Ph.D. Dissertation

David Nagy:

Quantifying the transport and fate of dissolved nitrogen at different scales in drained agricultural landscapes
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Front Page Photo:

The topography and field instrumentation of Silstrup and Tokkerup field with the conceptualized macropore settings of Silstrup.
Preface

This dissertation is the outcome of my PhD study at the Department of Agroecology, Aarhus University, Denmark, from December 2015 to July 2019. The PhD study was funded by Aarhus University and some of the data supplied by the Geological Survey of Denmark and Greenland in relation to the Pesticide Leaching Assessment Programme.(www.pesticidvarsling.dk).

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Aarhus University

Pouluum 7 August 2019

David Nagy.
Papers (included)

Paper 1.
Nagy, D., Rosenbom, A. E., Iversen, B. V., Jabloun, M., and Plauborg, F.: Estimating the degree of macropore flow to drainage at an agricultural clay till field for a 10-years period, Aarhus University, Manuscript

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Paper 2.
Nagy, D., Rosenbom, A. E., Iversen, B. V., and Plauborg, F.: Effect of preferential transport and coherent denitrification on leaching of nitrate to drainage, Aarhus University, Manuscript

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Paper 3.
Nagy, D., Moterjami S.K., Rosenbom, A. E., Iversen, B. V., and Plauborg, F.: Impact of drainage conditions on the fate of nitrogen in an agricultural tile-drained silty loam field, Aarhus University, Manuscript

(To be submitted)

Additional Papers


Summary

Nitrogen (N) is an essential part of the agricultural crop production cycle. Farmers generally apply high amounts of N fertilizer, in order to secure the high crop yield, which potentially increases the risk of N loss from the root zone. For keeping the N concentration of the groundwater and surface water below of the European limit for drinking water (11.3 mg N L\(^{-1}\)) and concurrently avoid the exacerbating the eutrophication of coastal and surface water, nitrogen leaching has to be mitigated. N leaching is an unavoidable part of the agro-ecosystem, due to the timing of mineralization of soil organic N, climate and current agricultural field management practices. One of the most widely used practice is the artificial subsurface drain system, which enables the excess water to be removed from the field with inadequate natural drainage and the main responsible for the nitrogen pollution of surface water. The aim of this PhD study was to identify the potential factors and processes at field scale that promotes the high loads of N transport to the artificial subsurface drainage.

The study includes a ten-year and one-year hourly-based dataset from two clay loam fields, Siltrup in the north-west and Tokkerup in the south-east of Denmark. Both fields are highly compacted macroporous soil with indicative hydraulic behaviour for preferential transport (PF). A Danish developed deterministic model, DAISY, was applied to describe the potential processes involved in N leaching. By using the dual permeability concept developed by the DAISY group, the model was calibrated and evaluated against hourly drainage loss of water and N, soil water N concentration, crop dry matter yield and crop N uptake. The water balance study of Siltrup field, which is presented in Paper 1, compared six different model concepts, using the dual-permeability approach by incorporating three different macropore settings and two different groundwater table boundary conditions. The study revealed, that the potential fraction of the total yearly precipitation transported by preferential flow to the drain was 70%. The model was capable of describing the dynamics of bromide transport based on the tracer experiment from 2000. The results of bromide leaching simulation estimated that 54% of the drainage is transported via vertical macropores being initiated in the plough layer. The follow-up study in Paper 2 allowed to identify elements, which dominantly affected the leaching of nitrate through this clay till. A large amount of N (48% to 80% of the total N-loss to drainage) was preferentially transported via macropores to drainage regardless of the application method and concurrent occurrence of precipitation. The current standard denitrification abiotic water reduction factor in DAISY had to be modified resulting in a reduction of approximately 50% in the denitrification of the field from a seasonal average of 75 kg N ha\(^{-1}\) to 35 kg N ha\(^{-1}\).
The study at Tokkerup (Paper 3), investigated the impact of drainage conditions by deploying two sampling wells with flow-magnetometers to continuously sample drain discharge in the main drain and ISCO samplers for flow proportional sampling of N concentration in the drainage water. The wells were deployed to capture discharge from a previously delineated area of a poorly (PD) and well-drained (WD) part of the field. During a no crop season of 2017-2018 (too wet for sowing winter wheat) a 100 kg N ha\(^{-1}\) mineral fertilizer was sprayed on the field in the autumn 2017. Using the hourly climate and leaching data, two DAISY models was set up to describe the leaching processes and their similarities and differences, involving preferential transport and concurrent denitrification between the two parts of the field. Model results were able to prove under no crop condition, that NO\(_3\)-N can be leached out dramatically faster by PF than expected. Macropore transport was, directly and indirectly, involved with the N loss to the drainage. Buried deep matrix ended macropores could transport NO\(_3\)-N to the top layer of the groundwater, which behaved as a rapid intermediary before the N were transported further to the tile drain system.

The DAISY model incorporates water, solute and heat transport, crop development, and nutrient conversion process that involve numerous parameters, which have a substantial impact on model calibration. Thereby DAISY, by being overparameterized, could lead to over-fitting or identifiability problems, as well as equifinality. To decrease the effect of the overparameterization and improve the calibration efficiency the Morris sensitivity screening method was applied on those model parameters, which were believed to have an impact on the multi-objective function. Included was drainage dynamics (DD) and cumulative drainage (DC), solute transport dynamics (ND, (nitrate) or BRD, (bromide)) and cumulative solute transport of nitrate and bromide (NC and BRC), respectively, harvested dry matter yield (DM yield), harvested N yield (N yield) and groundwater table fluctuations (GWT). The Morris screening method was applied separately on each objective alone, thereby creating a composite sensitivity screening.

The sensitive parameters were optimized by minimizing the multi-objective function, which was a sum of an error term between the field measurements (calibration objectives) and their simulated counterparts. The used performance measures were the normalized Root Mean Squared Error (nRMSE), normalized Mean Absolute Error (nMAE) and Kling-Gupta Efficiency (KGE). In Paper 1, Paper 2 and Paper 3 the differential evolution (DE) optimization was used for parameter optimization.
Danish summary


ændres, hvilket resulterede i en reduktion af denitrifikationen på ca. 50%, fra et sæsonennemsnit på 75 kg N ha$^{-1}$ til 35 kg N ha$^{-1}$ for marken.


De følsomme parametre blev optimeret ved at minimere multi--objektiv-funktionen, som var en sum af en afvigelser mellem feltmålingerne (kalibreringsmål) og deres simulerede modstykker. De anvendte evalueringskriterier var udtrykt ved den normaliserede kvadratrod-kvaderet fejl.
(nRMSE), normaliseret gennemsnitlig absolut fejl (nMAE) og Kling-Gupta-effektivitet (KGE). I Artikel 1, 2 og 3 blev optimering af differentiel udvikling (DE) brugt til parameteroptimering.
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1 Introduction

1.1 Artificial subsurface drainage

Optimizing agricultural production has been in focus of humanity since the early stage of civilization, but more particularly from the end of the 19th century when the population of the world started to increase rapidly. One of the most significant and worldwide used optimizations is to enable excess water to be removed from fields with poor natural drainage. Drainage in agriculture means the artificial removal of excess water from the field, the avoidance of erosion as a result of irrigation, and the general enhancement of agricultural land-use by improving optimum air and nutrition environment for the plant roots, thereby promoting root growth [Herzon and Helenius, 2008]. Besides the fast water transport, drainage networks under the root zone can facilitate the more rapid increase of the soil temperature. Thus it prevents a possible delay in planting in early spring [Fausey and Lal, 1989; Jin et al., 2008].

Denmark covers an area of 42,937 km2, of which roughly ~60% is agricultural land (Fig. 1) [Statistics Denmark, 2019]. The deployment of subsurface drainage in Denmark began at the end of the 19th century, and nearly half of the agricultural land has been systematically drained since then. A State Act authorizing subsidies for drainage and soil improvement and the general economic situation for agriculture have been of great importance for drainage activities [Mortensen, 1986]. However, this agricultural water management measure puts the aquatic environment into risk since it facilitates rapid transport pathways to the aquatic environment with reduced possibilities for the reduction of nitrate [Ernstsen et al., 2015]. Therefore, drainage can potentially cause surface and groundwater contamination, followed by eutrophication, threatening the local and regional ecosystems [Blann et al., 2009]. To counteract the effect of this type of diffuse pollution international and national regulations and laws have been placed by covering aquatic environments under the Nitrates Directive [EEC, 1991], the EU Water Framework Directive [EC, 2000], and the EU Groundwater Directive [EC, 2006]. To fulfil the aforementioned directives’ requirements, the Danish Commission of Nature and Agriculture recommended to locally (field scale) implement the requirements to ensure the identification of vulnerable and non-vulnerable areas to nitrate leaching in Denmark [Ernstsen et al., 2015]. Hence, monitoring programs and studies [Lindhardt et al., 2001; Jensen and Veihe, 2009; Ernstsen et al., 2015] were defined to allow measurements of the different nitrogen flows in water (drainage, groundwater, and surface water) and as well gaseous losses which may vary quite substantial in N concentration and amount, and thus pose different risks to the aquatic and aerial
environment. However, the monitoring capabilities of these environments, their deployment and operation are laborious and expensive.

1.2 Subsurface drainage modelling

Modelling exercises could ease and improve the understanding of nitrate flow routes, which are highly crucial to determinate the fate of applied fertilizer at field scale [David et al., 2009; Rosenbom et al., 2009; Hazen and Sawyer, 2010; Zhou et al., 2013; Cheng et al., 2014; Mollerup et al., 2014; De Schepper et al., 2015; Li et al., 2015; Mekala and Nambi, 2016]. Modelling studies with a primary focus on the drainage water flow have been set up to be able to compare the frequencies of modelled discharge to measured drain-water discharge [Feng, 2010; Hansen et al., 2013; De Schepper et al., 2015].

The contribution from drainage to aquatic environment can be assessed by applying large scale hydrologic and ecosystem models that are fully distributed physically-based models, with the inclusion of field scale models [Refsgaard et al., 1999]. Field-scale models, generally describe the water and solute transport with Richards equation and the advection-dispersion equation (ADE) in one dimension for the variably saturated zone, respectively. The lateral water flow to the drain in these models are approximated with Hooghoudt theory (HHT) [Hooghoudt, 1940], whereas solute transport towards the drainpipe is based on mass flow (advection). Most frequently used field-scale models that are commercially available or open-source and coupled with the HHT, are MACRO [Larsbo and Jarvis, 2003], RZWQM [Ma et al., 2012], HYDRUS1D [Šimunek et al., 2012], COUPMODEL [Jansson, 2012] and DAISY [Hansen et al., 1990; Hansen, 2002; Hansen et al., 2012b]. Several studies investigated the accuracy of the HHT against a measured drain flow, bromide and N concentration in drainage water [Carlson, 1971; Lovell and Youngs, 1984; Smedema et al., 1985; Kohler et al., 2001; Fox et al., 2004; Kohne et al., 2006; Fox et al., 2007; Larsbo et al., 2009; Mollerup et al., 2014]. Van Schilfgaarde [1957] demonstrated that HHT was able to predict the drainage flow accurately at nearly steady-state condition at field scale, whereas Carlson [1971] and Lovell and Youngs [1984] were able to validate the same findings in laboratory sand tank experiment under steady-state conditions. Smedema et al. [1985] were able to prove that the HHT, even though it is an approximation of the Laplace equation [Fetter, 2000], can be used in homogeneous-anisotropic soils. Due to the cross-platform application of HHT, modellers have been testing the potential use of it in different soil condition. Kohler et al. [2001] showed that HYDRUS SWMS_2D model with an HHT lower boundary condition instead of a node representation on a 2D plane performed satisfactorily and the discharge compared well with other models. A similar conclusion was reached by Larsson and Jarvis [1999] and Mollerup et al.
The former study was based on MACRO where the 1D model with a sink term based on HHT in nodes within the saturated zone representing lateral flow toward drains, where the authors were able to describe the mineral-N concentration in the drainage with reasonable accuracy. The latter study compared DAISY 1D-HHT with the two-dimensional DAISY version of the same model having an explicit drain representation (EDR). Mollerup et al. [2014] found in term of drainage transport of water and solute (nitrate and bromide), that the difference between the HHT and EDR was very small, and one-dimensional models with HHT are capable of describing the lateral transport towards the drain.

Albeit all of the aforementioned models and studies were successful in representing the drainage flow, each of them used a different type of conceptual representation of the soil that is equally or more important than the numerical drainage representation. Generally, the Richards and the ADE equation alone describe uniform flow and transport or called equilibrium flow and transport, due to the assumption that water contents and pressure heads are tightly coupled through the equilibrium retention curve [Simunek et al., 2003]. However, this conceptualization is unable to account for the presence of macropores and other structural features caused by profile heterogeneities, which can create a non-equilibrium flow or preferential flow (PF). Paper 1 reflects on the HHT equation in regards to drain flow from the matrix coupled with the preferential flow, by fixing the lower boundary to the actually measured groundwater table. In contrast to Paper 1, Paper 3, is using a parameterized low permeability aquitard, in order to model the measured groundwater table jointly with the measured drainage.

1.3 Preferential transport of water and nitrate

In the last three-decade, PF became the focus of the soil and agricultural sciences. Numerous field and laboratory studies suggested the potential risk of agrochemical and nutrient leaching through preferential pathways, by bypassing the soil matrix [Bergstrom, 1995; Tofteng et al., 2002; Fox et al., 2004; Gjettermann et al., 2004; Akay and Fox, 2007; Rosenbom et al., 2008; Petersen et al., 2012]. This type of flow behaviour limits the possibility of retention and degradation of compounds, such as nitrate, phosphorus, or pesticides. It increases the importance of the correct conceptualization of preferential transport since the commonly used Richards, and ADE equation alone is not adequate to describe fast transport of solute. Several preferential water and solute transport modelling approaches have been developed, most of them coupled with the Richards and ADE equation. According to Simunek et al. [2003], conceptual models including preferential flow can be bimodal single porosity equilibrium models [Børgesen et al., 2006] to account for increases in the hydraulic conductivity near saturation or non-equilibrium single porosity model.
[Ross and Smettem, 2000] by decoupling the water contents and pressure heads in Richards equation. Even though the approach of Børgesen et al. [2006] increases the conductivity at near saturation, it does not describe PF, due to the wetting front remains uniform with faster advance and no lateral transport between matrix and macropore. The other types of non-equilibrium models consider dual-porosity and dual-permeability concepts. The former theory describes the mobile-immobile water approach by restricting water movement in the matrix medium and allowing transport in the macropore region. Here the matrix can store, retain, and exchange water but prohibits it to advance. Germann [1985] has proposed an alternative approach, using the kinematic wave equation. The model describes the PF inside the macropore by a kinematic exponent and a macropore conductance parameter. The last type of non-equilibrium model is the dual-permeability concept. This model approach is able to describe the flow within the matrix and the macropore media. Of this type, the most well known variably saturated zone modelling systems, e.g. MACRO [Larsbo and Jarvis, 2003], HYDRUS [Šimunek et al., 2012] and RZWQM [Ma et al., 2012] are developed with similar approaches to describe the non-equilibrium transport within the soil. Gerke and van Genuchten [1996] described the matrix and macropore media with the Richards equation, whereas MACRO uses the kinematic wave approach for describing the PF and Richards equation to describe water flow in the matrix region. The alternative method of RZWQM is following a Poiseuille’s law based explanation for the macropore flow, assuming gravitational flow.

Nitrogen leaching by preferential pathways has been debated since the PF gained attention due to their ability to transport and increase leaching of agrochemicals. Several studies have investigated this phenomenon in term of laboratory, field and modelling experiment [Ahuja et al., 1993; Bergstrom, 1995; Mohanty et al., 1998; Larsson and Jarvis, 1999; Bergström and Djodjic, 2006; Gooday et al., 2008; Frey et al., 2012; Cheng et al., 2014; Frey et al., 2016]. Most of these studies investigated the possible leaching through surface connected macropores, implying that NO₃-N may be transported by PF if heavy rainfall occurs right after the application of fertilizer. This fast transport only from surface connected macropores agreed to by Bergstrom [1995] and Bergström and Djodjic [2006], who argued that N compounds which are stored in the matrix and thereby protected against PF, are more exposed to a slow convective transport. Although if the statement is right, it should be conditionally approached. Paper 1 and Paper 2 discuss the possibility of N leaching by buried macropores below the surface. As one of the main features of a structured soil, low permeability plowpan layers play a strong influence on the plough layer water pressure heads. Dye infiltration studies found plowpans to inhibit the vertical advection of dyed water through the soil matrix, and cause lateral movement until open earthworm burrows were encountered, e.g. Shipitalo (2004) found that vertical movement of the dye was mainly conducted by vertical
Consequently, N compounds, which are stored in micropores, can be intercepted by the lateral flow. Therefore as earlier modelling studies showed [Abbaspour et al., 2000; Rosenbom et al., 2009], it may be essential to incorporate discrete low permeable soil layers to simulate field observation more accurately. Although a discrete low permeable layer (plowpan) was not explicitly incorporated in Paper 1, Paper 2 and Paper 3, the subsoil has a significant lower hydraulic conductivity than the topsoil, and as such equivalent to a discrete low impermeable layer.

1.4 Denitrification modelling
Denitrification is the process where microbes use nitrate as an oxygen donor when decomposing organic matter in anaerobic conditions. In this way, N can be lost to the atmosphere in a gaseous form such as N₂ or N₂O, thereby limiting the N amount to be leached downward to the drainage or groundwater or taking up by the crops. The aforementioned models and others have developed submodels to describe the anaerobic process driven by the oxygen content, temperature, pH, and microbial biomass of the soil environment. Due to the number of different approaches, studies have been conducted in terms of effectiveness, accuracy, and complexity [Hansen et al., 1995; Ma and Shaffer, 2001; Manzoni and Porporato, 2009]. [Heinen, 2006] categorized the today available submodels as microbial growth models, soil structural models, and simplified process models. The first two categories are considered by all studies as complex models, which are challenging to parameterize due to the difficulty of obtaining information on the microbial processes and gaseous diffusion within the soil aggregates. Therefore simplified models are more practical at field-scale modelling since they determine denitrification based on easily measurable parameters such as degree of water saturation, soil temperature, and nitrate content of the soil. The potential denitrification calculated by either simple empirical relationship to CO₂ evolution rate or a first-order decay coefficient, which refers to the denitrification at optimal condition. The description of the abiotic reduction factors is the backbone of these simplified submodels. They fit the potential denitrification to the current soil condition resulting in the actual denitrification. Paper 2 applied this simple denitrification model and tested the sensitivity of the abiotic water function.

2 Objectives and Hypotheses
To avoid unacceptable leaching of contaminants such as nitrate through soil media into drainage/surface waters and groundwater it is imperative to be able to conduct high-quality leaching risk assessments accounting for the dominant flow and transport processes. In many soils such as those ones selected for this study, preferential transport through macropores are
dominating, but how much? To our knowledge, such estimates are lacking in the scientific literature. Therefore, this study is focusing on the following objectives:

(1) The ability of the DAISY model to describe the water and solute balance (bromide and nitrate) in artificially drained sandy clay loam soils (Paper 1, Paper 2, Paper 3).
(2) The sensitivity of model parameters incorporated in six different model concepts, including three different macropore settings and two groundwater levels as lower boundary conditions. The behaviour of the DAISY dual-permeability approach towards a multi-objective calibration procedure (Paper 1, Paper 2, Paper 3).
(3) Assessment of which macropore settings were capable of giving the optimal representation of the hydrogeological setting in the investigated clay till (Paper 1).
(4) The performance of the calibrated model concepts in regard to the degree of macropore flow to drainage (Paper 1, Paper 3).
(5) Denitrification modelling with respect to water saturation of the lower part of the plough layer (Paper 2, Paper 3).
(6) The effect of tile drain depth in terms of nitrate transport (Paper 3).

