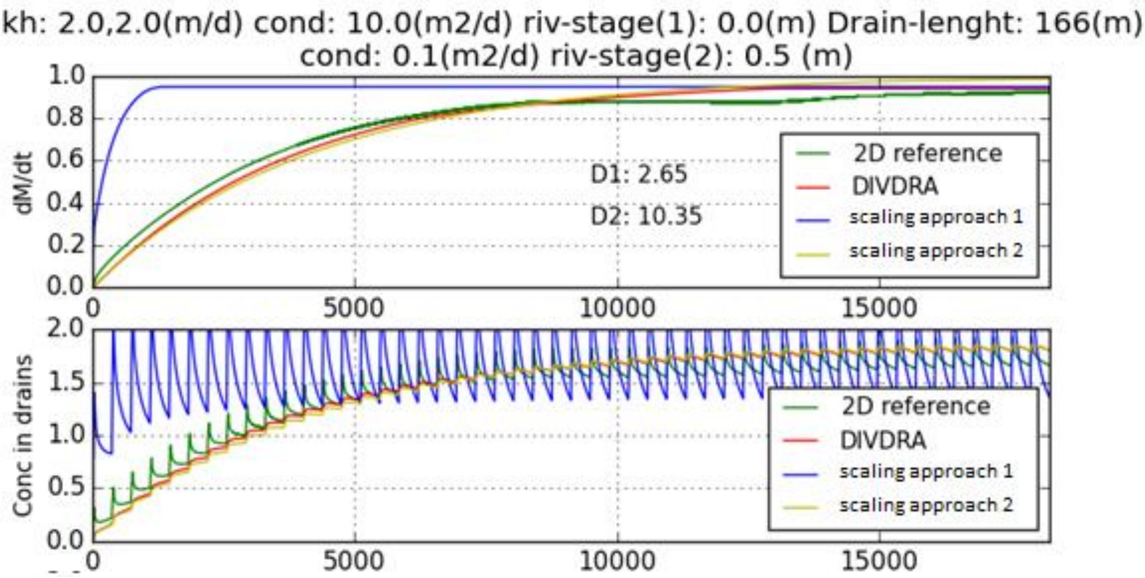


Figure 36 Stationary, homogeneous and conservative solute transport.

4.2.2 Stationary, stratified and conservative

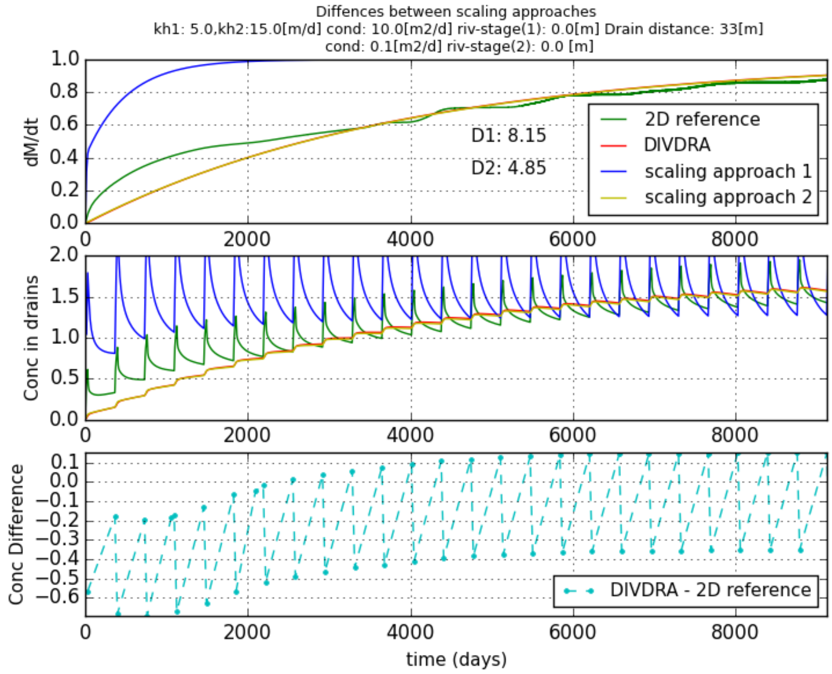


Figure 37 Comparison scaling approaches and 2D reference model for SPI:5.