The aim of the work is to test the following hypotheses by focusing on the above-mentioned objectives:

- Nitrate leaching to the drainage is facilitated by preferential transport in macroporous clay soils.
- Simplified models of denitrification based on abiotic reductions functions cannot satisfactorily well describe denitrification in heterogeneous soils.

3 Experimental data and theoretical background

3.1 Silstrup and Tokkerup
The study involves data from two heterogeneous clay fields, where one is located in the north-western (Silstrup) and one in the south-eastern (Tokkerup) part of Denmark. The former dataset is from the research activities of the Pesticide Leaching Assessment Programme (PLAP), organized under Aarhus University (AU) and Geological Survey of Denmark and Greenland (GEUS), and the latter is from a co-operation between Aarhus University and University of Copenhagen. Both fields are involved in ongoing long-term experiments.
Soil type and climatic conditions are considered to be some of the most important parameters controlling nitrate leaching. This study focuses on clay fields representative of the macroporous clay soil types in two different climatic conditions in Denmark (Fig. 1). The groundwater table is shallow at both fields, thereby enabling nutrition leaching to groundwater or drainage to be rapidly detected. Cultivation of the Silstrup and Tokkerup is done in line with conventional agricultural practice in the area. Both fields were accommodating separate studies under supervision in one of the managing organizations. In the case of Silstrup, Norgaard et al. [2015] conducted an experiment focusing on pesticide degradation based on 65 sixty-five soil samples taken from the plough layer. They were unable to explain pesticide leaching based on the microbial potential for degradation and mineralization in the plough layer, suggesting rapid bypass to the deeper horizon. For validation purposes, the soil water retention and hydraulic conductivity data were used in the water balance modelling in Paper 1. Katuwal et al. [2015], by using X-ray computed tomography for comparing fluid and chemical transport properties (tracer test), showed that tracer arrival time was explained mainly by the total macroporosity. In Paper 1, using the pre-existing knowledge based on the macroporosity and the available data on water and bromide transport, a dual permeability model was set up to prove the preferential flow transport in connection to the tile
drainage and to the groundwater. For further field description and management data, cf. Paper 1 and Paper 2.

In terms of the Tokkerup site, the experimental field and the surrounding area is used for conventional farming. The University of Copenhagen initiated a long-term experiment based on the preceding crop rotation data and the farmer experience on the field. The initial start of the experiment is described in Hansen and Jensen [2013], where they investigated the potential effect of drainage in relation to crop productivity. The field was divided into a poorly- and a well-drained part which resulted in the main drain depth of -66 and -120 cm at the poorly and well-drained part, respectively. Gyldengren [2016] investigated the drainage effect on crop production by using the groundwater and harvest data with the DAISY model. He identified significant harvested dry matter differences between the two-part of the field; however, he suggested, that there could be additional factors causing the reduction in harvested dry matter. As a continuation of the experiment, Holbak [2017] conducted a pedological experiment in the poorly-drained part of the field by identifying macroporosity, saturated hydraulic conductivity, and soil water retention. In Paper 3, all previous hydro-pedological knowledge was incorporated into the modelling dataset.

In order to identify the dominant transport processes at field scale, the dataset from both fields included hourly measured drainage, precipitation, temperature, relative humidity and wind speed with additional flow proportional sampling of the drainage water for laboratory testing of bromide and nitrate content.

3.2 DAISY dual permeability model

DAISY is a Soil-Plant-Atmosphere system model, which incorporates modules describing plant water uptake and plant growth, C-N turnover, heat and nitrogen dynamics in the soil. Each of these themes is incorporated into modules interconnected with each other. DAISY uses the Richards equation to solve the one-dimensional water transport in the matrix.

\[
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K \frac{\partial \psi}{\partial z} \right] + \frac{\partial K}{\partial z} - S
\]

(1)

, where \( \theta \) [VV^{-1}] is the volumetric water content in the soil, \( \psi \) [L] is the soil water pressure potential, \( K \) [LT^{-1}] is the hydraulic conductivity of the soil and \( S \) is a sink term, which represents the loss to the drain, macropore or plant water uptake. In order to solve the Richards’ equation, in this study, the van Genuchten (vG) soil water retention model was used [Van Genuchten, 1980].

- 8 -
\[ \theta = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha \psi|^n]^m} ; h < 0 \\ \theta_s ; h > 0 \end{cases} \]  

(2)

, where \( \alpha, n \) and \( m \) are empirical shape parameters, \( \theta_s \) and \( \theta_r \) are the saturated and the residual water content respectively of the given soil. One of the advantages of DAISY can accommodate several soil water retention and conductivity function. In this study, the commonly known, van Genuchten model is coupled with the Mualem hydraulic conductivity theory [Mualem, 1976] (vGM), where \( m \) is achieved as \( m = 1 - \frac{1}{n} \). The Mualem hydraulic conductivity is expressed as

\[ K = K_s S_e^l [1 - (1 - S_e^{1/m})^m]^2 \]  

(3)

, where \( K_s \) the hydraulic conductivity at saturation is, \( S_e \) is the effective saturation, which is calculated as, \( S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \) and the \( l \) is the shape form, which represents the pore connectivity.

When the Richards equation is solved, the water flux in the matrix is calculated by the Darcy equation,

\[ q = -K \left( \frac{\partial \psi}{\partial z} + 1 \right) \]  

(4)

, where \( q \) is the Darcy flux.

To model the water flow in the fast-medium in the soil, macropore parameters need to be specified. The fast flow domain in DAISY is described by a macropore module designed by Mollerup [2010] (web address: https://daisy.ku.dk/publications) and tested in a technical reports, prepared for and published by the Danish Environmental Protection Agency[Hansen et al., 2010b; Hansen et al., 2010a; Hansen et al., 2012a]. The macropore is a vertically oriented feature in the DAISY model, characterized by physical properties such as length and diameter. The macropores are divided into two different classes, depending on their bottom boundary; soil matrix or drain. The different lower boundary condition is essential for the macropore. If the macropore is characterized as matrix macropore and it is filled with water, after a certain pressure in the macropore, the water can be transferred back to the matrix from the macropore (Fig. 2.b). This condition cannot be applied to the macropores with drain connection since they empty instantly and as such cannot be filled.

Based on the experiment of Tofteng et al. [2002], the macropore flow is initiated when the matrix pressure exceeds a specific pressure potential called \( \psi_{init} \). If this pressure potential is exceeded the
macropore domain activates and water starts to fill up the macropore. When the pressure potential drops below a level called $\psi_{term}$, the macropore flow is terminated. In a specific case, when a macropore is filled with water, it can be transferred back to the soil matrix at a certain point. It is initiated when the pressure difference between the macropore and the matrix exceed a minimum pressure barrier $\psi_{barrier}$. All pressure parameters are common for all classes.

The approach of quantifying the water flow ($Q \ [VT^{-1}]$) to the macropore domain is calculated by soil water extraction from the matrix is based on a water movement in a confined aquifer towards a well,

$$Q = \frac{2 \pi K D (s_{well} - s_d)}{ln \left( \frac{r_d}{r_{well}} \right)}$$

(5)

where $K \ [LT^{-1}]$ is the saturated hydraulic conductivity, $r_{well} \ [L]$ is the radius of the well, $s_{well} \ [L]$ is the drawdown at the wall of the well, $s_d \ [L]$ is the drawdown at distance $r_d \ [L]$. In this case, a well represents a single macropore.

In the conceptual approach, the macropores are equidistantly placed, so the density of the macropores is approximated as:

$$M = \frac{1}{\pi r_{d,mean}^2}$$

(6)

Where $2r_{d,mean} \ [L]$, is the mean distance between two macropores. Then Eq. (5) with the physical term of the macropores can be expressed as:

$$Q_m = \frac{2 \pi K(\psi) \Delta z (\psi_{mx} - \psi_m)}{ln(\frac{r_d}{r_m})}$$

(7)

where $K(\psi) \ [LT^{-1}]$ the hydraulic conductivity of the soil matrix at is given pressure, $\psi_{mx}$ is the pressure potential in the matrix, $\psi_m$ is the pressure potential in the macropore, $r_m \ [L]$ is the macropore radius, $r_d \ [L]$ is the drawdown radius derived from the density of the equidistantly placed macropores, and $\Delta z \ [L]$ is the macropore height at the given calculation cell. The pressure potential of a macropore at a given position calculated from the surface until the actual water level ($z_{air}$) inside of a macropore (Fig 2.).
Figure 2. Macropore numerical schematics of the DAISY dual permeability approach. Pressure potential of macropore in respect to a calculation cell in case of a) matrix transport ($S_{mx\rightarrow m}$; Eq. 10) to the macropore, b) macropore transport ($S_{m\rightarrow mx}$; Eq. 11) to the matrix.

Figure 2. a) shows the abovementioned hydromechanics in $c_i$ calculation cell. The macropore potential ($\psi_m$) is relative to the centre of $c_n$, which is $z_{c,n}$ deep below the surface. Therefore the pressure potential of the macropore at depth.

$$z_{c,n} = \sum_{i=1}^{n-1} z_i + \frac{z_n}{2}$$

$$\psi_m = z_{air} - z_{c,n}$$

where $n$ is the number of discretized calculation cell.

By using Eq(6) and Eq(7) the Sink term ($S_{mx\rightarrow m} [VT^{-1}]$) can be expressed for the Richards’ equation as:

$$S_{mx\rightarrow m} = \frac{M Q_m}{\Delta z} = -\frac{4\pi M K(\psi) \Delta z (\psi_{mx} - \psi_m)}{\ln(\pi M \frac{r_m^2}{r_m})}$$

For the backward flow, from the macropore to the matrix is expressed similarly, but instead of the conductivity, resistance ($R_m = K(\psi)^{-1}$) from the macropore is used (Fig 2. b). To move water from the macropore to matrix, it is not enough that the pressure is higher in the macropore. It also needs to be positive, at least in part of the cell, moreover the pressure potential in the macropore has to be $\psi_m > \psi_{barrier} + \psi$. 
\[ S_{n\rightarrow m} = \frac{-4\pi M \Delta z (\psi_{mx} - \psi_m)}{R_m \ln(\pi M r_m^2)} \]  

(11)

The interaction between macropore and surface water follows the Poisseullies law [Hillel, 1998; Ma et al., 2012], and the only driver is gravity. The flow calculated as

\[ Q_{\text{infiltration}} = \frac{\pi r_m^4 \rho_w g (l + H_{\text{pond}})}{8 l \mu} \]

(12)

, where \( \mu \) is the dynamic viscosity of water, \( \rho_w \) the density of the water, \( g \) is the gravitational acceleration, \( l \) is the length of the macropore and \( H_{\text{pond}} \) is the height of the ponding water above the macropore. The infiltration rate is calculated in a similar manner as in Eq (10-11), based on the macropore density.

\[ i_{\text{infiltration}} = \frac{\pi M r_m^4 \rho_w g (l + H_{\text{pond}})}{8 l \mu} \]

(13)

When the hydrologic setup includes a subsurface drain at a certain level, and when the groundwater exceeds this level, the water tends to flow towards the drainpipe. The Hooghoudt equation gives a mathematical formulation of the parameters which are involved in a subsurface drain transport of a flat land [Hooghoudt, 1940]. In a steady-state condition, the drain flux per unit surface area is calculated as the following.

\[ q = \frac{8 K_b D_e h + 4 K_a h^2}{L^2} \]

(14)

, where \( K_a \) and \( K_b \) is the hydraulic conductivity of the saturated layer above and below the drain level, respectively. \( L \) is the distance between drains; \( D_e \) is the equivalent drainage depth depending on the vertical distance between the drain and an impermeable layer, \( D \). The midpoint water table height above the drain is denoted \( h \) and \( r \) is the radius of the drain. The \( h \) and \( r \) are used to calculate the equivalent drainage depth, according to van der Molen and Wesseling [1991]:

\[ D_e = \frac{1}{8} \frac{\pi L}{\ln \left( \frac{L}{r_m} \right) + F(y)} \]

(15)

, where \( F(y) \) is the function of the distance between the impermeable layer and the distance between the drain pipes. If \( D_e \leq D \), then \( D_e \) is used, due to the appearance of extra resistance as a result of radial flow near the drain pipe.

The drain flux is separated into two-part, one that flows to the drain above the drain level \( (q_a) \) and one that flows below it \( (q_b) \)
\[ q_a = \frac{4}{L^2} K_a h^2 \]  
(16)

\[ q_b = \frac{8}{L^2} K_b D_a h \]  
(17)

The drain flow may involve several layers above and below the drain level. Therefore the average conductivity is used in the equations.

\[ K_a = \frac{\sum_{i=0}^{N} f_{a,i} \Delta z_i K_{s,i}}{D_a}, \quad D_a = \sum_{i=0}^{N} f_{a,i} \Delta z_i = h \]  
(18)

\[ K_b = \frac{\sum_{i=0}^{N} f_{b,i} \Delta z_i K_{s,i}}{D_b}, \quad D_b = \sum_{i=0}^{N} f_{b,i} \Delta z_i = D \]  
(19)

where is \( N \) the number of the saturated layers above and below the drain level, \( K_{s,i} \) is the saturated conductivity of layer \( i \), and \( \Delta z_i \) is the thickness of the saturated cell \( i \). The \( f_{a,i} \) and \( f_{b,i} \) are the fraction of the saturated cell above and below the drain level, respectively. The drain flux is calculated in all saturated layer above and below the drain level and implemented as a sink term in the Richards equation.

\[ S_{\text{drain}} = \frac{f_{a,i} K_{s,i}}{K_a D_a} q_a + \frac{f_{b,i} K_{s,i}}{K_b D_b} q_b \]  
(20)
3.3 Uncertainty, sensitivity analysis, and calibration protocol

Uncertainty: Since the advent of mechanistic-deterministic models or process-based models, they have become one of the primary modelling tools for assessing and interpreting causal interactions between the environment, climate, and mankind. These tools allow researchers to simulate scenarios and conceptual ideas in a cost-effective manner. Although these tools are based on the mathematical formulation of physical, biological or chemical processes often describe a simplified version of reality, and often the models require a substantial amount of parameter input, which for some are empirical or even values without any physical meaning. Due to model development and a better understanding of environmental problems, new implementations have to lead to a more mathematical interpretation of physical phenomena which are build upon or related to other already characterized processes. This causes the risk of overparameterization of models, which could lead to over-fitting or identifiability problems. An over-fitted model, with small error term on a calibration dataset, could result in a significantly larger error on an evaluation-validation dataset, which could severely hinder the predictability of these models [Brun et al., 2001]. In practice, the performance of a process-based model is highly dependent on the setting of model parameters, which leads to another crucial problem; equifinality. As Beven and Freer [2001] described, overparameterized, complex, non-linear models with different parameter sets may lead to the same results. One particular example of the overparameterized model is DAISY. The model incorporates transport processes, crop development, and nutrient conversion that involve numerous parameters, which have a substantial impact on model calibration.

In order to overcome the drawbacks or uncertainty of these models, several measures can be taken. According to Refsgaard et al. [2007], multiple model simulation is a strategy to identify uncertainty about model structure. Instead of doing an assessment using one stand-alone model, the modelling should be carried out using different models of the same system which can be done by having different conceptual models based on different geological, in case of this study, pedological interpretations. This approach was attempted in Paper 1, by conceptualizing three different macropore settings with two different lower boundary conditions. By using different PF interpretation of the field, it allowed the assessment to focus and highlight those macropore features, which could be crucial for bypass transport at the field scale.

Sensitivity analysis: Further option is sensitivity analysis (SA) of parameters to help identify the most influential ones by measuring their relative impact on the model prediction. Some studies have shown, that SA is able to help the understanding of the model structure [Refsgaard et al., 2007], decrease the possibility of overparameterization and improve the calibration efficiency [van Griensven et al., 2006]. In the present study, the Morris sensitivity screening method
was utilized on those model parameters, which were believed to have an impact on the multi-objective function. The Morris screening method is based on the elementary effect (EE) of a given parameter [Morris, 1991] by changing one parameter at a time (OAT). The parameters are sampled from a predefined distribution by \( p \) discrete times. In case of a \( k \) number of input parameter, the screening method requires a \( M = p \times k \) parameter matrix. The influence of an input is assessed on the output by varying one input parameter by a predefined sampling increment \( \Delta \) while keeping the other parameters constant. An increment is defined as a multiple of \( 1/(p-1) \).

For a given mathematical model of the form \( Y = f(X_1, X_2, ..., X_n) \) with \( n \) parameters, \( EE_i \) for the parameter \( X_i \) can be expressed as:

\[
EE_i(X) = \frac{Y(X_1, ..., X_{i-1}, X_i + \Delta, X_{i+1}, ..., X_n) - Y(X)}{\Delta}
\] (21)

The number of model evaluations for the Morris method is of the order of \( r(n+1) \) where \( r \) is the number of values (trajectories) that the input is allowed to take within its range and \( n \) is the number of parameters. An extensive description of the method can be found in Campolongo et al. [2007] and Morris [1991]. In this study, a level \( p \) of 5 and a number of trajectories \( r \) of 10 were used.

The sensitivity measures proposed by Morris [1991] are the mean, \( \mu \), of the EE’s, which quantifies the importance of the parameters (i.e. additive affect) for the model output \( Y \) and the standard deviation \( \sigma \) of the EE’s, which indicates the non-linear and/or interaction effects of the model parameters on the model output \( Y \). Further, Campolongo et al. [2007] proposed the mean of the absolute values of the EE’s, \( \mu^* \), to overcome the cancellation of positive and negative EE’s on the mean, which was used in this study.

The parameters were ranked with regard to their sensitivity based on the Morris distance defined as

\[
\epsilon = \sqrt{(\mu^*)^2 + \sigma^2} \tag{22}
\]

which is the Euclidian distance (\( \epsilon \)) of \( \mu^* \) and \( \sigma \) from the origin (0, 0) [Jabloun, 2015]. This sensitivity ranking is an approximation as the interactivity and non-linearity are merged into one sensitivity index [Ciric et al., 2012]. In case a parameter shows high sensitivity or strong interaction, a high \( \epsilon \) will be obtained.
Figure 3. An example of the sensitivity screening output with three levels of sensitivity. Left: Parameter sensitivity to drainage dynamics (DD). Right: Parameter sensitivity to cumulative drainage (DC).

Sensitivity screening was done based on different sub-objectives. Each parameter was screened against each sub-objective separately, thereby creating a composite sensitivity, which takes into account the individual effect of all parameters on all objectives. The composite sensitivity screening aids the understanding of the model structure and gives a better overview of the parameter interaction, thus helping to reduce the uncertainty raised by the overparameterized model structure.