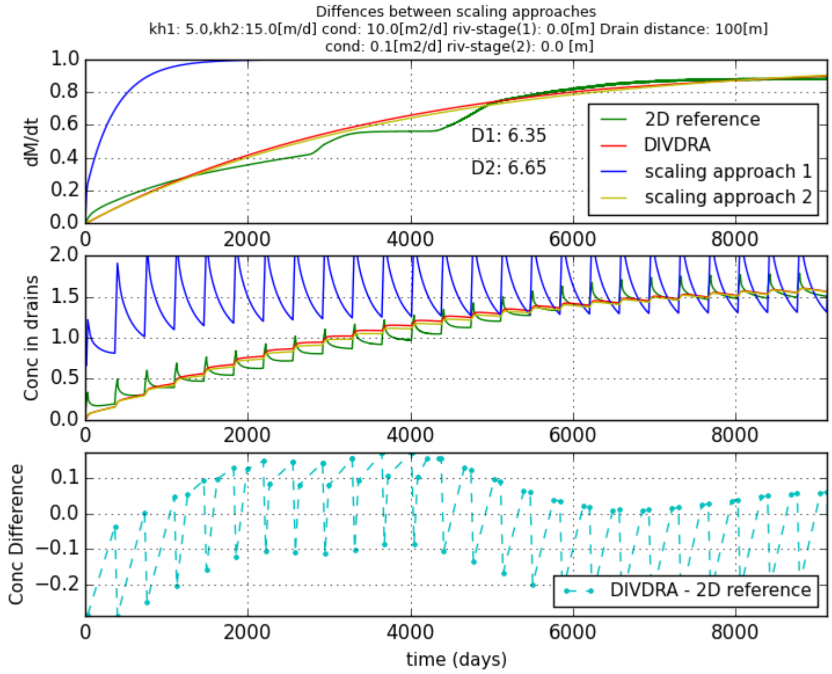


Figure 38 Comparison scaling approaches and 2D reference model for SPI:15

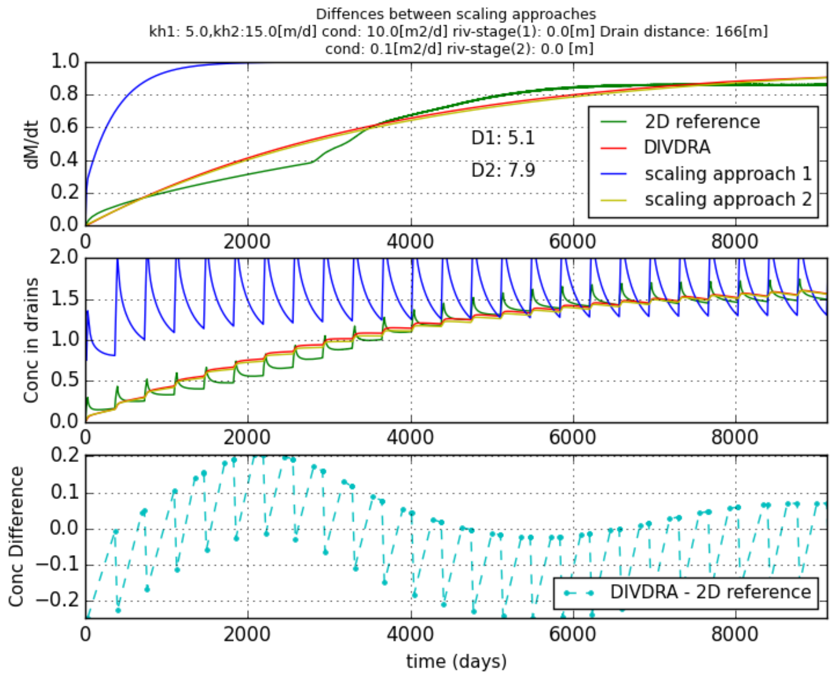


Figure 39 Comparison scaling approaches and 2D reference model for SPI:25

Overall Figure 37, Figure 38 and Figure 39 show a very similar trend for the scaling approach 2 and the DIVDRA equivalents. These figures have a different drainage distance that results in a different drainage depth for the primary or secondary drain (D_1 and D_2). The divided drainage depth for the primary and secondary drainage depths are also plotted in the graph (D_1 and D_2). Interesting is to conclude that a longer drainage distance also decreases the difference in concentration of the drainage system. Increased drainage distances imply an overestimation of the conservative tracer transport. This is also clearly visible for the travel time distribution for the different scaling approaches. The DIVDRA concept shows an underestimation for the conservative solute transport. These results in an increased negative concentration differences for a drainage distance of SPI:15. For Figure 37, Figure 38 and Figure 39 scaling approach 1 shows an increase for concentration in drains compared with the 2D reference model. This concentration differences have very high amplitude that gives a very high uncertainty. Therefore, this scaling approach could not be used for regulation or conservative solute transport indication.

For Figure 37, Figure 38 and Figure 39 at the top section on the x-axis the time is plotted versus the dM/dt on the y axis. This top figure shows the travel time distribution of the stratified soil profile. The second plot shows the conservative tracer transport through the system for the scaling approaches and reference model. The time is also plotted on the x