Calibration protocol: An optimal parameter set is sought “automatically” by minimizing an objective function, which is generally an error term between the field measurements (calibration objectives) and their simulated counterparts, such as Root Mean Squared Error (RMSE), Mean Absolute Error (MAE) or Kling-Gupta Efficiency (KGE). There is a large variety of optimization algorithm available for inverse modelling. In Paper 1, Paper 2 and Paper 3, for inverse modelling, the differential evolution (DE) optimization was used developed by Storn and Price [1997] and adapted in the R package by Mullen et al. [2011] and Ardia D. [2016]. DE is commonly known as metaheuristic method as it makes few or no assumptions about the problem which is being optimized. According to Ardia D. [2016], DE is the best for optimizing non-linear problems, or when the mathematical optimization problem has strongly non-differentiable characteristics. DE optimizes a problem by keeping a parameter set of a candidate solutions and generating new candidate solutions by incorporating existing parameters in accordance with its formulae, then keeping the parameter set which has the best fitness to the optimization problem. Further information in Storn and Price [1997].
3.4 Model parameterization

The model parameterization of the DAISY model, in terms of Silstrup, took two stages. In the first stage (Paper 1), the parameterization mainly focused on the hydraulic setup with the potential conceptual understanding of the field and the identification of probable hydraulic parameters within the model for sensitivity screening. The selected parameters were from the vGM model (Eq.2), and from the DAISY dual permeability model. Each soil water retention parameter was assessed based on available water retention and hydraulic conductivity measurement [Lindhardt et al., 2001; Iversen et al., 2011]. The vGM model was fitted to the measured retention points from every horizon and sampling plane (North - East) and by this creating a corresponding uncertainty range for each soil water retention parameter. Due to the small number of consecutive samples from the field, a uniform distribution was assumed within the uncertainty range. By reason of limited prior detailed information on macropore distribution at the field, the macropore distribution-survey study of Nielsen et al. [2010] was used, which was conducted on a similar clay field in Denmark. The potential model conceptualizations included 3 different approaches with a sequential setup of macropores types. The macropore types included macropore ending in a drain (DM), macropores ending in the matrix (MM), and a macropore feature representing a deep fracture throughout the soil profile (FR). The sequential setup includes a) DM alone, b) DM + MM and DM + MM + FR with each setting to exposed to two different groundwater measurement as a lower boundary condition. More details are given in Paper 1.

In the second stage (Paper 2), all hydraulic parameters were retained for further calibration, but the parameter range limited to 10% of either side from the calibration value. Additionally, crop, soil organic matter (SOM) and denitrification model parameter were included. The denitrification default water reduction function was replaced with the parameterized version of the power reduction function of Grundmann and Rolston [1987]. The initial value for the crop parameters was taken from DAISY library.

Regarding the parameterization of Tokkerup (Paper 3), the soil horizon distribution of well-drained (WD) and poorly drained (PD) were taken from Gyldengren [2016] and Holbak [2017], respectively. From the latter study, the pedological profile description and hydraulic measurement were taken for setting the uncertainty range for the vGM and macropore parameters using the methodology from Paper 1, and pedotransfer functions were used on the extracted soil texture information from the former study. In this study no crop parameter was assessed, however, the denitrification model was parameterized in the similar manner as in Paper 2. Additionally, the HHT were added with a parameterized aquitard hydraulic conductivity and thickness.
4 Main findings from this study

4.1 Plough layer induced macropore transport

In *Paper 1*, the one-dimensional DAISY process-based model dual permeability approach was tested and calibrated against 10 years of hourly measured drainage dataset and evaluated by a tracer test. The modelling exercise showed that DAISY could model water flow to the drainage system with high precision for a long-term period accounting for PF, which showed major importance. As Refsgaard et al. [2007] suggested, different conceptualization of the clay till profile was used to account for the conceptual uncertainty, which appeared when different macropore descriptions from previous studies [Akay and Fox, 2007; Nielsen et al., 2010; Petersen et al., 2012; Cheng et al., 2014] were considered. The conceptualization included macropore settings with a) only drain-connected macropores (DM), b) macropores ending up in the drain (DM) and the matrix (MM), and c) DM and MM macropores where an MM-type is present through the entire soil column, representing a fracture (FR). (Fig. 4)

![Diagram](image)

**Figure 4.** The three macropore settings applied in the clay till profile. The depth [cm] is given as height above soil surface: a) Only macropores ending in the tile drain (DM), b) same as a) but including macropores ending in the matrix (MM), and c) same as b) but including macropores...
representing a fracture (FR) penetrating the entire soil profile (horizons A-C) and a highly permeable matrix horizon D (Paper 1).

Two groundwater table measurements, P3 and P4, (Fig. S3, Paper 1) were collected at the southern and northern borders of the field, respectively, the results showed that the groundwater table measured at P4 did not truly reflect the water balance of the field, which indicate the importance of a correct lower boundary. The concept with macropore setting b) exposed to groundwater fluctuations measured in the southern part (P3) of the field gave the best description of the drainage of the field.

![Figure 5](image.png)

Figure 5. Measured and simulated drainage and SWC dynamic response to the heavy rain event on 8 June 2003 (Paper 1).

All conceptual macropore settings were screened for situations with fast drainage response to a distinct heavy rain event in a relatively dry period with SWC at 25 cm depth and drain flow in July 2003 (Fig. 5). The models were able to simulate the rapid PF phenomena in the drainage and a rapid wetting front in a soil matrix during an unsaturated condition, which is in alignment with findings of Nimmo [2012].
Figure 6. Simulated accumulated water and nitrate input from the matrix and macropore domains to the drainage system and measured counterparts at Siltrup (2006-2007) and the poorly and well-drained part at Tokkerup for period 2017-2018.

Further results of this model study (Paper 1) revealed that 70% of the overall drainage was supplied via macropores and of the applied tracer 54% leached directly from the plough layer. Based on the different conceptual settings, the majority of drainage seemed to be primarily the result of rapid precipitation infiltration from the surface to the plough layer, and from there via preferential pulse flow to the drain or below through macropores. The applied Br tracer test and modelling revealed that in this heterogeneous soil with yearly soil tillage (harrowing and ploughing) and, therefore, most likely a temporary increase of the soil porosity in the plough layer, the buried macropores could have a more significant impact on transport than surface-connected macropores (Fig. 6). These findings are in agreement with Shipitalo [2004] and Frey et al. [2012], where they explained the possibility of water build-up above a more compact soil horizon with the only vertical flow and transport possibility, through preferential transport.
4.2 Dynamic denitrification modelling

In the follow-up study (Paper 2), the main focus moved towards the effect of preferential transport, denitrification and their combination on leaching of nitrate to the drainage system during the previously assessed period at Silstrup. The results revealed a dominant effect of these processes on the drainage leaching of nitrate from this clay till field. A large amount of N (48% to 80% of the total N-loss to drainage) was preferentially transported via macropores to drainage system regardless of the application method and concurrent occurrence of precipitation.

Heinen [2006] investigated the sensitivity of denitrification reduction factors and found that the most sensitive factor was the water reduction factor, as it controlled the majority of the denitrification. In regards to the water balance study of Silstrup (Paper 1), the build-up of the water above a low-permeable layer such as a plough pan or compacted subsoil could lead to gaseous loss of N [Frey et al., 2012]. However, preferential flow dynamics could reduce the residence time of the solute in the plough layer and thereby introduce the need for adjustment of the current standard denitrification water reduction factor. The results in Paper 2 revealed the need for a modification of this reduction factor for both the fast and slow SMB (Soil Microbial Biomass) pools resulting in approximately 50% reduction in the denitrification from a seasonal average of 75 kg N ha⁻¹ to 35 kg N ha⁻¹.

![Figure 7](image)

Figure 7. Modified water reduction functions of denitrification of slow and fast pools in DAISY at Silstrup field and the poorly and well-drained part of the Tokkerup field with the default reduction function of DAISY.

On the data gathered from the field experiment of Tokkerup (Paper 3), similar modelling research was conducted with relation to the drain depth and the possibility of denitrification. The
outcome of the calibration showed that NO$_3$-N could be leached out dramatically faster by PF than it is expected. Macropore transport, directly and indirectly, governed the N loss to the drainage. It was shown that buried matrix-ended macropore transported NO$_3$-N to the top layer of the groundwater, which behaved as a rapid intermediary before it transported further to the drain system. Denitrification, in the presence of preferential flow, was shown to be significantly lower than calculated with the standard parameters, probably due to the short residence time of the N. The modelling results also implied that denitrified mineral N is not originating from the added mineral fertilizer but rather from the slowly mineralized organic N.

Figure 7 shows the default DAISY relative water content and denitrification reduction relationship (similar for both the slow and fast pools) and the calibrated reduction functions for the field at Silstrup and for the poorly and well-drained part the field at Tokkerup. All the three calibrated models showed a significant alteration from the original default denitrification reduction function, especially for the fast pool.

By extending the view on the importance of a low permeability layer or plough pan in simplified denitrification models, which are incorporated in all well-known C/N turnover models, have to be calibrated in a field dependent way. It might be that denitrifying bacterias are not consuming NO$_3$ with the same efficiency in the Spatio-temporal pattern. Therefore the relationship between denitrification and water saturation has to be approached a more dynamic way, rather applying a default relationship(Paper 2, Paper 3).

4.3 The sensitivity of the dual permeability parameters
The sensitivity of the dual permeability parameters of the DAISY model was explored in Paper 1, Paper 2, and Paper 3. All three studies have shown that the diameter of the macropores show little to no effect on any of the objectives in relation to water and solute transport, which is consistent with the study of R. Ahuja et al. [1993], who stated that to determine the maximum flow rate, one only needs to adopt a relevant pore size, instead of identifying the distribution of the macropore sizes in a given field.
5 Conclusion
The overall study shows that preferential transport at a heterogeneous field, such as Silstrup and Tokkerup, has a high potential to facilitate nitrate leaching to the drainage or to the deeper-lying groundwater. Drainage transport modelled by the HHT may be accurate for sandy soils, where the waterfront is uniformly descending towards to the drainpipe, however, in a macroporous soil, it is imperative to depict the direct preferential connection to the drainage system. Although several models have implemented one way or another their aspect of preferential transport, current research still lacks the modelling of long term effect of this phenomena. This study highlights, that the potential quantity of water and solute (bromide and nitrate), which can be transported by PF from the plough layer, is caused by an induced pressure build-up within the plough layer due to an underlying low permeability layer.

Denitrification is difficult to model, especially as no direct long-term measurements in the field is possible. Hence, the present study shows big differences in the amount and in the calibrated water reduction functions compared to the defaults in DAISY.

Modelling with DAISY operates with a substantial amount of parameters, which is challenging to control. However, with the right sensitivity testing, calibration and assessment of the input parameters, the uncertainty of the model outcome can be reduced. Even though the DAISY dual permeability approach has not been frequently tested, its combination of the extensive crop, carbon-nitrogen modelling could be a powerful tool for understanding the fate and transport of nitrogen and hence how to mitigate nitrogen leaching. The DAISY model has also shown that a one-dimensional Darcy flow-based model with an extended module to describe preferential flow made the model capable of capturing water and solute dynamics in a given field, both in short and long term.

6 Recommendations for future research
Macropore transport in the last 3 decades received much attention in regards to pesticide, phosphorus and colloid transport. Although several models have implemented one way or another their aspect of preferential transport, current research still lacks modelling the long term effect of this phenomena. Macropore transport is seldom associated with nitrogen leaching. However, evidence of this study shows that nitrogen leaching is significantly affected, facilitated by macropore transport. Modelling of fate and transport of nitrogen in artificially drained clay soils with the use of uniform or composite soil water retention and hydraulic conductivity alone may
be misleading, and this study recommends to apply a dual permeability approach such as the inclusion of the DAISY macropore flow concept with the Darcy based matrix flow.

It is also recommended to apply isotopic N to identify the relative importance of sources that are isotopically distinct. These methods could help to delineate, the composition of leached N in the drainage, by separation of the added mineral N from the mineralized organic at the field.

Further, future research should aim at changing the concept for modelling denitrification in DAISY to reduce the uncertainty of this important element of the nitrogen balance, which was found surprisingly high in the present study of heterogeneous clay soils with a high possibility of preferential transport. It seems imperative to model denitrification in DAISY more dynamic using the parameterized power function of Grundmann and Rolston [1987].
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Estimating the degree of preferential flow to drainage in an agricultural clay till field for a 10-year period
Estimating the degree of preferential flow to drainage in an agricultural clay till field for a 10-year period

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Key points:

- 1D-numerical model based on Richards equation incorporating macropore settings can describe the drainage including bromide transport
- Simulations reveal, up to 70\% of the drainage was transported rapidly from surface via macropores through the variably-saturated clay till.
- Vertical macropores initiated in the plow layer are estimated to facilitate the transport of 54\% of the drainage.

Abstract

In order to assess the risk of contaminants like nitrate and pesticides being transported through a variably-saturated macroporous clay till to drainage, the conceptual understanding of the preferential water flow is crucial and hence the degree of water percolating rapidly through vertical macropores or slowly through the low-permeable matrix. This study compared six different model concepts, using the dual-permeability module of the one-dimensional model DAISY, incorporating three different macropore settings and two different groundwater tables set as lower boundary conditions. The three macropore settings included vertical macropores supplying water
directly to \textit{a}) drainage, \textit{b}) drainage and matrix and \textit{c}) drainage and matrix including fractures supplying water to the matrix in the saturated zone. The model study was based on ten years of coherent climate, drainage, and groundwater data from an agricultural clay till field. The estimated drainage obtained with the six model concepts was compared to the measured drainage. No significant discrepancies between the estimated and measured drainage were identified. The model concept with the macropore setting \textit{b}) exposed to groundwater fluctuations measured in the southern part of the field part gave the best description of the drainage. Bromide leaching tests were used to evaluate the mass balance of the model concepts. The estimated water balance of all six concepts revealed that 70\% of the precipitation input to drainage was transported via macropores. According to the results of bromide leaching simulation, 54\% of the drainage was estimated to be transported via vertical macropores being initiated in the plow layer.

Keywords: Preferential flow, Macropore settings, Field-scale, Automated calibration, Morris screening.

1. Introduction

Preferential flow (PF) is a general term for non-uniform, non-equilibrium water flow processes, which can occur in low permeable drained clay tills given the presence of macropores/discontinuities/continuous voids such as earthworm, root channels, sand lenses, and fractures. Today, it is well-recognized that such macropores can provide the main transport pathways for leaching of agrochemicals and nutrients from the soil surface to drainage and groundwater. The occurrence of PF and the associated solute transport have been observed and demonstrated under several field and laboratory conditions [Akay and Fox, 2007; Gjettermann et al., 2004; Larsbo et al., 2009; Nielsen et al., 2010; Petersen et al., 2012; Rosenbom et al., 2009; Stamm et al., 2002; Tofteng et al., 2002]. Studies have documented that drainage is affected by the presence of macropores, especially earthworms [Akay et al., 2008b; Frey et al., 2016; Köhne et
al., 2006; Larsson and Jarvis, 1999; Petersen et al., 2012; Vogel et al., 2000] providing a direct hydraulic connection between the soil surface and the tile drain. This direct connection may result in rapid transport of nutrients [Cheng et al., 2014; Gärdenäs et al., 2006; Köhne et al., 2006; Larsbo et al., 2009; Larsson and Jarvis, 1999; Mohanty et al., 1998] and other contaminants from the surface into the tile drain system. Bypassing the soil matrix and its retarding capacity (sorption and degradation), the contaminants are transported via tile drains to nearby surface water bodies, such as lakes and rivers, with no or limited possibility of further reduction or retention along this path [Blann et al., 2009; Hansen et al., 2012a; Hinsby et al., 2012; Kronvang et al., 2005]. This direct connectivity phenomenon was verified by Akay and Fox [2007], who conducted infiltration experiments in soil columns with an artificial macropore placed directly above or shifted from the subsurface tile drain pipe. The setup of their experiment allowed the length of the artificial macropores to be varied without disturbing the soil column. The macropores were classified as either surface-connected or buried macropores. They observed that the water arrival time to the tile drain through surface-connected macropores was eight times faster and about two times faster for buried macropores than in a soil column with only matrix flow. At field scale, Petersen et al. [2012] showed a direct connection of macropores to the subsurface tile drains by injecting smoke to the tile drain pipes and counting the surface-emitting macropores on sandy loam. They analyzed two 35-m-long tile drain sections for the spatial distribution of emitting macropores while the water table dropped from about 0 cm to 20 to 50 cm below drain depth. From 65 and 96 emitting macropores were identified along the tile drain sections, separately.

Geologies incorporating such highways for flow and transport in the shape of macropores connecting the surface/plow layer with the deeper part of the soil can as described make them vulnerable in regard to rapid leaching of contaminants to drainage and groundwater. It is, therefore, imperative to be able to account for these highways when assessing the risk of leaching of contaminants through the variably-saturated drained clay till. As demonstrated by Germann [2018] this is not straightforward, since the hydromechanics of the macropores and the interaction with the lower-permeable soil matrix still pose a scientific challenge in terms of avoiding too crude a description thereof.

Nevertheless, within the last four decades, different numerical models have been developed, incorporating reality-simplified processes/concepts describing PF and coherent solute transport.
With the macropore setting being very complex and varying in space and time, the well-documented models like RZWQM2, MACRO, HYDRUS1D and DAISY [Hansen et al., 2012b; Larsbo and Jarvis, 2003; Ma et al., 2012; Šimůnek and van Genuchten, 2008] cope with the water flow and solute transport in one dimension using the Richards (1931) equation for capillary flow in the matrix domain and apply different approaches for the macropore domain. Hence, in these models, the soil pore space is divided into two domains: A low-permeable matrix domain with a relatively large storage capacity and a high-permeable macropore domain with a relatively low storage capacity.

The Root Zone Water Quality Model, RZWQM2 describes the macropore flow capacity using Poiseuille’s Law based on gravity flow in cylindrical pores. The water exchange between the domains is based on the radial or lateral Green-Ampt equation that accounts for the infiltration front in the matrix surrounding the cylindrical pores or cracks, respectively. Using pore-scale physical laws in RZWQM2 poses a disadvantage in that it assumes full saturation in macropores and simplifies the geometry of macropores, which are usually tortuous [Simunek et al., 2003]. The governing equation for the macropore domain of the dual-permeability model in MACRO [Larsbo and Jarvis, 2003] follows the kinematic wave approach described by Germann [1985], where the macropore flow is controlled by a kinematic exponent, which reflects the macropore size, distribution, tortuosity and ignores capillary flow. In MACRO, the mass transfer between domains in the absence of gravity is described by the Richards equation recast as a diffusion equation for a homogeneous medium, where the water content gradient is the driving force. In HYDRUS 1D [Šimůnek and van Genuchten, 2008] uses the approach of Gerke and van Genuchten [1996] who applied the Richards equation for both matrix and macropore domain. This dual permeability approach requires more, rarely available, specific knowledge about water retention and hydraulic conductivity functions for both matrix and macropore domains and their interface. The mass transfer between the two domains is similar to MACRO, using the first-order mass transfer coefficient and assuming it is proportional to the difference of the pressure head between the two domains. Also, HYDRUS 1D has incorporated different approaches to simulate the flow in the macropore domain, such as the mobile-immobile and dual porosity model, which requires fewer input data. DAISY has been modified by Mollerup [2010] based on the laboratory experiments of Tofteng et al. [2002] and Gjettermann et al. [2004] and the field experiment of Petersen et al. [2012]. Tofteng et al. [2002] showed with an artificial macropore attached to the bottom of a
sandbox that macropores were able to conduct water on pressure potentials as low as -30 cm, which indicates that macropore flow can alter from a typical retention/conductivity function. These findings are essential since tillage increases the porosity of the plow layer [Petersen et al. 1997], while macropore continuity may be reduced [Roseberg and McCoy, 1992], and a compacted layer – the plow pan, which often occurs at the transition zone between the plow layer and the subsoil – may cause accumulation of water and thus initiate macropore flow [Frey et al., 2012].

All of the models mentioned are simplifications of reality and as such, have pros and cons in regard to their description of the hydromechanics of the macropores and the interaction with the surrounding matrix and drainage. Additionally, they need to be able to account for plant cover and fate processes (mineralization-immobilization-turnover, sorption, degradation, effects of soil management, etc.) in an assessment of the leaching risk of agrochemicals.