axis and the concentration of the conservative tracer is plotted on the y axis. The bottom plot shows the differences between the DIVDRA model and the 2D reference model is plotted for the same time scale on the x axis and the differences in concentration of the conservative tracer on the y axis. This scale bar changes per scenario, due to the minimum and maximum concentration differences that are plotted instead of a fixed scale.

DIVDRA and scaling approach 2 shows a lower travel time compared to the 2D reference model, Figure 38 for concentration in drains. This is also clearly visible in the dM/dt curve between 200 days and 500 days. Figure 37 shows a decreased drainage distance that shows the highest concentration difference between 0 and 2000 days. For Figure 39 the differences between the upscaled models and 2D reference model are critical between 500 and 3500 days.

4.2.3 Stationary homogeneous decay

The DIVDRA approach shows less amplification compared to the 2D reference model and at certain time steps. This results in high difference of concentrations for tracer solute, as shown in Figure 40. Concentration estimations between 0 and 4000 days are underestimated by the DIVDRA approach. The small increase of concentration shows the delay of the decay in the system. Increasing the drainage distance decreases, the difference between the decay DIVDRA and decay of the 2D reference model slightly as shown in Figure 41**.** For the scaling approaches 1 and 2 the travel time through the system is too short to get decay. Therefore, the conservative tracer line of the 2D reference model is almost equal to the scaling approach 2.

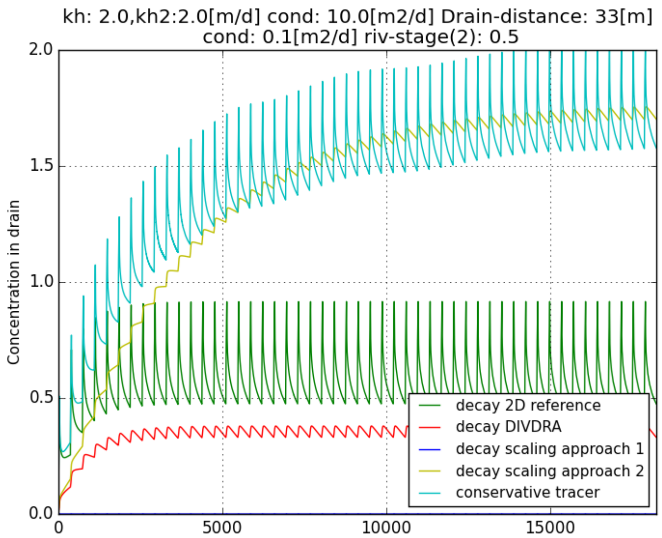


Figure 40 Compare tracer with decay for upscaling approaches also a 2D reference model without decay is plotted for homogeneous model