The purpose of this study was to evaluate whether it is possible with the DAISY model to capture the water balance (climate, groundwater fluctuations, water content in the profile and in drainage) of a well-described agricultural clay till field that is tile-drained and prone to preferential transport [Ernstsen et al., 2015], during a 10-year period with/without macropores, and if so to estimate the degree of macropore flow and the associated transport of bromide to the drains during the period.

2. Materials and Methods

2.1 Field characteristics

In this study, data originated from a tile-drained agricultural clay till field included in the monitoring program PLAP (Pesticide Leaching Assessment Programme of Denmark) [Lindhardt et al., 2001]. The field is situated at Silstrup in the northwestern part of Denmark (56°55'56"N 8°38'44"E). The field was established in 1999 and has been used for agricultural purposes since 1942 and systematically drained since 1966. The field has been farmed from 1983 without any plot experiments conducted [Lindhardt et al., 2001]. The field and the surrounding area are dominated by Weichselian glacial clay till deposits in combination with thin meltwater sand lenses. The underlying geology comprises dislocated slices of clay till and meltwater sand/gravel forming "drains" down to the groundwater. The southern rim of the field contains dislocated clay and silt mixtures in the depth interval of 4-8 m. This material is underlying half of the field (Figure S1). According to the geological survey of the field, the top layer of this mixture is the most permeable
part of the whole field and seems to dominate the hydraulics of the field-setting [Abiltrup, 1999].

In general, the field is heavily fractured and contains high-density of macropores. In the upper 2 meters of soil, dominated by bioturbation and desiccation cracks, the macropore density was estimated to be 400 pores m\(^{-2}\) [Lindhardt et al., 2001] with diameters of 2-5 mm, using the methodology from Klint and Gravesen [1999].

The size of the field is 1.69 ha (185 × 91 m). Highest points of the field vary from 41 to 45 m above sea level (m.a.s.l.) (Figure S3). The groundwater head potentials (in m.a.s.l.) measured in February 2000 from several piezometers and monitoring wells surrounding the field (Figure S4) indicated that the groundwater tends to flow towards the southwest, which is opposite to the topographical slope of the field. This water movement gives the idea that the significant part of the field is hydraulically connected to the layer with the silty-clay Oligocene deposit, which can be considered as an aquifer, overlaid by a clay till [Freeze and Cherry, 1979] (Figure S1). The pedological profile investigation was carried out in the northeastern corner of the field where two profiles were excavated (N-North face, E-East face). The most common horizon subdivision was Ap-Bv-Bt(g) and Ap-BC-Cc, with an average depth of Ap (plow layer) and Bv/BC of 31 and 140 cm, respectively. The textural analysis showed a plow layer with 18-25% clay and more variable clay content in the underlying soil of up to 43% clay in the eastern profile. This clay content probably decreases towards the southern part of the field since Hansen [1976] found 15% and 24% clay in the topsoil and the underlying soil, respectively. The field was also mapped with a DUALEM21 ground conductivity meter (GCM). The processing and inversion of GCM data were done by Aarhus Workbench using the Aarhus Inv inversion code [Auken et al., 2015] (Figure S2).

The soil hydraulic measurements for soil water retention (SWR) and hydraulic conductivity were conducted on 100-cm\(^3\) and 6280-cm\(^3\) soil cores, respectively. The cores were sampled at three depths corresponding to the Ap-, B-, and C-horizon. The mean retention points showed that the water content gradually decreased with pF (logarithm of the soil water potential [\(\psi\), in cm H\(_2\)O times -1]) because of the relatively uniform pore size distribution, which is consistent with loamy-clay soil types (Table S1).

The SWR, saturated \((K_s)\) and unsaturated \((K(\psi))\) hydraulic conductivity were determined by the methods described in Iversen et al. [2004] and Iversen et al. [2011]. The unsaturated hydraulic conductivity showed high variability at -10 cm H\(_2\)O pressure potential and was significantly lower.
than the saturated conductivity. The variability in saturated hydraulic conductivity showed differences by two to three orders of magnitude, which indicates the presence of macropores (Figure S5).

2.2 Field-scale monitoring and field management

The tile drain system of the field consists of five parallel tile drains at approximately 110 cm depth 18 m apart, established in a south to north direction. They are connected with a transverse tile drain at the northern end of the field. Drainage flow in the drainage outlet well, and soil water content were measured hourly and automatically from 2000 to 2010. The drainage flow was calculated from a measured water level above the Thomson weir V-notch [Lindhardt et al., 2001] using a pressure transducer (Druck PDCR 1830, Druck Limited, UK) and soil water content was measured with horizontally installed 30-cm-long TDR (Time Domain Reflectometry) probes at various depths (0.25, 0.6, 0.9, 1.1, 1.9 and 2.1 m with three replicates per depth) in the variably-saturated zone, where the pedological profiling had been conducted [Lindhardt et al., 2001]. The measurements were obtained using probes made at Aarhus University and a Campbell CR10X data logger controlling a Tektronix 1502C cable tester (Tektronix Inc., Beaverton, OR, USA). The hourly measured water content (three replicates) were averaged to daily response data, due to the hourly measurements containing a significant amount of missing data due to instrument failure. Further, as the water content measurements were sampled in the northern corner of the field, these measurements may not represent the water flow dynamics and variability of the whole field and especially not the PF [Nimmo, 2012] as the 30 cm long probes integrate by far the size of a macropore, and water flow in bigger pores happens so fast that it may not be captured by hourly measurements. Germann [1985] reported velocities of the wetting shock fronts in the range of 0.3 to 1 mm/s. However, the hourly measured drainage flow was kept at its hourly time resolution as it integrates the whole field response to measured hourly rainfall data.

Hourly weather data has been recorded from 29 April 2000 to 31 December 2010. The weather data includes wind [ms⁻¹], global radiation [Wm⁻²], air temperature [°C] and vapor pressure [Pa] in order to calculate the evaporative demand using the Penman-Monteith Reference Evaporation equation [Allen et al., 1998]. The wind speed measurements at 10 m height were scaled to 2 m, assuming logarithmic wind profile and neutral atmosphere [Allen et al., 1998]. Hourly precipitation [mm] was sampled with a tipping bucket gauge (Lambrecht meteo GmbH,
Göttingen, Germany) at the upper northeastern end of the field (Figure S2). Water samples were collected flow-proportionately at the drainage outlet [Ernstsen et al., 2015] for in-lab determinations of bromide (Br\textsuperscript{−}) and nitrate (NO\textsubscript{3}) concentrations. The hydraulic response data also included daily groundwater table measurements in piezometers situated at the northern (P4) and southern (P3) end of the field (Figure S3). P4 was placed in clay till in the North, whereas P3 hit dislocated clay-silt layers (Figures S1 and S2). With the earlier mentioned difference in geology from South to North, a contrast of up to 1.5 meter in the groundwater level was measured during the summer period and, hence, slower drainage with a lower amount may have taken place in North compared to South. Unfortunately, this cannot be documented by monitoring data since only TDR has been deployed at the northern end of the field.

The annual precipitation varied from 686 mm to 1146 mm with an average of 838 mm for the above-considered time interval. Most of the precipitation records (96%) were obtained from the field, but where the gauge malfunctioned (4% of the records) precipitation was obtained from the nearby meteorological station. The precipitation was obtained at open field conditions 1.5 m above the soil surface and was corrected to true ground based on factors provided by Allerup and Madsen [1979]. This correction was conducted in order to overcome induced errors, mainly due to wind turbulence, which causes the 1.5 m precipitation to be underestimated.

In the course of the data period of 2000-2010, five different types of crops were grown: fodder beet (2000, 2008), spring barley (2001, 2005, 2009), pea (2002), maize (2003), winter wheat (2004, 2007) and winter rape (2006). All crops were harvested and analyzed for dry matter yield and nitrogen content, and the phenological development stages of the plants were recorded. To identify the possible solute transport routes, 30 kg ha\textsuperscript{-1} Potassium Bromide (KBr) was sprayed on 22 May 2000.

2.3 The DAISY model

DAISY is a soil-plant-atmosphere system model incorporating modules describing plant water uptake, plant growth, C-N turnover, and water, heat, and nitrogen dynamics in the soil [Hansen, 2002]. Each of these processes is incorporated into modules that are interconnected with each other. In this study, the main focus will be on the soil water module [Hansen, 2002; Hansen et al., 1990; Hansen et al., 2012b; Mollerup, 2010].
DAISY uses the Richards equation \cite{Richards, 1931} to solve the one-dimensional water flow in a variably-saturated subsurface porous medium. In DAISY, the Richards equation includes the closed form of the van Genuchten SWR model \cite{Van Genuchten, 1980}, which is coupled with the Mualem hydraulic conductivity theory \cite{Mualem, 1976} applied to the matrix domain. In terms of soil solute balance, the model applies the convection-dispersion equation with the ongoing transformation processes and uptake by plants.

For the modeling of PF, DAISY assumes two flow regimes: a matrix flow regime where the convection-dispersion equation for solutes is applied, and a macropore regime where only convection is considered. The mass exchange between the two regimes is governed by the water flow through the sink-source strength of the two domains and the model does not consider storage of solutes in the macropores; hence the macropores are only considered as a fast pathway for transport of solutes \cite{Hansen, 2002}. The fast flow domain in DAISY is described by a macropore module described by Mollerup \cite{Mollerup, 2010} (web address: \url{https://daisy.ku.dk/publications}) and tested in a technical reports, prepared for and published by the Danish Environmental Protection Agency \cite{Hansen et al., 2010a; Hansen et al., 2010b; Hansen et al., 2012c}.

Here a macropore is a vertically oriented feature characterized by physical properties such as length, diameter, and density. The macropores are divided into two classes specified by their lower boundary. One class of the macropores ends in the soil matrix, while the other class can be set to end directly in the tile drain. When water is transferred from the matrix to the macroporous domain ending in the matrix, the water is instantaneously moved to the top of the current water level in the macropores. If the pressure difference between the macropore and the matrix exceeds a predefined soil water pressure barrier potential ($\psi_{\text{barrier}}$) water will be transferred back to the matrix from the macropore. For the macropores ending in the tile drain, the lower boundary condition has a constant pressure head of zero, meaning that water will be transferred directly into drainage without building up in the macropores.

The macropore flow is initiated when the matrix potential exceeds a specific pressure potential called $\psi_{\text{init}}$. Hence, if this pressure potential is exceeded, the macropore domain is activated, and water starts to fill up the macropore. When the pressure potential drops below a level called $\psi_{\text{term}}$, inflow to the macropore is terminated. All pressure threshold parameters apply to all macropore classes. The macropore domain concept consists of an equidistant distribution of macropores
where the water flow in the domain is quantified by soil water extraction from the matrix, which is based on the water movement in a confined aquifer, towards a well where the well is represented by a single macropore. The interaction between macropores and surface water follows Poiseuille's Law [Hillel, 1998] the same way as in the RZWQM2 model [Ma et al., 2012]. The only driver of the water flow is gravity. The macropore model does express viscous flow, as Germann [2018] suggested since the water flow is lumped to an instantaneous transport within a macropore. Due to the velocities of wetting shock fronts, which is the range of 0.3 to 1 mm s⁻¹, the model could not represent the hydro-mechanical aspects of a turbulent flow, since the basic time step is one hour.

When the hydrologic setup includes a subsurface tile drain at a certain depth, drainage from the soil matrix domain will only be initiated when the groundwater level rises above this depth. This inflow to the tile drain assumed installed in a flat landscape, is described by the Hooghoudt equation [Hooghoudt, 1940].

2.4 Model concepts

The soil profile in the one-dimensional DAISY model was described based on the pedological survey of the Silstrup field with three different horizons:

- A-horizon – Plow layer to a depth of 31 cm
- B-horizon – Layer from 31 cm to 140 cm depth
- C-horizon – Layer from 140 cm to 500 cm depth

The discretization of the profile was into 1-cm layers to 50 cm depth, 5 cm to 110 cm depth, and 10-cm intervals to 500 cm depth including additional steps at the upper and lower boundaries of the horizons. The tile drain was set at a depth of 110 cm and 18 m apart according to the field characteristics described above. The C-horizon was extended to 500 cm in order to account for the fluctuating groundwater table. To avoid having an unrealistic impermeable layer as a lower boundary condition as the Hooghoudt equation requires, a Dirichlet boundary condition defined by the measured groundwater level was applied to the Hooghoudt equation [Fetter, 2000].

The van Genuchten-Mualem (vGM) retention conductivity model was used to describe the water retention and conductivity in all three layers for the matrix domain. The retention parameters ($\theta_s$, $\theta_r$, $l$, $n$, and $\alpha$) of this model and saturated hydraulic conductivity $K_s$ [$LT^{-1}$] were estimated
by fitting the vGM model to the laboratory-measured water retention. The uncertainty boundaries were established by fitting all retention and conductivity data from the corresponding samples of the horizons and combining to create a retention and conductivity range. (Table 1 and Figures 3, 4). The unsaturated hydraulic conductivity was fitted to the measured $K(\psi)$ available from different soil cores (Table 1, Figure 4) for each horizon. The outcome of the fitting gave saturated hydraulic conductivities that were one to two orders of magnitude lower than conductivities measured directly on the undisturbed soil cores (Table S2). The initial SWR and hydraulic conductivity parameters were obtained from the best fit of the combined vGM models (Figures 3, 4). In Table 1, the columns Min and Max show the range of the uncertainty boundaries of the parameters assessed from the fitted results.

To incorporate PF, well-connected macropores need to be included in the model. Using the macropore module of DAISY, up to six conceptual types of macropores (DM1, DM2, MM1, MM2, MM3, FR) can be included. To represent the macropore structures in the field, three different macropore settings have been included in the model (Figure 1, Table 2). The division into the different settings was based on a field study of Nielsen et al. [2010] conducted on a similar macroporous, sandy-clay loam soil. Because the macropore distribution in a given field is unknown and difficult to describe by soil textural parameters [Lamandé et al., 2011], the following conceptual considerations have been applied.

Matrix macropore 1 (MM1) represents all small macropores created by bioturbation or agricultural processes after plowing. This kind of macropore always ends at the bottom of the plow layer. MM2 and MM3 represent the wide (up to 5 mm in diameter) and long macropores created by large earthworms or old root channels. They are present below the depth of the tile drain, facilitating in most periods of the year a direct connection to the groundwater table. The difference between MM2 and MM3 is the starting depth. MM2 starts at the soil surface, whereas MM3 starts at the bottom of the plow layer. This difference defines a surface-connected macropore as MM2, and a buried macropore as MM3, consistent with Akay and Fox [2007] and Rosenbom et al. [2009]. Matrix macropores are able to increase the fast storage capacity in a clay till which can slow down the breakthrough of the solute transport. The macropores ending in the tile drain (DM1, DM2) are numbered according to the starting depth. The field description [Lindhardt et al., 2001] indicates that the field is heavily fractured, which is the reason for including a long macropore passing
through the system to represent a well-connected fracture system of a field in a one-dimensional model (Figure 1, Table 2).

Figure 1. The three macropore settings applied in the clay till profile. The depth [cm] is given as height above soil surface: a) Only macropores ending in the tile drain (DM), b) same as a) but including macropores ending in the matrix (MM), and c) same as b) but including macropores representing a fracture (FR) penetrating the entire soil profile (horizons A-C) and a highly permeable matrix horizon D.

The concepts represent a clay till profile with: a) only drain-connected macropores (DM), b) macropores ending up in the drain (DM) and the matrix (MM), and c) DM and MM macropores where an MM-type is present through the entire soil column, representing a fracture (FR). With the matrix-macropore-concept applied in DAISY, water cannot percolate out of the bottom of the MM macropore but only through its sides, while water can build up inside the macropore if the
surrounding matrix has sufficiently low permeability. Given this model constraint, a thin, permeable sand layer (even though not present) needed to be added at the bottom of the model profile to facilitate constant drainage of the FR macropore. The soil texture properties of this sand layer “D–horizon” (Figure 1) was taken from the soil database at the Department of Agroecology “Jordprofil databases” [Madsen et al., 1992], and the vGM parameters were generated by HYPRES [Wösten et al., 1999].

The initial macropore parameters (Table 2) were extracted from the field study of Nielsen et al. [2010], where they counted the stained macropores along a drain trench after a tracer experiment. MM1 density $\rho_{MM1}$ was set to 100 m$^{-2}$ to represent the large amount of bioturbation. The remaining macropore properties were set arbitrarily since they were considered to be applied in the model calibration process. The initial fracture diameter and distribution ($d_{FR}$ and $\rho_{MM1}$) were taken from Rosenbom et al. [2009] and Lindhardt et al. [2001], respectively.

To apply realistic boundary conditions for the model, hourly precipitation, evapotranspiration, and crop developments were used as the upper boundary condition and the depth to groundwater table was used as a lower boundary condition. The latter was monitored on a daily basis. Given the large difference in groundwater table level monitored in piezometer P4 in the northern part of the field and P3 in the southern part (Figure S1) during the summer, the flow through the profile exposed to both conditions was evaluated for all three macropore settings a), b), and c):

i. M.settings a) + P3
ii. M.settings a) + P4
iii. M.settings b) + P3
iv. M.settings b) + P4
v. M.settings c) + P3
vi. M.settings c) + P4

In such a clay till it is imperative to account for the fluctuating groundwater table and coherent drainage to be able to account for the water balance in the system over time addressing the field including the degree of macropore flow. This study should be seen as a “learning” study, which can help to delineate the degree of preferential flow and transport through fields where one can only have knowledge about the fluctuations of the groundwater table and knowledge about the presence of tile drains.
2.6 Model performance and objective function

In order to calibrate the six model concepts towards the desired performance by fitting monitoring data, an automatic calibration procedure was set up. Efficiency criteria were defined as mathematical measures to evaluate model performance, e.g., how well a given model fits the available observations [Krause et al., 2005]. Several studies have discussed which efficiency criteria to use in a hydrological modeling context [Krause et al., 2005; Muleta, 2011; Singh et al., 2016; Willems, 2009]. According to Krause et al. [2005], most of the efficiency measures that use the squared deviation tend to be sensitive to peak flows, which is an inherent characteristic in tile-drained soils. In this study, the Normalized Mean Absolute Error (nMAE) was used to avoid giving extra weight to peak drainage. This performance measure was chosen with reference to Muleta [2011], who tested efficiency measures based on the minimization of the squared, absolute, and log of the error terms.

For proper automated calibration, several different objectives might need to be considered in order to not push errors into an unexamined domain of the model. The objective function for the calibration procedure in the present study synthetizes four different sub-objectives. Primarily the hourly drainage and cumulative drainage observations were taken into account in order to take control of the dynamical behavior of the model and the water quantity leaving the clay till profile. To further constrain the model and to have a better representation of the soil water dynamics, the daily soil water content represented by TDR measurements at 25 cm (SWC25) and 60 cm depth (SWC60) were added to the objective function as two sub-objectives. Since the model was constrained to different objectives with different units, the four MAEs represented in Eq. (1) were normalized by the mean of the corresponding observations in order to aggregate them into one objective function, to be used for automated calibration.

\[
nMAE_{\text{year}}^{\text{obj}} = \frac{1}{N} \sum_{i=1}^{N} \frac{|\text{sim}_{\text{year},i}^{\text{obj}} - \text{obs}_{\text{year},i}^{\text{obj}}|}{\text{obs}_{\text{year}}^{\text{obj}}} \tag{1}
\]

where \(N\) is the number of observations of a given objective within a year and
\[
\bar{obs}_{year} = \frac{1}{N} \sum_{i=1}^{N} obs_{year,i}
\]  

(2)

\[
\bar{nMAE}^{obj} = \frac{1}{K} \sum_{k=1}^{K} nMAE_{year,k}
\]  

(3)

where \(K\) is the number of calibration years.