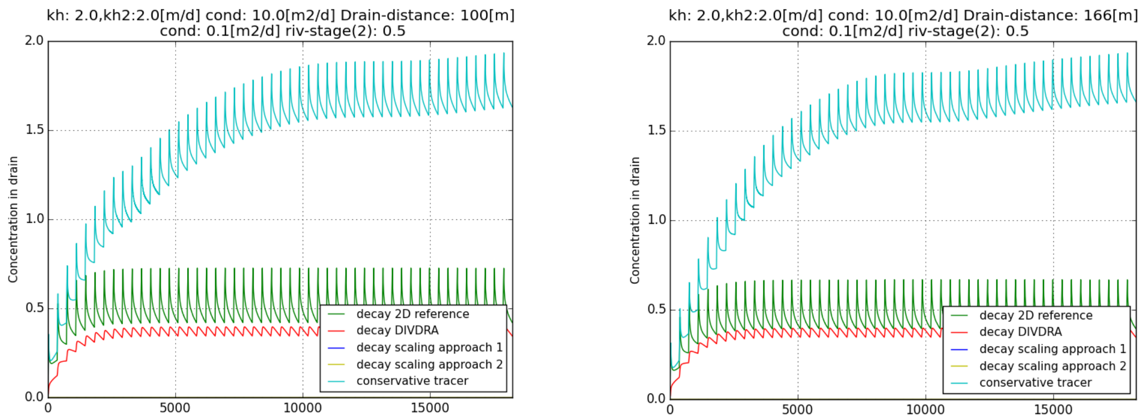


Figure 41 Comparison BPI:4 and BPI:7, effect on decay by increasing drainage distance

4.2.4 Stationary, stratified and decay

In Figure 42 the amplitude is increased due to the shorter drainage distance, because the DIVDRA approach has a minimal amplification. The maximum concentration difference could be around 0.5 on a scale of 2.0 [mass/volume]. Between 0 and 1000 days the DIVDRA approach has also underestimation of the concentration of tracer in the system. After 10000 days the average concentration in the system is comparable.

The difference between the stationary stratified and stationary homogeneous model with decay is minimal. Also for an increase in drainage distance the averaged concentration in the drains moves more to the averaged concentration of the DIVDRA model. Clearly visible for the scaling approach 1 is that with decay the amplitudes become larger, for Figure 42 till Figure 47. Therefore the variation of concentration in the drains differs from 1.0 to 2.0 within a minimal amount of days. This makes it extremely unreliable to use as scaling solution.

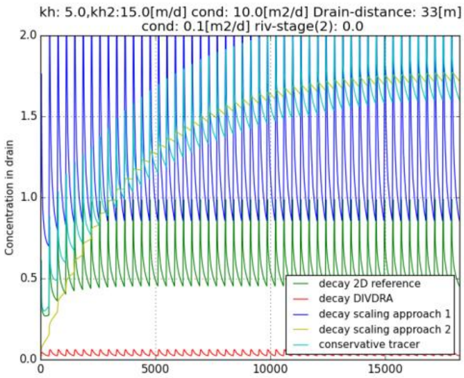


Figure 42 Comparison tracer decay for stratified soil profile with different scaling approaches (SPI:5)

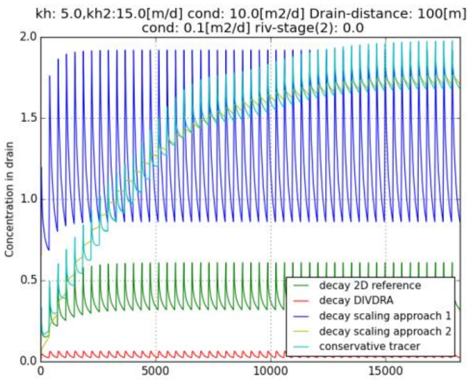


Figure 43 Comparison tracer decay for stratified soil profile with different scaling approaches (SPI:15)