Given the substantial differences between years, the nMAE was calculated for each objective on a yearly basis. The mean of the yearly nMAEs was used as a measure of the performance of the model during the years included in the calibration period. Thus, the final multi-objective function was expressed as:

\[
nMAE^{Final} = nMAE^{Drainage} + nMAE^{Cum.Drainage} + nMAE^{SWC25} + nMAE^{SWC60}
\]  

(4)

For the evaluation of the model concepts, nMAE (range \([0, +\infty]\)) was used primarily as it is the inverse version of Volumetric Efficiency (VE) proposed by Criss and Winston [2008]. Besides nMAE, also standard evaluation measures, nRMSE (Normalized Root Mean Squared Error) with the normalization of the maximum deviation of the inspected period (range \([0, +\infty]\)) and KGE (Kling – Gupta Efficiency) (range \([-\infty,1]\)) [Gupta et al., 2009] are presented. According to Singh et al. [2005] and Moriasi [2007], nRMSE and nMAE values, less than half the standard deviation of the measured data may be considered low and that either is appropriate for model evaluation. In terms of KGE, a model results higher than 0.5 is considered satisfactory. These values further called threshold.

2.7 Sensitivity analysis and calibration procedure

A calibration year was defined as a period from 1 April until the following 31 March, in order to cover one drainage and average crop growing period. The selected calibration period was from 1 April 2003 to 31 March 2008. This period was chosen to cover a broad range of yearly precipitation characteristics with marked differences in total amount and seasonal distribution.

The Morris sensitivity screening method [Campolongo et al., 2007; Morris, 1991] was applied to the model parameters that were believed to have an impact on the multi-objective function. The
sensitivity screening was done based on the different sub-objectives. Each parameter was screened against each sub-objective separately and selected as sensitive based on either one, two, three, or all four sub-objectives. The non-sensitive parameters were set to their nominal values. The sensitive parameters were calibrated by the DEoptim algorithm.

The Differential Evolution Optimization (DEoptim) [Storn and Price, 1997] was used to calibrate the model. DEoptim is a global optimization genetic algorithm, which uses biology-inspired operations of crossover, mutation, and selection on a population in order to minimize an objective function over the course of successive generations. For the search of the global optimum, the multi-objective function was used.

The sensitivity analysis and the calibration were carried out with the R statistical programming language [R Core Team, 2017]. The RDAISY toolbox [Jabloun et al., 2014], with the combination of the “sensitivity” package [Pujol et al., 2017] and “DEoptim” R packages [Mullen et al., 2009] was used to perform the sensitivity screening and the model calibration.

3. Results and discussion

3.1 Simple calibration of the DAISY crop parameters

The dynamics of soil water content and the matrix-macropore interface depend not only directly on soil physics, but also on evaporation and plant water use. The actual evapotranspiration was determined by the reference evaporation, the crop coefficient for the corresponding vegetation and water transport capability of the given crop root system. Therefore, the crop module of DAISY was calibrated to the measured phenological development stages and harvested dry matter yield (Figure S9). According to Plauborg et al. [2010], by matching the simulated dry matter yields with the measured ones, the simulated evapotranspiration may be at the right level for Danish conditions as the standard crop parameters included in the DAISY crop database are assessed from experiments in a temperate climate and based on the strong relation between accumulated transpiration and biomass production [Hsiao et al., 2007; Steduto et al., 2007; Steduto et al., 2009]. However, a check of the most essential parameters for transpiration such as crop development was carried out as these parameters may show differences between genotypes within species. Further details on crop calibration can be found in Hansen et al. [1990], [2002] and [2012b].
3.1 Impact of macropores on model performance

The performance of the model applying the groundwater table measurements from P3 before (single permeability model) and after the introduction of macropores (the dual-permeability model, macropore setting b)) without calibration of parameters was tested. The two model setups yielded 1.09 and 1.37 nMAE, respectively, for the drainage sub-objective when tested for the drainage year 2006-2007. Even though the single permeability model “mathematically” performed better than the dual-permeability model, it was not capable of capturing the rapid drainage dynamics (Figure 2). This is in agreement with the findings of Akay et al. [2008a].

![Figure 2](image)

**Figure 2.** Performance of the single (S) and dual (D) permeability model setups in describing measured drainage during the period 1 September 2006 to 31 March 2007. Values in brackets are for the entire calibration period 1 April 2003 to 31 March 2008.

The non-calibrated dual-permeability model concept b) + P3 was parameterized with the initial parameter values described in Tables 1 and 2. The model was able to depict the drainage dynamics, but the proportion of water leaving the clay till profile via drainage was almost twice that of the measured (Figure 2).

3.2 Sensitivity analysis of the six model concepts

For the model setup of concepts a), b) and c), 26, 32, and 35 parameters, respectively, were identified as probable sensitive parameters (Table 1 and 2). The difference in the number of parameters was due to the macropore parameters specified for each macropore setting. Besides the macropore parameters of the concepts, all parameters related to the SWR and hydraulic
conductivity were kept for horizons A, B and C as well as the thickness of the A- and B-horizons. The latter two were included based on the variation in horizon thickness from the pedological profile description. In addition, Table 1 presents the uncertainty boundaries (columns Min and Max), which were used in the sensitivity analysis. For the A-horizon, the uncertainty range was extended for the vGM parameters, after the inspection of the SWR range from PLAP [Iversen et al., 2004; Lindhardt et al., 2001]. Data for the A-horizon shows a very high air-entry pressure (Figure 3), which could indicate a prolonged infiltration rate. By inspecting the resistivity map of the field, the corner where the sample was taken has the highest clay content of the whole field (Figure S2). The macropore parameter ranges were based on the macropore studies of [Nielsen et al., 2010; Rosenbom et al., 2009].

According to the Morris sampling strategy, 270 to 360 parameter sets were obtained depending on the concept. As previously mentioned, in order to identify the important parameters, the sub-objectives (Drainage, Cumulative Drainage, SWC25, and SWC60) were separately screened. The results of the sensitivity screening were turned into the Morris distance ($\epsilon$) [Ciric et al., 2012; Jabloun, 2015], which represents the Euclidean distance of the parameter from (0,0) on the $\mu^* - \sigma$ coordinate system [Campolongo et al., 2007]. Thus, all the sensitive parameters that have an impact on either one or more sub-objectives were considered for the calibration procedure. The sensitivity criteria for Drainage, Cumulative Drainage, SWC25, and SWC60 were set to $\epsilon \leq 0.2, 0.2, 0.1, \text{ and } 0.1$, respectively. The criteria were set arbitrarily by observing the sensitivity screening outputs (Table 1, Figure S6-S8).

The sensitivity screening gave values of 14/16, 13/15, and 19/19 for model concepts a), b) and c) with lower boundary P3/P4, respectively. All non-sensitive parameters were excluded from the calibrations.

**Table 1.** Optimization of hydraulic parameters of the matrix for macropore settings a), b) and c). Initial values and selected minimum and maximum uncertainty boundaries are based on laboratory measurements (Table S1). Best calibration for macropore setting b) shows the result from the best calibration being restricted by the two different fluctuating groundwater tables monitored in wells P3 or P4. The macropore setting shows the settings for which a given matrix parameter is active. Sensitivity lists the macropore settings for which a given parameter is sensitive given the lower boundaries P3 and P4. Gray rows are the non-sensitive parameters.
The sensitivity screening showed that for the concepts the A- and B-horizon water retention and hydraulic conductivity parameters dominated (Table 1, Figure S6-S8). This was anticipated due to their strong influence on the sub-objectives (SWC25 and SWC60). In the macropore domains, the pressure parameters were also found to be sensitive in all concepts, with the exception of $\psi_{\text{barrer}}$ in model concept $b)$ - P3 (Table 2). The most interesting result of the sensitivity screening of all the model concepts was that the MM dead-end macropores had almost zero influence on the flow through the profile. This is probably because the MM macropore is filled up with water quickly without being able to release water through the low permeable surrounding matrix at the bottom of the macropore. The MM macropores contribute very little thereafter to the rest of the hydraulic environment. Neither did the diameter of the macropores show any effect on any of the objectives,
which is consistent with the study of R. Ahuja et al. [1993], who stated that to determine the maximum flow rate, one only needs to adopt a relevant pore size, instead of identifying the distribution of the macropore sizes in a given field.

Table 2. Optimization of hydraulic parameters of the macropores for macropore settings a), b) and c). Initial values and selected minimum and maximum uncertainty boundaries are mostly based on Nielsen et al. [2010] (Table S2). Best calibration for macropore setting b) is restricted by the two different fluctuating groundwater tables monitored in wells P3 or P4. Macropore setting shows the settings for which a given macropore parameter is active. Sensitivity lists the macropore settings for which a given parameter is sensitive given the lower boundaries P3 and P4. Gray rows are the non-sensitive parameters.
3.3 Calibration of the water balance of the six model concepts

In over ~30000 model runs the multi-objective function (nMAE) was minimized to 0.75-0.85 for all six model concepts using data from the period 1 April 2003 to 31 March 2008. The calibrated sub-objectives are shown in Table 3.

The outcomes of the calibration of macropore settings a), b), and c) did not differ significantly from each other, although, according to KGE settings, a) performed significantly better than the other concepts (Table 3). The more complex macropore setting c) (incorporating a fracture together with the D layer) underperformed (nMAE=0.81-0.85) compared to setting a) (nMAE=0.79/0.81) and b) (nMAE=0.75/0.79). This may be because the fracture concept cannot be incorporated in DAISY; not being in direct contact with the tile drain has no significant impact on the drainage. The different lower boundary condition (P3 and P4) had little influence on the calibration outcome, but the performance measures disagreed on which of them had the greatest impact on the modeled field. If nMAE is taken into account, P3 outperforms P4 in all model concepts; for KGE and nRMSE, the exact opposite is true. According to the threshold, the multi-objective resulted in satisfactory results in all model according to nMAE and KGE, but non-satisfactory by nRMSE.
Table 3. The calibrated performance measures nMAE, nRMSE and KGE of the sub-objectives (Drainage, Cumulative Drainage (Cum. Drainage), SWC25, and SWC60) for the three different macropore settings \((a), \(b),\) and \(c)\) in combination with the two lower boundary conditions \((P3\) and \(P4)\) for the calibration period 1 April 2003 to 31 March 2008. Coloring range from worst to best concept(red to green) per objective, bold values indicate objectives which are better than the threshold \((nMAE, nRMSE - SD_{obs}/2, KGE - 0.5)\).

<table>
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<th>b) + P3</th>
<th>c) + P3</th>
<th>a) + P4</th>
<th>b) + P4</th>
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</tbody>
</table>

3.3.1 Soil water retention and hydraulic conductivity.

The calibrated hydraulic parameters for the A horizon differed in all concepts compared with the initial SWR range from PLAP (Figure 3). The calibrated models showed a more realistic representation of sandy clay loam, while the SWR range from PLAP showed a very high air entry pressure, which is more characteristic for clay soil. The constant water content at the wet end was reduced to higher water pressure from -50 to around -4 cm, reflecting conceptually that air entry pressures in all concepts were increased, thereby increasing the potential for infiltration and redistribution within the plow layer. The SWR of the B- and C-horizons remained within the observed ranges.
In order to validate the calibrated SWRs of the A-horizon, the observed SWR ranges from previous studies conducted on this field [Katuwal et al., 2015; Naveed et al., 2016; Norgaard et al., 2015], where 65 soil samples were taken from the whole field in a 60 x 165 m grid, are superimposed in Figure 3 (orange band) over the data from PLAP and the calibration. As Figure 3 shows, all calibrated SWRs mimic the shape of the SWR range of the studies. Thus, it can be concluded that the calibrated SWRs of the A-horizon are representative of the field.

![Figure 3. Laboratory measurement ranges of SWR (black error bar) of A-, B- and C-horizons from the East and North pedological faces (Figure S5, Table S1-S2.) from PLAP; the SWR uncertainty boundary based on the fitted laboratory data (gray ribbon); calibrated concepts’ SWR for all horizons; assessed SWR measurement ranges (brown error bar) and uncertainty boundary (orange)](image-url)

- 55 -
ribbon) (Literature) only for the A-horizon from Katuwal et al. [2015], Naveed et al. [2016] and Norgaard et al. [2015].

The calibrated hydraulic conductivities were all within the observed ranges (Figure 4), although the C-horizon conductivity was at the higher end of the observed range. For the applied two different lower boundary conditions (P3, P4), the models showed no significant difference between the calibrated concepts in SWRs and the measured unsaturated hydraulic conductivity.

3.3.2 Soil water content at 25 and 60 cm

The SWC measurements at 25 cm depth were well described by the six models (Figures S10 and S11, upper graph). The model concepts captured the groundwater fluctuations and plant water uptake in the growing season, which is causing drying in the A-horizon, and the models reacted to the sudden saturation from the surface due to precipitation. There are discrepancies compared to the measured values due to the expected heterogeneity of the drained field not taken into account by the TDR point measurements. The ability to describe the SWC measurements at 60 cm depth was not as good as for the upper depth, due to the measured soil water content at 60 cm depth not responding to plant water uptake and the groundwater changes like at 25 cm depth, especially in the growing season 2003. Hence, the estimated soil water content at 60 cm depth did not capture the relatively stable and close to saturation content observed during 2003, whereas it did capture the dynamic and level of the water content in 2004 (Figures S10 and S11, middle graph). The discrepancy between measured and estimated soil water content in 2003 could be explained by the low rooting depth at this locality in the field where TDR was permanently installed, given that all the model concepts predicted the soil water content well at 25 cm depth during both 2003 and 2004 and at 60 cm depth during 2004.
Figure 4. Laboratory measurement ranges of $K(\psi)$ (black point) of A-, B- and C-horizons from the East and North pedological faces (Figure S5, Tables S1, S2,) from PLAP; $K(\psi)$ uncertainty boundary based on the fitted laboratory data (gray ribbon); calibrated concepts’ $K(\psi)$ for all horizons; assessed $K(\psi)$ measurements (brown points) and uncertainty boundary (orange ribbon) (Literature) for only the A-horizon from Katuwal et al. [2015], Naveed et al. [2016] and Norgaard et al. [2015].

3.3.3 Calibrated drainage dynamics of the six model concepts

In the drainage year 2006-2007 (part of the calibration period), the dynamics of the drainage were captured completely when applying the three macropore settings (Figure 5), although they did not capture timing and some of the amplitude of the measured drainage in March 2007. In this period, the temperature was around or below zero degrees, which could indicate that the precipitation fell
as snow, which is not well captured by the rain gauge at 1.5 m above the soil surface. Some measurements in this period were taken from the nearby experimental station (Geonor, rain gauge, weighing principle) and hence not fully representative of the field. The measured peak in drainage could be caused by snowmelt due to an increase in air temperature. The discrepancy between the estimated and measured could thus be explained by the numerical interpretation of the precipitation by the sub-model for snow accumulation and melt incorporated in DAISY. In this sub-model, low temperatures determine the amount of snow-rain mixture and the possible snowmelt is determined by global radiation, air temperature and heat flux on the ground surface [Hansen et al., 1990]. The timing of the fast increase in estimated drainage (due to snowmelt) was, therefore, delayed around a week in the simulated results, which may be explained partly by the too low precipitation input to the model.

![Figure 5. Performance of the six model concepts (including three macropore settings a), b) and c) using the groundwater table from P3 and P4) to describe measured drainage during the period 1 September 2006 to 31 March 2007. nMAE, nRMSE and KGE of the six concepts are given for the presented period and in brackets for the whole calibration period of drainage from 1 April 2003 to 31 March 2008.](image-url)
The other significant disagreement between the model results and the measurements was in mid-December 2006, most likely caused by measurement errors, where measurements indicate zero flux in the drainage, while in this month the model predicted one of the highest fluxes (Figure 5). In general, however, all six concepts performed well. The best calibration result was achieved with model concept \( b) + P3 \), where nMAE was 0.53 for the calibration period for drainage. The comparison of the outcome of applying the two different groundwater tables revealed that all P3 concepts outperformed those using P4 as the lower boundary condition in terms of nMAE. It was also clear that P3 setups performed much better during the single sudden flow events such as in October 2006 where the groundwater seems to supply less drainage from the field than with P4 setups. The dynamics of the drainage including zero fluxes were perfectly captured applying P3, whereas with P4 the simulated fluxes tended to be high during the period with measured zero flux, probably because the groundwater kept supplying water to the drains. It is also worth pointing out that P4 setups performed better for nRMSE and KGE than for nMAE, even though there are visible discrepancies between the observed and modeled flow. This is a clear example of what Muleta [2011] concluded, that using squared deviations tends to overestimate the goodness of fit because peak flows will be given excessive weight.

3.4 Evaluation of model performance

3.4.1 Drainage and Soil water content dynamics

The evaluation periods chosen were 1 May 2000 to 31 March 2001 and 1 April 2008 to 31 March 2009. The latter period was chosen because the drainage events were more frequent in this year, with drainage occurring on 224 days, whereas in the following year there were only 115 days of drainage. Both selected periods included continuous drainage over the winter period with distinct peak flows, but also included sudden cloudburst-induced drainage in the dry periods. Similar to the calibration, all model concepts performed well in terms of predicting the dynamics of the drainage (Figure 6). The results show that the model concept, including macropore setting \( b) \) performed better than settings \( (a) \) and \( c) \). Due to the importance of the DM and MM macropores for water transport, the pressure parameters were left close to saturation in order to initiate imbibition, in accordance with Tofteeng et al. [2002]. In the evaluation period of 2008 the \( b) \) setting seemed to perform the best with nMAE_{2008} values for the P3 and P4 lower boundary conditions of 0.5 and 0.55, respectively. In the evaluation period of 2000, setting \( a) \) performed the best for P3,
with $n\text{MAE}_{2000} = 0.39$, and setting $b)$ performed the best for P4, with $n\text{MAE}_{2000} = 0.37$. In the 2000-2001 period, setting $b)$ performed marginally worse than the other settings for P3, although the amplitude of the measured drainage matched the $b)$ setting better in the winter season. When comparing the lower boundaries, P4 captured the winter period better with setting $b)$ in the year 2000 than P3, although the individual sudden drainage events were underpredicted in contrast to concept $b) + P3$. Additionally, the same identified groundwater induced drainage surplus appeared here as well with P4, at times when the measurements showed zero flux. Overall, applying the P3 groundwater condition tended to give a better description of the dynamics of the drainage. The reason could be that P3 is installed in a dislocated clay and silt layer that is hydraulically more well-connected to the groundwater aquifer than P4, which is placed in a clay till.
Figure 6. Performance of the six model concepts (macropore settings a), b) and c) applying the groundwater table from P3 and P4) to describe measured drainage during the evaluation period 2000-2001 and 2008-2009. The nMAE, nRMSE and KGE of the six concepts are given for the presented period, and in brackets the nMAE for the whole calibration period of drainage from 1 April 2003 to 31 March 2008.
Figure 7. Measured and simulated drainage and SWC dynamic response to the heavy rain event on 8 June 2003.

For situations with fast drainage response to heavy rain, a distinct heavy rain event was screened for model response in SWC at 25 cm depth and drain flow on 8 June 2003 (Figure 7). All macropore settings and lower boundary setups were able to depict the sudden increase in water content, as well the immediate water transport to the drain. For the lower boundary, P3 model concepts were able to simulate the dynamics better. This drainage response is more dependent on the accumulated water above the B-horizon rather than direct transport from the surface. These findings are consistent with the observation of Rosenbom et al. [2008] and Nimmo [2012] that water/solutes can be preferentially transported even though the matrix is only partially saturated below the plow layer during the summer season. Therefore it can be concluded that the DAISY model with Richards’ equation combined with Mollerup’s approach [Mollerup, 2010] of PF is capable of describing PF in unsaturated conditions. Although the model does not account for viscous flow, still as a Darcy-based model, it may indeed represent preferential flow to the drainage over the assessed 10 year period. [Germann, 2018]
3.4.2 Transport pathways

The water balance and distribution of different flows and transport pathways to the drain system as a result of the conceptual descriptions of the field were evaluated for the drainage year 2008 – 2009. As a percentage of the annual precipitation, the concepts did not differ significantly from each other (Table 4), although the transport to the drainage with P3 showed higher matrix and macropore water transport to the drain.

**Table 4.** Accumulated water contribution to drainage from matrix and macropores (DM1, DM2 and the sum of the two) and percolation through the matrix and macropore at 1.1 m depth (depth of drain) in mm and as a percentage of the annual precipitation (997 mm) for the period 2008-2009 for all six model concepts (settings a), b) and c) applying groundwater tables from P3 and P4).

<table>
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<tr>
<th>Concept</th>
<th>Matrix contribution to drainage</th>
<th>Macropore contribution to drainage</th>
<th>Matrix percolation</th>
<th>Macropore percolation</th>
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<tr>
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The optimal fit to the field measurements was achieved by model concept b) + P3 (Figure 8) estimating a high macropore contribution to drainage (113 mm, 70% of total drainage). In contrast to a) + P3, the matrix contribution to drainage was somewhat higher, although the macropore input remained of the same magnitude (Table 4). Since macropore setting a) does not consider MM macropores, only leaching through the matrix can bypass the tile drain and enter the groundwater. The amount of percolation to the groundwater was similar for all macropores (34-36% of the
annual precipitation). This indicates that even though settings b) and c) include the MM and FR macropores as extra transport pathways, no more water percolation to the groundwater (sum of matrix and macropore percolation) appeared. Hence, the simulated degree of contribution from the macropores and matrix to drainage appeared to be a good indication of reality. For setting c) the distribution followed a) and b) when applying P3 and it had a relatively similar outcome to setting b). The implemented fracture gave no input to macropore percolation. The simulated results with concept c) + P4 did not follow the other results.
Figure 8. Simulated accumulated drainage input from the matrix and macropore domains, accumulated matrix and macropore percolation, and measured drainage with the corresponding nMAE, nRMSE and KGE for 2008-2009 drainage at 1.1 m drain level for all six concepts.

3.4.3 Bromide transport

Another essential point of the model evaluation was to compare Br\textsuperscript{−} transport of the application 22 May 2000 (Figure 9). After the application of 30 kg KBr ha\textsuperscript{−1} which is the equivalent of 20.14 kg Br\textsuperscript{−} ha\textsuperscript{−1}, Fodder beet and Spring Barley were sown in 2000 and 2001, respectively. This showed even though Br\textsuperscript{−} is considered a conservative tracer by hydrologists with limited interactions with the soil microbiome and crop, Br\textsuperscript{−} has been proven to be taken up by crops to a substantial degree [Shtangeeva, 2017]. In this modeling case, with P3 as the lower boundary condition, 61%, 57% and 52% of the applied amount was taken up by the sown fodder beet in macropore setting a), b) and c), respectively, whereas the corresponding uptake for P4 was 59%, 60%, and 54%. This amount of Br\textsuperscript{−} uptake was not unprecedented in beet crops, as Kohler et al. [2005] found 50% of initially applied Br\textsuperscript{−} in harvested sugar beet. However, it has to be mentioned that in the present study no crop calibration has been done towards Br\textsuperscript{−} uptake.
Figure 9. Simulated accumulated Br$^-$ transport to drainage from matrix and macropore domain and measured Br$^-$ transport in the drain flow with the corresponding nMAE (threshold$_{BR} = 2.14$, threshold$_{BRC} = 0.27$), nRMSE (threshold$_{BR} = 1.9$, threshold$_{BRC} = 15.3$) and KGE (threshold = 0.5) for 2000-2001 for all the six model setups (BR = Br$^-$ dynamics, BRC = Cumulative Br$^-$ transport).

Two heavy rain events occurred around the day of the application of Br$^-$, the first event causing little drain flow, but the second almost instantly initiating drain flow. The instantaneous occurrence of Br$^-$ in the drainage at a 5.1 mg/L concentration reflects the presence of macropore flow. Figure
shows that the Br$^-$ was retained throughout the summer period but started to leach out during the drainage season and the breakthrough ended mid-November. However, due to some retardation in the matrix and in crop residues, later appearances of Br$^-$ can be observed.

As shown in Figure 9, macropore settings with the P3 boundary condition (nMAE$_{BR}$ = 0.85-0.93, nMAE$_{BRC}$ = 0.14–0.21) performed significantly better than any other with P4 (nMAE$_{BR}$=1.07-1.19, nMAE$_{BRC}$ = 0.45–0.64), even though P4 setups performed marginally better for this specific year in terms of drainage dynamics and cumulative drainage. For concept a) + P4, considerable transport of KBr resulted, where $K_{s,B}$ (1.46 cm$^{-h}$) was 2.25 times larger than the average $K_s$ (0.65 cm$^{-h}$) for all setups, and therefore more Br$^-$ leached to the drain through the matrix. For this concept, $K_{s,C}$(0.19 cm$^{-h}$) was also one magnitude lower than $K_{s,B}$, which allowed the water to build up above the C-horizon, which is the reason for the high proportion of matrix water in the drainage (Table 1). Also, if matrix leaching is included, the different concepts with P4 resulted in percolation levels that were 1.5-2 times higher than in P3. This supports the hypothesis that the observed lower boundary at P4 had no or limited hydrological connection to the field.
**Figure 10.** The summarized Br\textsuperscript{−} solute inflow (+) and solute outflow (−) by depth below the surface for all six simulated concepts.

For all model concepts, the macropore transport of Br\textsuperscript{−} from the field to the drain substantially outweighed the matrix transport. As suspected, the DM1 macropore class transported the majority of the solute, indicating that the solute did not move further down in the matrix and was being held in the plow layer (A-horizon) to some degree. As Animation S1 shows, after the spraying of the Br\textsuperscript{−} the plume starts to diffuse into the plow layer after the first few hourly rain events, and when the pressure potential exceeds the threshold, all macropores related to the plow layer (DM1, MM1, MM2) are activated and facilitate the transport of Br\textsuperscript{−} to the drainage or below the drain level. On 25 October 2000, 156 days after the application, the rainy season initiated the Br\textsuperscript{−} movement in the plow layer again and allowed Br\textsuperscript{−} to slowly diffuse towards the B-horizon (Animation S2). The animation shows that although the plume had already reached the middle of the B-horizon, the majority of the Br\textsuperscript{−} transport to the drain or below was caused by the remaining concentration
in the plow layer. The summarized solute inflow(+) and solute outflow(-) show (Figure 10) that the transport mechanism was mainly driven by the Br⁻ build-up above the plow layer, causing large amounts of PF leaching the soil column.

4 Perspective

The present study and results call for further studies to understand the transport of agro-chemicals, such as the optimization of the model concept b) + P3 with respect to transport of Br⁻, nitrate, and applying pesticides. Such future studies could reveal how nitrogen leaching will be affected in the plow layer by mineralization and denitrification processes and further transported to the drainage systems through DM macropores. In the present study, all concepts proved that the majority of drainage was caused by the DM1 macropores, which collected the water mainly from the plow layer. This reveals that there is a high risk of applied soluble agrochemicals and nutrients, which are incorporated to the plow layer (such as injected slurry), being leached to the tile drain system [Larsson and Jarvis [1999].

5. Conclusions

In this study, a one-dimensional model code including different macropore settings and a representation of artificial drainpipes in an agricultural clay till field was tested in order to describe the measured water and mass balance with a focus on drainage. The modeling exercise showed that Darcy flow-based models with coupled dual permeability capabilities could model with high precision for a long-term period while accounting PF. Two groundwater table measurements, P3 and P4, were collected at the southern and northern borders of the field, respectively, the results showed that the groundwater table measured at P4 did not truly reflect the water balance of the field, which indicate the importance of a correct lower boundary. The concept with macropore setting b) exposed to groundwater fluctuations measured in the southern part (P3) of the field gave the best description of the drainage of the field.

Further, the results of this model study revealed that 70% percent of the overall drainage was supplied via macropores and of the applied tracer 54% leached directly from the plow layer. Based on the different conceptual settings, the majority of drainage seemed to be primarily the result of rapid precipitation infiltration from the surface to the plow layer, and from there via preferential pulse flow to the drain or below through macropores. The applied Br⁻ tracer test and modeling
revealed that in this heterogeneous soil with yearly soil tillage (harrowing and plowing) and, therefore, most likely a temporary increase of the soil porosity in the plow layer, the buried macropores could have a more significant impact on transport than surface-connected macropores.

6. Acknowledgment

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Supporting Information for

[Estimating the degree of macropore flow to drainage in an agricultural clay till field for a 10-year period]

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Figures S1 to S17
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Introduction

The supporting information of this paper includes all extra datasets that are necessary for a deep understanding of the presented problem. The datasets cover the topographical information, geological mapping and groundwater potential heads of the Silstrup field. Besides the field information, the laboratory results of the soil water retention and conductivity test are presented. Additional figures describe the sensitivity output for each sub-objective and for each macropore setting with the P3 and P4 lower boundary conditions. Further, the tables and extra figures include the final calibrated result for each test scenario with their respective retention and conductivity calibrated parameter values.
Field characteristics and field instrumentation

Figure S1. A geological model of the Silstrup field. M marks the location of groundwater wells and P the locations of the piezometers for monitoring groundwater level.
Figure S2. Apparent resistivity measurement of the field.
Figure S3. Topography and field instrumentation of the Silstrup field.
Figure S4. Potential head (m.a.s.l.) contour lines of the field measured in February 2000.
Field instrumentation description supplement [Lindhardt et al., 2001]

The automated system consists of various items of hardware and sensors and commercially available software tools in which dedicated software codes have been implemented. The central unit is a Campbell CR10X 2M datalogger (Campbell Sci, UK). User communication from office PC to this datalogger is established via a modem using fixed telephone lines or GSM phone transmission. The data are collected automatically every night.

An automated monitoring system has been installed for measurement of precipitation, barometric pressure, soil temperature, soil water content and drainage flow. Further, the datalogger was programmed to control ISCO samplers (ISCO 5800 Refrigerated Sampler, Teledyne ISCO, USA) to take flow-proportional samples of the drainage water from which total nitrogen and nitrate were assessed from standard analysis methods in the lab.

Precipitation
Precipitation is measured on site with a tipping bucket rain gauge (Type 1518 Wilh. Lambrecht, BmbH, Germany). The gauge is accurate to 0.1 mm and is well suited to measuring high precipitation intensity. Sampling is carried out every minute and hourly values are stored.

Soil water content
Soil water content is measured using a CR10X-controlled Time Domain Reflectometry (TDR)-system. The central unit in the TDR-system is the cable tester from Tektronix 1502C (Tektronix Inc., Beaverton, OR, USA). The soil water probes are developed at Research Centre Foulum and consist of a 40-m coaxial cable (Mikkelsen Electronic A/S, DK) connected through a solid plastic box to three 30-cm steel rods spaced about 2 cm apart. The accuracy of the soil water measurements is around ±1 vol %.
Soil water content is measured in two profiles at each site at the depths of 0.25, 0.6, 0.9, 1.1, 1.9 and 2.1 m, with three replicate probes at each depth. Soil water content is measured and stored every hour.
Soil water retention data from PLAP

The laboratory SWR measurements were done on 100-cm³ soil samples, with nine replicates at each horizon and face. The mean of the SWR measurement of the corresponding Face and Horizon is presented below. The saturated and unsaturated hydraulic conductivity measurements were done on 6280-cm³ large, undisturbed soil columns. The measurements and measurement algorithm were done by Iversen et al. [2004].

Figure S5. Soil water retention measured in the laboratory (mean of 7-9 soil cores ±SD, Table S2) at various soil water potentials (Table S1) on soil samples from the North and East pedological profiles (top figure) in the A-, B- and C-horizons. Unsaturated hydraulic conductivity ($K_{\text{unsat}}$) is presented as a function of Log10 of the soil water potential and the saturated hydraulic conductivity ($K_s$) (mean of 4-5 soil core ±SD)(bottom figure).
Table S1. Laboratory measured mean soil water retention of function of Log10 of soil water potential, bulk density and porosity. (P = Profile, H = Horizon, BD = Bulk Density)

<table>
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<th>D.</th>
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<tr>
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<td>±SD</td>
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Results of Morris sensitivity screening

Figure S6. Morris sensitivity screening output with Morris distance of M.setting a), red lines represent the sensitivity threshold with respect to the sub-objectives.
**Figure S7.** Morris sensitivity screening output with Morris distance of M.setting b), red lines represent the sensitivity threshold with respect to the sub-objectives.
Figure S8. Morris sensitivity screening output with Morris distance of $M$.setting $c)$, red lines represent the sensitivity threshold with respect to the sub-objectives.
Calibrated model results

Figure S9. Simple calibrated harvested dry matter (DM) for concept a), b) and c) with lower boundary P3 and P4 and nMAE, nRMSE[\%], and KGE of the six concepts. FB: Fodder Beet, SB: Spring Barley, P: Pea, M: Maize, WW: Winter Wheat and WR: Winter Rape
Figure S10. Calibrated soil water content at depth of 25 cm (upper) and 60 cm (middle) for M.settings a), b) and c) with lower boundary P3 (GWT, lower). nMAE, nRMSE[%, and KGE are given for the whole calibration period (2003-2008) for drainage.
Figure S11. Calibrated soil water content at depth of 25 cm (upper) and 60 cm (middle) for M.settings a), b) and c) with lower boundary P4 (GWT, lower). nMAE, nRMSE[\%], and KGE are given for the whole calibration period (2003-2008) for drainage.
Figure S12. Performance of the six model concepts (M. settings a), b) and c) applying the groundwater table from P3 and P4) when describing measured drainage for the evaluation period 2000-2001 and 2001-2002. nMAE, nRMSE[%] and KGE of the six concepts are given for the presented period with nMAE values in brackets for the whole calibration period of drainage (2003-2008).
**Figure S13.** Performance of the six model concepts (M. settings a), b) and c) applying groundwater table from P3 and P4) in describing measured drainage for the evaluation period 2002-2003 and 2003-2004. nMAE, nRMSE[%] and KGE of the six concepts are given for the presented period with values in brackets for the whole calibration period of drainage (2003-2008).
Figure S14. Performance of the six model concepts (M. settings a), b) and c) applying groundwater table from P3 and P4) in describing measured drainage for the evaluation period 2004-2005 and 2005-2006. nMAE, nRMSE[\%] and KGE of the six concepts are given for the presented period with values in brackets for the whole calibration period of drainage (2003-2008).
Figure S15. Performance of the six model concepts (M. settings a), b) and c) applying groundwater table from P3 and P4) in describing measured drainage for the evaluation period 2006-2007 and 2007-2008. nMAE, nRMSE[%] and KGE of the six concepts are given for the presented period with values in brackets for the whole calibration period of drainage (2003-2008).
Figure S16. Performance of the six model concepts (M. settings a), b) and c) applying groundwater table from P3 and P4) in describing measured drainage for the evaluation period 2008-2009 and 2009-2010. nMAE, nRMSE[%] and KGE of the six concepts are given for the presented period with values in brackets for the whole calibration period of drainage (2003-2008).
Figure S17. Simulated accumulated drainage input from matrix and macropore domains, accumulated matrix and macropore percolation, and measured drainage with the corresponding nMAE, nRMSE[\%] and KGE for 2000-2001 drainage at 1.1 m drain level for all the six model setups with values in brackets for the whole calibration period of drainage (2003-2008).
Table S4. Final calibrated parameters of concepts a), b) and c) with lower boundary conditions P3 and P4. Non-sensitive parameter for P3 and P4 marked in gray color.

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<th>c)</th>
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<td>P4</td>
<td>P3</td>
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**Animation S1.** Simulated bromide transport in the macropore and the matrix media from 22 May 2000 to 31 May 2000 of concepts a), b) and c) with lower boundary conditions P3 and P4. The animation can be downloaded from the following [Link](#).

**Animation S2.** Simulated bromide transport in the macropore and the matrix media from 15 October 2000 to 31 December 2000 of concepts a), b) and c) with lower boundary conditions P3 and P4. The animation can be downloaded from the following [Link](#).
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Denmark.
Effect of preferential transport and coherent denitrification on leaching of nitrate to drainage
Effect of preferential transport and coherent denitrification on leaching of nitrate to drainage

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Abstract. To protect the quality of the aquatic environment, it is imperative to be able to assess the leaching of nitrate through various hydrogeological settings. Numerical model concepts have been developed in order to describe this leaching and possible routes of nitrogen at field scale often without being evaluated in regard to their ability to account for dominant preferential transport and coherent denitrification, which is the rule than the exception in soils. This study evaluates on whether it is possible to describe 10-years of nitrate concentrations measured in drainage from a tile-drained agricultural clay till field in Denmark by applying the soil-plant-atmosphere model DAISY capable of accounting for preferential transport and denitrification. A DAISY model concept including macropores capable of capturing the water and bromide balance of the field within this specific timeframe was able to predict the water transport to drainage, dry matter, and N-yield of the harvested crops, while it was unable with the standard default denitrification model to predict dynamics and quantity of N-loss to drainage. This was caused by a fast saturation of the plow layer, where nitrate seemed to be denitrified almost instantly, and no surplus nitrate remained to be transported to the drainage. To circumvent this and describe the measured N-loss, modification to the water reduction function affecting denitrification was conducted. The denitrification had to be reduced approximately 50% from a seasonal average of 75 kg N ha⁻¹ to 35 kg N ha⁻¹ added with 48% to 80% of the total N-loss to drainage had to be preferential transported from the plow layer. This study hence reveals that by not accounting for preferential transport and coherent denitrification, there is a high risk of underestimating leaching of nitrate to the aquatic environment.

Keywords: Preferential transport, Denitrification, Modeling, N-leaching, Drainage

1 Introduction

Nitrogen is an essential element of crop growth and development. The input of agricultural
nitrogen fertilizers, however, causes one of the most substantial amounts of non-point source nitrogen pollution of surface water (including drainage) and groundwater despite the Nitrate Directive [EEC, 1991]. One of the most widespread impacts on inland surface water and coastal seawater is eutrophication, which is induced by unnatural enrichment of nitrogen and phosphorus. In order to increase agricultural production from the arable land, artificial subsurface tile drains are widely deployed all around Denmark to remove excess water from fields with poor natural drainage. Nevertheless, this agricultural water management measure puts the aquatic environment into risk since it facilitates rapid nitrogen transport pathways to the aquatic environment with limited possibilities for the reduction of nitrate [Ernstsen et al., 2015] followed by eutrophication [Blann et al., 2009]. Bergstrom [1995] argued that nitrate would be transported evenly through the matrix media and unlikely via preferential flow pathways. In contrast, Larsson and Jarvis [1999] showed the importance of macropore flow in regard to nitrate transport in structured soils. Mohanty et al. [1998] found water flow better described by using bimodal unsaturated hydraulic functions accounting for preferential flow of water than obtained with the commonly used unimodal hydraulic functions. Recently, Cheng et al. [2014] have shown that the leaching of nitrate from an undisturbed soil column of loam on average was 2.31 times faster than from a packed soil column. Besides the contamination threat towards the aquatic environment, agricultural fertilization practices pose a risk as one of the accelerators of global warming, since it is a source of nitrous oxide (N₂O) emission. Hofstra and Bouwman [2005] concluded by statistical modeling including studies with 336 denitrification measurements in contrasting crop management systems and landscapes that the possible magnitude of gaseous N loss was around 10 kg N ha⁻¹ year⁻¹ from a well-drained field with the uncertainty of 2-46 kg N ha⁻¹ year⁻¹. The authors classified the results based on drainage conditions, such as well-drained and poorly drained with a contribution of 13 and 22 kg N ha⁻¹, respectively. According to Knudsen et al. [2000], in Denmark, the general “rule of thumb” for sandy clay loam and clay loam is a loss of 20-40 kg N ha⁻¹ year⁻¹ due to denitrification. Besides nitrogen being a pollution factor, nitrogen is one of the most limiting nutrients for vegetation, which regulates crop productivity in the agricultural ecosystem. The proportion of various nitrogen compounds in the system depends both on the form and the amount of the input of nitrogen (organic or inorganic), but also on transformations in the soil. Although inorganic nitrogen is responsible for both plant production and facilitation of eutrophication, the labile N compounds account for less than 5% of the total nitrogen in soil [Jarvis et al., 1996; Brady et al., 2008]. Nitrogen is present in organic form as plant residues, but since it is not soluble to water,
plants have limited access for this storage. Microorganisms (bacteria and fungi) convert the organic nitrogen into ammonium and nitrate (mineralization), and this inorganic nitrogen can be mobilized by the root system of plants. The excess available inorganic nitrogen is either transported to surface waters by subsurface tile drain systems or the groundwater if not being immobilized or denitrified [Reddy and Ronald, 2008].