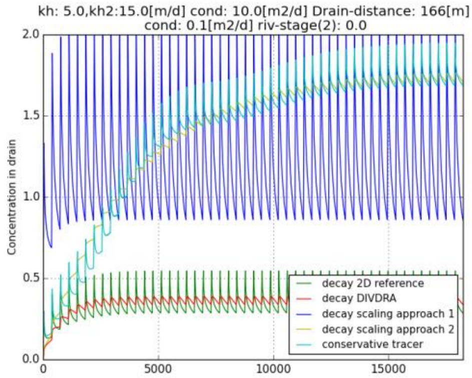


Figure 44 Comparison tracer decay for stratified soil profile with different scaling approaches (SPI:25)

In Figure 42, Figure 43 and Figure 44 the effect of drainage distance is clearly visible between the different scaling approaches. The difference between DIVDRA and 2D reference model is large for 33 and 100 meter drainage distance. Although the drain distance of 166 meter shows less difference between the scaling approaches. For this increased permeability the DIVDRA approach at 100 meter is not reprehensive for the concentration curve of the 2D reference model. Although if the permeability of the model decreases also the 100 meter drainage distance becomes more reprehensive for the concentration in the drain after decay, see Figure 45, Figure 46 and Figure 47.

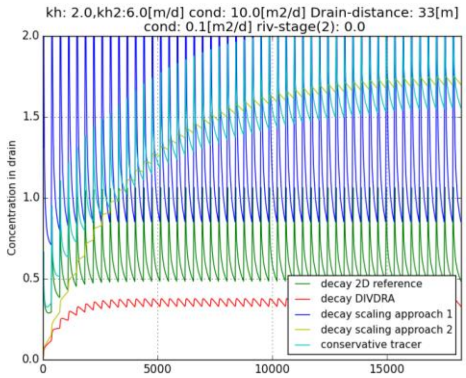


Figure 45 Concentration in drains over time with decay for different scaling approaches (SPI:1)

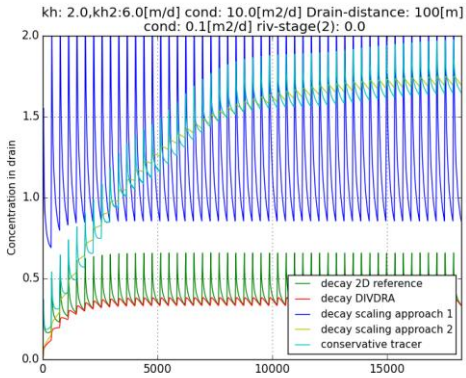


Figure 46 Concentration in drains over time with decay for different scaling approaches (SPI:11)

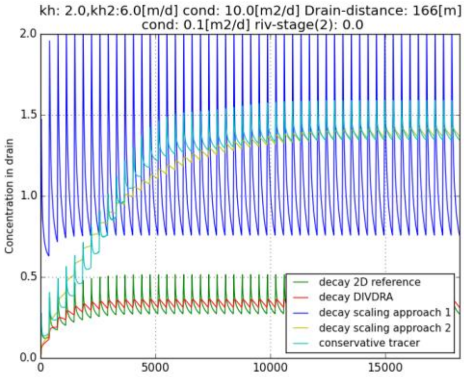
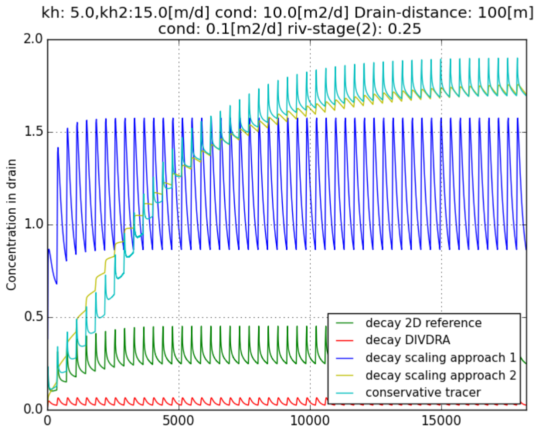


Figure 47 Concentration in drains over time with decay for different scaling approaches (SPI:21)

For scaling approach 1 the variations in output concentration of the drains have high amplitude. This makes it not useful as scaling approach for solute transport, see Figure 45, Figure 46 and Figure 47 The scaling approach 2 also shows high differences with the 2D reference mode this because all the extraction wells are in every layer that disables the decay process in this model. Remarkable is also the change in amplitude, when the drainage distance increases the amplitude decreases. This is a result of the concentration differences near the drains. Shorter drainage distances increase the amount of drains and therefore the concentrations differences near these drains.



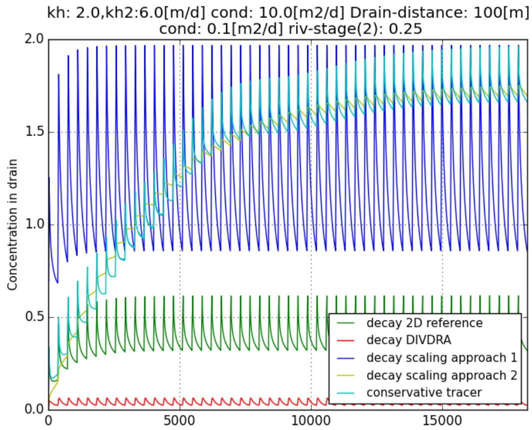


Figure 48 Comparison between SPI:15 and SPI:11

In Figure 48 the difference in drainage level of the secondary drainage level shows the effect on the different scaling approaches. For scaling approach 1 the amplitude increases with a decrease of the permeability of the soil profile. Also the amplitude of the 2D reference model increases when the permeability decreases. Therefore, the concentration of the tracer in the drains changes more per time step than for the models with a higher permeability. Comparing Figure 48 with Figure 46 the difference between drainage levels is also visible. For a drainage level of 0.0 meter at the secondary drainage level the amplitudes of scaling approach 1 is higher compared to a drainage level of 0.25 meter. The decay of DIVDRA is higher for this model and therefore the output concentration of the tracer in the drain is decreased. This could be an implication of an overestimation of the travel time in the system. An increased drainage level would increase the primary drainage depth and this increase the average travel time of the solute transport for DIVDRA

Overall to use an analytical solution that describes groundwater fluxes as DIVDRA several assumptions are required. As a result, these assumptions the discharge areas will be perfectly distributed. When the stage or conductance's are low enough it will fit perfectly for DIVDRA. When the stages of the largest drainage system are the lowest or the conductance is relatively high, there is a dominant groundwater flux to this system. Therefore, there is only a primary drain system in the model, the secondary drainage system can be ignored. On the other when the conductance is high for drainage systems and when the stages are very low, the discharge fluxes of the drainage systems are equal divided and also DIVDRA works perfect for this system. DIVDRA become less optimal when the drainage systems parameters for conductance or stage are in between these scenarios. Then it is clearly visible that overestimations or underestimations are made with the DIVDRA concept. DIVDRA has fewer subs regional under stream and therefore the relatively long flow lines are ignored. For the DIVDRA concept this sub regional under stream is not present. Due to this assumption the travel time in the DIVDRA concept should decrease compared to the 2D reference model. The sub region flux is not represented for DIVDRA and therefore an increased difference can be expected.

5. Conclusion and recommendation

The implementation of "DIVDRA in MODFLOW" for NHI-WQ will give a profit in computational time for groundwater flow. The fluxes within the cell of 250 by 250 meter to the drains are calculated with the "DIVDRA in MODFLOW" concept. Fluxes a cross the cell boundaries will be calculated with MODFLOW. To fit the different time of calculation methods the DIVDRA concept is only used in the saturated zone of the model. METASWAP will calculate the groundwater fluxes in the unsaturated zone. The profit in computational time that can be established is maximal for the solute transport in MT3DMS. A high resolution numerical model needs 120 minutes (averaged) to calculate steady state solute transport whereby the analytical (DIVDRA) model is done in several seconds.

Output of the models shows the results of scaling approach 1 for varies parameters. The overall impression of scaling approach 1 is overestimates the solute transport compared to the reference model and other scaling approaches. Therefore, the solute travels faster through the 13 meter of saturated soil. The differences between the 2D reference model and scaling approach 1 are too high for the conservative tracer without decay and especially for a tracer with decay. This would make it not useful as upscaling approach for 2D groundwater flow.