Today, models applied to assess the water and solute transport includes discrete representation of soil layers, which with their hydraulic, chemical and biological properties drives the organic and inorganic compounds through the simulated soil profile [Manzoni and Porporato, 2009]. Such models are often one-dimensional and apply Richard’s equation [Richards, 1931] paired with the advection-dispersion equation, and depict the subsurface drain transport with the widely used Hooghoudt equation [Hooghoudt, 1940]. Besides the equilibrium water and solute transport, several of these models have included preferential pathways in order to simulate the rapid transport throughout the soil media [Simunek et al., 2003]. The ability of these models to describe preferential transport and coherent denitrification in relation to leaching of nitrate has however seldom been evaluated in detail, which is imperative for being able to protect the aquatic environment against nitrate pollution.

The objective of this study was to evaluate, by using one-dimensional physically based root zone model DAISY [Hansen, 2002], the effect of preferential transport and denitrification on leaching of nitrate to drainage during a 10-years period as measured for an agricultural clay till field included in the Danish Pesticide Leaching Assessment Programme (PLAP; Lindhardt et al. [2001]; web address: http://pesticidvarsling.dk). This was conducted by (a) testing the performance of the preferential flow and transport model concept developed by Nagy et al. (2019) for this specific field in describing the measured loss of nitrate to drainage, and (b) improving this model performance by optimizing the concept regarding sensitive, hydraulic, crop, nitrification and denitrification parameters [Hansen et al., 2012].

2 Material and Methods

2.1 Long-term field experiment

The experimental field (1.69 ha) has been included in PLAP and is located in Silstrup (56° 55'56"N 8° 38'44"E) on the North West side of Denmark [Lindhardt et al., 2001] (Fig. 1). The field was set up in 1999 with the knowledge that since 1942 the field has been used for agricultural purposes and artificially drained in 1966 with a systematically and uniform layout of the drain
pipe system. The field was farmed from 1983 without the use of plot experiments, and since the monitoring started in 1999, the field has been cultivated with crops in a rotation following Danish standard agronomic procedures concerning soil tillage, fertilization and spraying with pesticides. The field and the surrounding area are dominated by Weichselian glacial clay till deposits in mixture with thin meltwater sand lenses. The field is heavily fractured and contains high-density of macropores. In the top 1 m, traces of agricultural processes are highly visible, dominated by bioturbation and desiccation cracks and the macropore density was approximated to 400 pores m$^{-2}$ [Lindhardt et al., 2001] with diameters of 2-5 mm utilizing the methodology from Klint and Gravesen [1999]. The most common horizon subdivision is between the topsoil or plow layer (Ap horizon) and subsoil (B horizon) with average depths of 31 cm and 140 cm, respectively. The textural evaluation showed a plow layer with 18-25% clay and an even more varying clay content within the underlying soil up to 43%. The loss of pesticides has from the start of the monitoring program been followed by flow proportional sampling of water from the drainage system and grab samples of water from deep groundwater wells installed at the border of the field. In addition to pesticide leaching assessed from the water samples also nitrate concentration in the same water, samples have been measured. Further details on the monitoring program are given by Lindhardt et al. [2001]. In the present study, Silstrup data is included from the period 2000-2010. Silstrup has an average yearly precipitation of 838 mm. The groundwater table is located relatively deep for the duration of the dry seasons with a depth of 2-4 m, whereas during the wet season it varies between 0.5 – 1.5 m. On average, the drainage was occurring 168 days per year with a mean magnitude of 0.5 mm d$^{-1}$ corresponding to 8.45 m$^3$ d$^{-1}$ from the whole field. Most of the drainage occurred during the wet season (late autumn and winter), although occasional sudden preferentially induced flow was observed during the spring and summer period. Further hydrological details can be found in Nagy et al. [2019] and Lindhardt et al. [2001].

[Figure 1 about here.]

**Management and measurements:** From 2000 through 2010, crops of spring barley (SB) and winter wheat (WW) were grown in rotation with winter rape (WR), fodder beets (FB), pea (P), and maize (M) (Fig. 2). No catch crop has been cultivated. Every single year, the total amount of N fertilizers applied was adjusted to accommodate the selected crop considering the nutritional effects of the previous crops in rotation. On average for 2000–2010, the annual N-application was 197 kg N ha$^{-1}$ yr$^{-1}$. The climate data was recorded from 29 April 2000 until 31 December 2010 on an hourly basis. The data include wind speed [m s$^{-1}$], global radiation [W m$^{-2}$], air temperature [$^\circ$C] and vapor pressure [Pa] to be able to determine the evaporative demand utilizing the Penman-
Monteith Reference Evaporation equation [Allen et al., 1998]. The wind speed measurements at 10 meters height were scaled to 2 meters, assuming a logarithmic wind profile and neutral atmosphere [Allen et al., 1998]. Hourly precipitation [mm] was sampled with a tipping bucket gauge (Lambrecht meteo GmbH) at the upper Northeast end of the field [Lindhardt et al., 2001; Nagy et al., 2019]. At the tile drain outlet, hourly drainage discharge was measured using the Thompson weir method [Lindhardt et al., 2001]. ISCO samplers (Teledyne ISCO, Lincoln, NE, USA) had been utilized to get samples of drainage water. Drainage water was sampled time proportionally (hourly) until 2004 and hereafter sampled proportional with sub-samples collected for every 3000 L of drainage flow during the winter months (September–May) and 1500 L during the summer season (June–August). Each week, all the collected subsamples were pooled, and a sample was analyzed nitrate in the laboratory [Ernstsen et al., 2015]. The soil water was sampled with PRENART SUPER QUARTZ suction cups (Prenart, DK)) consisting of porous Polytetrafluoroethylene (PTFE) mixed with quartz. Four suction cups were installed at a depth of 1 m and four at a depths of 2 m at the edge of the field [Lindhardt et al., 2001]. The sampling bottles are 1- or 2-liter glass bottles, and samples were taken every 7 days.

**N-concentration and transport:** In the period 2000–2010, the nitrate-N concentrations in drainage at Silstrup varied between 0.5–34 mg N L\(^{-1}\) and 20 percent of the time exceeded the European limit for drinking water (Fig. 2). Slightly elevated nitrate-N concentrations were measured during M2002 (15.47 mg N L\(^{-1}\)), P2003 (13.96 mg N L\(^{-1}\)), WW2006/2007 (12.68 mg N L\(^{-1}\)) and in extreme WW2004/2005 (22.10 mg N L\(^{-1}\)), FB2008 (34.29 mg N L\(^{-1}\)) was two and three times more than the allowed EU limit for drinking water supply (11.3 mg N L\(^{-1}\)). Most of the N leaching occurred throughout the fall- and wintertime, and generally, the daily fluxes were below 1 kg N ha\(^{-1}\) d\(^{-1}\). For a short period of time, the concentration hit the range of 1–2 kg N ha\(^{-1}\) d\(^{-1}\) and hardly ever been above 2 kg N ha\(^{-1}\) d\(^{-1}\) (Fig. 2). The yearly drainage transport of nitrate-N coming from the field was between 3–23 kg N ha\(^{-1}\) yr\(^{-1}\), corresponding to 1–16% of the annually applied N fertilizers (Fig. 2). Even though N was applied every year at nearly the same plant development stages, no immediate effects on nitrate-N concentrations in the drainage were observed. This applied to both mineral and organic N fertilizers [Ernstsen et al., 2015]. Figure 2 presents the water and NO\(_3\)-N leaching accumulated seasonally. One season was comprised from the 1 April of the given year until the 31 March of the next year to represent the significant crop growing and N fertilization season. This seasonal approach is an alteration from the standard use of hydrological year, as United States Geological Survey (USGS) defines it as the period between 1 October of one year and 30 September of the next (U.S.G.S, 2016).
2.2 The DAISY-model

DAISY is a one dimensional physically based root zone model being able to model water balance, carbon and nitrogen turnover, solute balance, heat balance and crop production based on input of climate data, soil texture, and various management strategies [Hansen, 2002]. The water balance includes surface and subsurface matrix and preferential flow processes, as well as plant uptake and flow to tile drains. It puts great emphasis on nitrogen balance and modeling of processes in the nitrogen cycle, mineralization-immobilization, nitrification, and denitrification. Further, it simulates uptake and leaching of ammonium and nitrate to drains and groundwater [Hansen et al., 2012].

Soil N pools: Nitrogen (N) is present in two different fractions in the soil as organic or inorganic forms. These two fractions are in a constant exchange with each other through mineralization and immobilization. According to Jarvis et al. [1996], inorganic N represents approximately 5% of the total soil N, although it may change after fertilization for a short period. Hence, organic N, which occurs in many forms, including proteins, urea, amino and nucleic acids and nucleotides is by far the largest N fraction of the soil.

Although the microbial state of N may cover only 3-5%, most of the transform processes (mineralization, immobilization, and denitrification) are mediated by the microbial community. In DAISY, soil N is divided into six different pools (Fig. 3), and some N in an inert pool (not shown in Fig. 3). The pools are separated into two distinct groups, pools with slow turnover rate (denoted 1), and pools with higher turnover rate (denoted 2). Thereby the soil organic matter pool 1 (SOM1) mainly contains chemically stabilized compounds which are relatively resistant to biological degradation. The other organic matter pool (SOM2) is physically stabilized and more labile, although temporarily resistant to biodegradation due to sorption to soil colloids. Added organic matter refers to manure, crop residue or green manure and typically divided into AOM1 – cell wall material and AOM2 cell extractable substances. The main driver of the C/N turnover is the soil microbial biomass (SMB), which controls the turnover processes of the dissolved
organic matter even though it only represents a small quantity of the total organic matter [Hansen, 2002].

**Mineralization-immobilization turnover:** Net N mineralization or net N immobilization is determined by the microbial activity and the overall N balance. If the content of N in the assimilated organic substance is higher than that required by the biomass for growth, ammonium is excreted to the soil solution. On the other hand, if the content of N in the assimilated organic substance is lower than that required by the biomass for growth, ammonium or nitrate is assimilated from the soil solution and transformed into nitrogenous organic compounds [Hansen, 2002]. The measure used in DAISY for the available organic substrate is the content of carbon in the organic matter. Hence, the simulation of net mineralization of N is based on the simulation of the turnover rate of soil organic carbon. The potential decomposition rate of organic carbon in various pools in the soil is described by first-order kinetics but is affected by the abiotic factors (soil water content, soil temperature, pH (5 to 8), oxygen pressure) and availability of inorganic N. The potential N mineralization rate is strongly related to the carbon turnover as every sub-pool has a C:N ratio and the decomposition of carbon leads to mineralization of N carbon according to this ratio. Hence, the potential background N mineralization from dead native organic matter in the soil is highly dependent on the distribution of the dead native soil organic matter between SOM1 and SOM2, which in turn is strongly related. By default, the C:N ratio for SMB1 and SMB2 is assumed to be 6 and 10, respectively, however, it can be specified differently if required.

**Denitrification:** In the present model, denitrification is simulated using a rather simple index type model considering the decomposition of organic matter, volume of anaerobic microsites expressed simply in terms of soil water content, soil temperature, and the concentration of nitrate in soil solution. This is a typical way of using a simplified model for denitrification (1), according to Heinen [2006]:

\[
D_a = \alpha f_N f_S f_T f_{\text{pH}}
\]  

(1)

where, \(D_a\) is the actual denitrification rate, \(\alpha\) represents the potential but may in different models have different formulation, \(f_N\) is a dimensionless reduction function for nitrate content in soil or it represents the nitrate content in the soil (depending on the exact formulation determined by \(\alpha\), \(f_S\) is a dimensionless reduction function for water content in the soil, \(f_T\) is a dimensionless reduction function for temperature in the soil, and \(f_{\text{pH}}\) is a dimensionless reduction function for soil pH. The \(\alpha\) parameter can be considered in two ways depending on the model concept; either \(\alpha\) represents the potential denitrification rate \(D_p\) (same units as \(D_a\)) or represents a first-order denitrification
coefficient (constant) $k_d$. For both cases, $\alpha$ can be a constant parameter or can be related to carbon dynamics. In the DAISY model, the potential denitrification rate (in case of anoxic conditions and sufficient nitrate concentration in the soil solution) is expressed as a linear function of the CO$_2$ evolution rate:

$$\xi^*_d = \alpha^*_d \xi_{CO_2}$$  \hspace{1cm} (2)

where $\xi^*_d$ is the potential denitrification rate of the soil, $\xi_{CO_2}$ is the CO$_2$ evolution rate simulated by the mineralization - immobilization - turnover model (MIT-model), and $\alpha^*_d$ is an empirical constant, which was taken from Lind [1980], who measured the relationship between easily decomposable organic matter and denitrification capacity. The actual denitrification rate is determined either by the actual microbial activity at the anaerobic microsites, or the transport of nitrate to the anaerobic microsites represented by the left and right solution, respectively, in Eq. 3. In the case of ample supply of nitrate, the actual denitrification rate is determined by multiplying the potential denitrification rate by a modifier function. Hence, the actual denitrification can be simulated as:

$$\xi_d = \min\{f_T f_S \xi^*_d; K_d N_{ni}\}$$  \hspace{1cm} (3)

Where $\xi_d$ is the actual denitrification $K_d$ is an empirical proportionality factor when denitrification is governed by the microbial activity at the anaerobic microsites and $N_{ni}$ the nitrate concentration in the soil. The maximum transport of nitrate to microsites can be assumed to be relative to the nitrate concentration in the soil ($N_{ni} = \theta C_{ni}$, where $C_{ni}$ is the concentration in the soil solution, and $\theta$ is the soil water content). In Eq 3, the modifier function $f_S$ is assumed to be a function of the soil water content. Many models use a power reduction function of the form [Grundmann and Rolston, 1987]:

$$f_S = \begin{cases} 0 & S < S_t \\ \left(\frac{S - S_t}{S_m - S_t}\right)^w & S_t \leq S \leq S_m \\ 1 & S_m \leq S \end{cases}$$  \hspace{1cm} (4)

where $f_S$ is the dimensionless power water reduction function in the range [0, 1], $S$ is the dimensionless degree of water saturation or water-filled pore space; $S$ is always in the range [0, 1], $S_m$ is close to full water saturation above which $f_S=1$, $S_t$ is a threshold value for $S$ below which $f_S=0$, $w$ is a curve shape parameter determining the steepness of the curve [Heinen, 2006]. The
temperature modifier function $f_T$ is an Arrhenius like function \cite{Rodrigo et al., 1997} by correlating the exponential rate of biological processes to the increasing temperature. According to Heinen [2006], based on a sensitivity test on Eq.(1), $f_S$ is the most sensitive within all modifiers. Therefore, this study is only focusing on the water saturation effect on denitrification in the aspect of calibration Eq. (1).

2.3 Initial model concept

Nagy et al. [2019] conceptualized the water and solute transport for the clay till field Silstrup with three different macropore settings and three different horizons (A, B and C). The macropore settings were included vertical macropore transport supplying water directly to 1) the drainage pipes, 2) to drainage pipes and the matrix 3) to drainage pipes and the matrix added with fractures supplying water to the matrix in the saturated zone. The best-calibrated concept with drainage ending macropores (DM1, DM2) and matrix (MM1, MM2, MM3) ended macropores (Fig 4a), yielded indices for the evaluation of measured and simulated drainage, 0.12/0.48 nMAE (normalized Mean Absolute Error) and 0.87/0.82 KGE (Kling –Gupta Efficiency) and for the bromide drainage transport 0.14/0.85 nMAE with 0.85/0.52 KGE. Further details in Nagy et al. [2019] (Fig. 4b, 4c).

[Figure 4 about here.]

2.4 Objectives included in the automated calibration procedure

The soil and hydrological parameters are adjusted in order to improve the bromide (Br) transport as the hydrological model by Nagy et al. [2019], which was not calibrated on Br transport. Especially a better performance of the model could be expected just after the application of 30 kg KBr ha$^{-1}$, corresponding to 20.14 kg Br$^{-}$ ha$^{-1}$ (cf. Fig. 9 in Nagy et al. [2019].) Therefore new objectives have been included in the calibration procedure, such as the harvested dry matter DM yield, harvested N yield - N yield, N drainage flux dynamics - ND [kg N ha$^{-1}$ h$^{-1}$] and cumulative N transport - NC [kg N ha$^{-1}$ h$^{-1}$], Br$^{-}$ transport dynamics – BRD1 [kg Br$^{-}$ ha$^{-1}$ h$^{-1}$] and cumulative transport – BRC1 for the whole tracer experiment period [kg Br$^{-}$ ha$^{-1}$ h$^{-1}$], Br$^{-}$ transport dynamics – BRD2 kg Br$^{-}$ ha$^{-1}$ h$^{-1}$] and cumulative transport – BRC2 [kg Br$^{-}$ ha$^{-1}$ h$^{-1}$] for the period of initial Br$^{-}$ breakthrough (1 April 2000 - 1 June 2000) and to not compromise the earlier findings from Nagy et al. [2019], the drainage dynamics - DD [mm h$^{-1}$] and cumulative transport – DC [mm] including soil water content measurement [cm$^3$ cm$^{-3}$] at depth 25cm - S25 and 60cm - S60 were
According to Muleta [2011] and Nagy et al. [2019], the mean absolute error was used for calibration. Since the model was constrained to different objectives with different units, the objectives in Eq. (5) were normalized by the mean of the corresponding observations in order to aggregate them into one objective function, which is eligible for automated calibration [Criss and Winston, 2008; Nagy et al., 2019].

\[
\text{nMAE}_{\text{season}}^{\text{obj}} = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\text{sim}_{\text{season},i}^{\text{obj}} - \text{obs}_{\text{season},i}^{\text{obj}}}{\text{obs}_{\text{season}}^{\text{obj}}} \right|; \text{obj} 
\]

\[
= \{\text{ND, NC, DD, DC, SWC25, SWC60}\}
\]

where \( N \) is the number of observations of a given objective within a year and

\[
\overline{\text{obs}_{\text{season}}^{\text{obj}}} = \frac{1}{N} \sum_{i=1}^{N} \text{obs}_{\text{season},i}^{\text{obj}}
\]

\[
\overline{\text{nMAE}_{\text{season}}^{\text{obj}}} = \frac{1}{K} \sum_{k=1}^{K} \text{nMAE}_{\text{season},k}^{\text{obj}}
\]

where \( k \) is the number of calibration years. Due to \( \text{DM yield} \) and \( \text{N yield} \) has only one value per season, a seasonal aggregation is not possible. Thus, nMAE was calculated for all season and normalized by the mean of the observations. The same applied to the \( \text{Br}^- \) (\( \text{BRD1}, \text{BRC1}, \text{BRD2}, \text{BRC2} \)) objectives due to the tracer experiment were held for one season in 2000-2001. The multi-objective function calculated for the automated calibration is expressed as:

\[
\text{nMAE}_{\text{final}}^{\text{obj}} = \sum_{\text{obj}} \overline{\text{nMAE}_{\text{season}}^{\text{obj}}} ,
\]

\[
= \{\text{N yield, DM yield, ND, NC, BRD1, BRC1, BRD2, BRC2, DD, DC, S25, S60}\}
\]

For further evaluation purposes nRMSE [%] (normalized Root Mean Squared Error), normalized on the difference on the minimum-maximum deviation of the observation and KGE (Kling-Gupta efficiency measure were calculated. KGE is presented by Gupta et al. [2009]). Singh et al. [2005]
and Moriasi [2007] suggested if MAE or RMSE of the model lower than half of the standard deviation (SD) of the measured data, the model may be considered as an adequate representation of the measured data. On the other hand, KGE with a range of $-\infty$ to 1, if KGE is above 0.5, the model can be considered as satisfactory.