The comparison between the scaling approach 2 and the DIVDRA concept is specially to look at the benefits of DIVDRA instead of scaling approach 2. Scaling approach 2 is much easier to implement, no analytical formula or intermediate calculation steps are required. Differences between these concepts are minimal in some cases without decay. This implies that the addition of DIVDRA for solute transport shows no major improvement for the scenarios in this research study. Although when decay is added the differences starts to occur and the benefit of DIVDRA is visible.

Scenarios and upscaling approaches with an overestimated travel time will show lower output concentrations. The scenarios with an underestimation of the travel time show a lower output of solute concentration than the 2D reference models. These differences become a risk for solutes where decay influences the concentration in soil. This could affect the regulation and policy makers.

Increased amplitude for the concentration in drain with a low permeability scenario will increase the uncertainty of the output concentration. This because the concentration per time step vary a lot. This makes it difficult to determine a reliable output concentration. Scaling approach 2 and the DIVDRA approach are comparable for conservative tracer without decay. The conservative tracer transport with decay shows more differences. This is a result of different travel times for scaling approach 2 compared to the DIVDRA approach.

Differences between 2D reference model and DIVDRA decreases with an increase of the drain distance. Because the model has only the primary drainage systems that influence the discharge fluxes. If the drain distances decreases, the secondary drains have an increased discharge flux that become higher than the primary discharge flux. This results also in one main drainage system and discharge flux that minimalize the difference between these scaling approaches.

Drainage levels effects DIVDRA drainage levels and therefore the averaged travel time distribution. An increased drainage level should decrease the discharge flux of the secondary drainage system. Therefore, the difference between the 2D reference model and the scaling approaches decreases.

Although the difference for decay should increase if the short flow lines are ignored. This reduces the influence of decay on the solute concentration. That will decrease the output concentration of conservative tracer of the DIVDRA approach. This is an overestimation of the travel time which results in an increase of decay. An underestimation of the travel time distribution results in an overestimation of the output concentration in the drains.

To improve the scaling concept, the travel time distribution has to be optimised. The travel time depends on the flow lines through the system. To optimize the flow line, the occurrence of sub region under stream. This important process is underestimated in all of the scaling approaches. Therefore, the decay is over or underestimated and the outcomes could not be used for regulation or policy makers. Improving the sub region under stream makes the DIVDRA scaling approach more reliable and to use as a replacement for the high resolution model.

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First I would like to thank Gijs Janssen and Jacco Hoogewoud for their time and the opportunity to write my master thesis at Deltares. The last nine months they learned me a lot, like programming in Python and working with groundwater models. I always liked our update meetings very much, these meetings often turn out to become interesting discussion. Furthermore, I would like to thank everyone at Deltares Utrecht for an excellent time for the last nine months.

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8. Appendices

Appendix I: Subroutine for drainage depth DIVDRA

$$dq_y = \frac{q_i L_i - q_{i+1} L_{i+1}}{L_i}$$
$$dy = sum(q_y)$$

Ratio fluxes based on discharge fluxes ($m^3\ d^{-1}$)

For the Drainage Depth dividation the Q_i are used as flux component because it is a ratio between fluxes and depth.

$$D_i = \frac{q_i}{q_{tot}} * D_{tot}$$

Translation into python script:

$$D_i = \frac{f_i}{f_{tot}} * D_{tot}$$

$$z_{top} = f_{top}\phi_{avg} + (1 - f_{top})\phi_{drain}$$

Assumption for saturated zone: $\phi_{avg} - \phi_{drain} = z_{top}$

So the z_{top} is water table. D_2 is summation from water table to z_{bot} of D_2

For D_1 the z_{bot} of D_2 is the top, to the $-D_{tot}$ of system.

$$q_{d,1,i} = \frac{Q_i}{\frac{D_i}{dz} * z_{top}}$$

Looking at the units:

$$\frac{m^2}{d} = \frac{\frac{m^3}{d}}{m}$$