### 2.5 Parameters

The hydrological parameters were taken from Nagy et al. [2019] as it considered to be a reasonable baseline for the calibration (Table 1 and 2). All initial hydraulic parameters represented presented in Table 1, and 2 were given a ±5% uncertainty boundary range in order to see which parameter would be influential on the “new” objectives.

[Table 1 about here.]

For the fast flow domain, the macropore model of DAISY using the conceptualization of Nagy et al. [2019] was applied (Table 2). The details of the mathematical and physical description of the macropore domain can be found in Mollerup [2010].

[Table 2 about here.]

To be able to evaluate the model behavior considering the “new” objectives conditions, one has to determine essential input parameters important for calibrating N loss by crop harvest, nitrate leaching and gaseous N\textsubscript{2} loss due to denitrification (Table 3). Only crop parameters influencing dry matter formation was selected as the data available did not allow a calibration of the N uptake parameters.

[Table 3 about here.]

The simple photosynthesis description in DAISY requires a value for the quantum efficiency at low light ($Q_{\text{eff}}$) [(g CO\textsubscript{2} m\textsuperscript{-2} h\textsuperscript{-1})(Wm\textsuperscript{-2})\textsuperscript{-1}], a maximum assimilation rate ($F_m$) [g CO\textsubscript{2} m\textsuperscript{-2} h\textsuperscript{-1}] and a temperature factor for assimilating production, referred to as a piecewise linear function (PLF) [Vries, 1989; Hansen et al., 2012]. Also to get more control over the crop production the conversion efficiency (growth respiration) (E) [(g CH\textsubscript{2} O ) (g DM)\textsuperscript{-1}] [Vries, 1989; Manevski et
al., 2016] was taken into the calibration besides the Photosynthetic Active Radiation extinction coefficient \(\text{PAR}_{\text{ext}}\) and the temperature sum at emergence \(T_{\text{sum}}\), Table 3.

Additionally, the crop uptake reflection factor of \(\text{Br}^-\) \(\text{CURF}_{\text{BR}}\) \(\text{[Hansen, 2002]}\), the SOM fraction ratio of the plow layer \(\text{SOM}_{\text{ratio}}\) which describes the ratio \(\text{SOM}_1:\text{SOM}_2\) has been added as a parameter, as well as parameters from the denitrification module for both fast and slow pools: the anaerobic denitrification constant \(\alpha_d^*\) \[((g \text{ NO}_3-\text{N h}^{-1})/(g \text{ CO}_2-\text{C h}^{-1}))\] and the empirical proportionality factor \(K_d\) from Eq. 2 and 3, respectively, and \(S_i\) and \(w\) from Eq.4 (Table 4).

The initial values of the selected crop and denitrification parameters were based partly on the values recommended for DAISY in the model library (https://DAISY.ku.dk/, Hansen et al. \[2012\]) and on literature screening. Due to the lack of data on the crop growth, N uptake, and partitioning during the growth season, no extensive calibration of the crop models was possible.

### 2.6 Sensitivity analysis

The range of crop parameter values is biologically constrained by the diversity of crop and their cultivars. Given the lack of knowledge associated with the range of the variability that is genetic for most of the crop model parameters, uniform distribution for each parameter was assumed with \(\pm 20\%\) uncertainty bound except \(\text{PAR}_{\text{ext}}\) where the bounds were set \(\pm 50\%\). All denitrification related parameter was given \(\pm 10\%\) uncertainty bounds except for the water reduction function the ranges, which were taken from Heinen \[2006\]. The SOM fraction ratio varied within from 0.43 to 2.33, which indicate fractions of \(\text{SOM}_1:\text{SOM}_2\) as 0.3:0.7 to 0.7:0.3 and \(\text{CURF}_{\text{BR}}\) could vary from 0 to 1, where 1 means no crop uptake.

Key parameters directly related to crop development, leaf photosynthesis, and net mineralization of plough layer as one of the input source of denitrification were tested for sensitivity by the Morris sensitivity screening \[Morris, 1991; Campolongo et al., 2007; Nagy et al., 2019\] in order to help finding sensitive parameters that has the most influence on objectives presented in section 2.4.

The results of the sensitivity screening were turned into the Morris distance \((\epsilon)\) \[Ciric et al., 2012; Jabloun, 2015\], which represent the Euclidean distance of the parameter from \((0,0)\) on the \(\mu^-\sigma\) coordinate system \[Campolongo et al., 2007\]. The decision on sensitivity threshold was made by K-Means Clustering \[Jain and Dubes, 1988\]. For each objective, the parameters were clustered
into 3 groups (Low, Medium, High) by its $\epsilon$.

### 2.7 Calibration methodology

The overall objective function was based similar to the mathematical formulation, which was used in Nagy et al. [2019], by calculating the normalized Mean Absolute Error of each objective described in section 2.6 annually for the period of 2000-2007. In order to stabilize the N dynamics, 4 years were run prior to 2000 as a warm-up period. The calibration of the model was done by differential evolution (DEoptim, Ardia D. [2016]) in conjunction of RDAISY R package [under development] and RDAISY toolbox [Jabloun et al., 2014].

### 3 Results and discussion

#### 3.1 Sensitivity screening results

Overall six soil matrix parameters per horizon (A, B, C), the SOM ratio for the A horizon plus two horizon depth parameters, two macropore parameters per macropore type (DM1, DM2, MM1, MM2, MM3), two soil water pressure parameters for macropores, four denitrification parameter per pool (slow/fast) and one Br$^-$ parameter called as soil-hydraulic parameters (SH) and eight parameters per crop as crop parameters (CP) were tested for sensitivity. All parameters were selected as a sensitive parameter, which belongs to group High, at least in one of the objectives (Fig. 5). However, to put more emphasis on the $ND$ and $NC$ objectives, parameters which belonged to sensitivity group Medium of $ND$ and $NC$ was also selected as sensitive and added to the calibration parameters (Fig. 5). All selected parameters which were involved in sensitivity analysis against 12 objective functions were listed with their associated sensitivity group (Fig. 5). Parameters with black are the selected sensitive parameters and gray letter the non-sensitive. Even though a large amount of parameter has been evaluated, only 16 CP and 21 SH parameters showed to be sensitive to the objective functions. All the sensitive CP parameters were as expected sensitive to $N$ yield since all crop parameters are related to crop growth and therefore directly affecting the crop N uptake.

[Figure 5 about here.]

SH parameters showed more diversity regarding sensitivity towards the objectives. This is in contrast to CP parameters, which mainly were sensitive towards $N$ yield and $DM$ yield. There was
no single parameter, which showed to be sensitive for all objectives. Only one SH parameter, $S_t$, affecting the denitrification reduction factor had an effect on $DM$ yield (Fig. 5). As also seen in Fig. 5, no matrix and macropore SH parameter was sensitive in the objective function for $DM$ yield. Therefore, it can be inferred that the crops were not affected by water stress. Furthermore, no macropore SH parameters were sensitive in the objective functions for $DM$ yield and $N$ yield. Even though the uncertainty bound was only $\pm 5\%$ for the SH macropore parameters, the $N$ dynamics, and quantity objectives ($ND$, $NC$) showed no sensitivity on the preferential transport. This could mean that the $N$ transport is not affected dramatically by the preferential transport change although earlier studies showed macropore influences on water and solute movement [Larsson and Jarvis, 1999; Nagy et al., 2019]. However, the denitrification parameter, $S_t$, showed one of the highest impacts on $NC$ objective, which represents the $N$ quantity in the drainage water. This high sensitivity might be related to the fact that the denitrification is limiting the amount of $NO_3$-N, which would be transported by hydrological means.

3.2 Model calibration

Through the calibration procedure, it was found that the $ND$ and $NC$ objectives were not responsive to the initially selected crop and hydraulic parameters. Since the $Br^-$ transport in the drainage simulated by the baseline model showed agreement to the accumulated measured transport with underprediction of initial breakthrough after spraying of KBr (Fig. 4). The simulated $Br^-$ uptake by FB was verified by Nagy et al. [2019]; thus, the solute leaching to the groundwater seems to be a good approximate to the reality. If all these conditions are probable, $NO_3$-N can be only limited by gaseous loss; therefore, the denitrification model parameters had to be involved in the sensitivity and calibration process.

As mentioned above, the sensitivity and the calibration process were done by minimizing the mean nMAE performance measures. For a broader evaluation, also KGE and nRMSE(%) is presented in Table 5. The calibrated objective results show that significant improvements were achieved in all solute transport accounts ($BRD1$, $BRC1$, $BRD2$, $BRC2$, $ND$, $NC$), without compromising any of the water balance objectives ($DD$, $DC$, $S25$, $S60$). By observing the $N$ yield and $NC$ objectives, one can see that $N$ transport $ND$ was improved without creating nitrogen stress in the crop. $Br^-$ transport improved during the tracer experiment period, as the model were able to provide a
reasonable fit for the initial breakthrough (Table 5, BRD2, and BRC2). (Fig. 6).

Table 6 shows the calibrated parameters and their initial value. There was no substantial change within the SH parameters. The SOM\textsubscript{ratio} increased, the SOM1 became 0.63, and SOM2 became 0.37 from the initial 0.5.

The most significant changes appeared for parameters directly related to the denitrification reduction function ($S_{t,\text{fast}}$, $w_{\text{fast}}$, $S_{t,\text{slow}}$, $w_{\text{slow}}$; Table 6), which may indicate that the default reduction function in DAISY overestimated this type of N loss.

### 3.3 Water and bromide transport

The improvement of Br$-$ transport yielded a larger initial breakthrough (Fig. 6) without compromising the water balance. The Br$-$ transport mainly responded to the change of the matrix pore distribution (van Genuchten “n”) in the horizon of A and B ($n_A$ and $n_B$, Fig. 5), although it could be the interaction of multiple parameters.

The crop uptake reflection factor increased only slightly from 0 to 0.34 %. The FB dry matter yield decreased from 14.5 Mg DM ha$^{-1}$ to 13.7 Mg DM ha$^{-1}$. However, the Br$-$ uptake in fodder beet increased from 11.6 kg Br$-$ ha$^{-1}$ to 12.1 kg Br$-$ ha$^{-1}$, which resulted in a 2% (0.5 kg Br$-$ ha$^{-1}$) higher Br$-$ uptake of the initially sprayed 20.1 kg Br$-$ ha$^{-1}$. The 0.5 kg Br$-$ ha$^{-1}$ proportionately removed from all Br$-$ leaching routes and macropore leaching remained at the same magnitude. Therefore, it can be inferred that the matrix and macropore interchange did not change significantly (Fig. 7).

### 3.4 Nitrogen transport and harvest

Considering the calibrated Br$-$ transport, the overall leached quantity of Br$-$ did not change
substantially. This contrasted with N transport, which responded differently to the calibration. The original model captured the N dynamics and in one instance the magnitude of the cumulated transport during the WW2003-2004 season. The application of N fertilizers was not reflected in simultaneous or subsequent increases of N flux from the field as well as no significant additive effect from crop type could be identified.

Figure 8 shows that the denitrification in the original model significantly out weighted the N loss by drains (measured NO$_3$-N) with one order of magnitude with an average seasonal loss of 75 kg N ha$^{-1}$ (18 - 151 kg N ha$^{-1}$), due to denitrification from slow and fast pools combined. Hence, it seems that denitrification limited the amount of N transported to the drainage. Nagy et al. (2019) discovered that most of the water build up above the plow pan in the A horizon. This could lead to this rapid denitrification, according to Eq. (1) to (4) where one of the modifying components is the $f_S$ water factor.

In DAISY, $f_S$ had been set as default in order to increase linearly from 0 to 1 as a function of $S$ from 0.7 to 1.0 [Hansen, 2002] (Fig. 9). This linearity does not fit the real condition for denitrification since the stagnation of the water above the plow pan, as it presented in Nagy et al. [2019], should allow the N almost instantaneously to denitrify. In the calibrated model, $f_S$ dynamics based on Eq. (4) has been changed, which resulted in a steeper reduction of the denitrification (Fig. 9). By allowing the separation of the reduction factor for both the fast and the slow pool, the calibration of the model showed that the denitrification from the fast pool was shrunk to the range approx. from 0.9 to 1.0 relative saturation, while the slow pool remained like the default version of DAISY.

The modified $f_S$ showed a high impact on the N leaching as the reduced denitrification enabled the model to depict the amount of N transported to the drain. The main increase appeared in the directly connected macropore flow (DM1 flow, cf. Fig. 4.), which mainly drained water from the A horizon. Since the mineralization process is faster from the fast pool, the available mineral N was not readily reduced to gaseous N, but instead transported through preferential pores to the
The average seasonal denitrification was reduced to 34 kg N ha\(^{-1}\) (9 – 62 kg N ha\(^{-1}\)), which is more than 55% percent reduction, which instead was made available for crop uptake, flow to the drainage system or the groundwater.

The harvested DM and N did not show significant differences before and after calibration (Fig. 10). Some crop N and DM yield were closer to the measured values after calibration, but although the surplus of N was increased by the lowered denitrification, this additional N was not taken up by the crops. Overall, the objectives of \textit{DM yield} and \textit{N yield} were improved with the modified crop parameters (cf. Table 5 and Fig. 10). However, none of the models showed a satisfactory match for N yield. For both the original and the calibrated model, the comparison between measured and simulated N yield showed differences of more than 10 kg N ha\(^{-1}\) and even 20 kg N ha\(^{-1}\) for maize 2002 and winter wheat 2007. As earlier stated, a calibration of the N uptake parameters in the crop models governing the N uptake during the season was not possible as the data available did not contain samples of biomass and hence N uptake during the season.

3.5 Evaluation of the model performance related to nitrogen loss routes

The period 2007-2008 involving crop rotations of WW2006-2007 and FB2008 was selected to test the performance of the calibrated model to simulate N transport to drains and loss to groundwater. Season 2009-2010 was excluded from the evaluation since a few water balance discrepancies were discovered. Some of the precipitation input and drainage transport was not aligned or missing. Thereby, the measured values cannot be reliable. Besides data from this calibration independent evaluation period, data series of N concentration sampled with suction cups at depths of 1 m and 2 m for the period from 2000 to 2010 were used to validate the N transport to both drainage and groundwater.

3.6 Nitrogen transport in drainage water and deep leaching to groundwater

The N flux was remarkably improved according to all performance measures for the period 2007-2008 (Fig. 11). For the original modeling of the two cropping seasons, the average KGE was below zero, indicating that the observed mean N flux was better predicted than the simulated one. In contrast, the calibrated model gave satisfactory results with KGE of 0.56 and 0.5 for the objective \textit{ND} and \textit{NC}, respectively, which in the case of solute transport modeling is an excellent result [Singh et al., 2005; Moriasi, 2007]. Although the comparison for the drainage season 2008-
2009 was improved even after calibration, less N loss to the drain system was simulated. The difference in simulated and measured N uptake in FB could not explain this difference.

The loss due to denitrification has changed similarly for the calibration period 2000-2007 from seasonal 75 to 35 kg N ha⁻¹, which is similar to a 50 % percent reduction in total. In season 2007-2008, after the WW2006-2007 crop, a satisfactory match between measured and simulated accumulated N losses to the drainage could exclusively be explained from the reduced denitrification loss (Fig. 11).

As mentioned above, soil N concentration in soil water sampled with suction cups was used for validation purposes. The soil water N concentration had similar behavior before and after the calibration apart that the dynamics were better matched after calibration (Fig. 12). During the WW2003-2004 crop drainage period, the calibrated model was able to depict the ~25 mg N L⁻¹ measured peak as well as the fluctuations from 2002 to 2004. However, both models underestimated the N concentration substantially in the period after WW followed by FB 2007-2008. Again, these differences could not be explained by an overestimated high N uptake (cf. Fig. 10). Although the drainage input of N massively increased due to the change in denitrification, the simulated N concentration only improved nRMSE 5%-point for the whole period, which is equal to ~1 mg N L⁻¹. Visual and mathematical inspection of the N concentration show, of course, a decent improvement on the soil N dynamics, but with this pronounced change in denitrification, the expected raise could be expected higher, if the more available N was not transported further down to the lower soil matrix (Fig. 1a) as DM1 and DM2 macropores start either from the surface or from the bottom of the plow layer (A horizon). However, both are conceptually described to transport water and nutrients to the drainage system, and water build up is not allowed in the model. Besides three other MM type macropores are present in this conceptual system with the possibility to transport water and solute: from surface to the bottom of the plough pan (MM1), from the surface to below the drain level at 150 cm depth (MM2) and from the bottom of the plough layer to below the drain level at 150 cm depth (MM3).
The latter two have the capability to transport N from the surface/plow layer below the drain level bypassing the entire B horizon. This limits the transport through the mentioned horizon by matrix flow. The conceptual description of deep macropores points out another possible rapid transport route for N from the plow layer towards the groundwater. By comparing the measured suction cups samples with the simulated concentrations at 2 m depth, a remarkable 30 %-point decrease can be observed in the nRMSE and 0.3 nMAE performance measure (Fig. 13). Rosenbom et al. [2009] concluded that deep fractures might result in deep leaching of agrochemicals and nutrient. However, these flow phenomena were outside the scope of the present study.

4 Conclusion
This study aimed to evaluate, by using one-dimensional physically based root zone model DAISY [Hansen, 2002], the effect of preferential transport and denitrification on leaching of nitrate to drainage during a 10-years period as measured for an agricultural clay till field included in the Danish Pesticide Leaching Assessment Programme (PLAP; Lindhardt et al. [2001]; web address: http://pesticidvarsling.dk). The results reveal a dominant effect on the leaching of nitrate through this clay till field. A large amount of N (48% to 80% of the total N-loss to drainage) was preferentially transported via macropores to drainage regardless of the application method and concurrent occurrence of precipitation. The current standard denitrification water reduction factor, $f_s$, needed modification with a reduction of approximately 50% in the denitrification of the field from a seasonal average of 75 kg N ha$^{-1}$ to 35 kg N ha$^{-1}$. The crop model provided acceptable results, and further studies are needed to improve the simulation of N uptake in crops. Overall, this study delineates the importance of accounting for preferential transport and coherent denitrification in the assessment of the leaching risk of nitrate to the aquatic environment.

5 Author contribution
David Nagy(DN) carried out the development of the conceptualization and methodology under the co-supervision of Annette E. Rosenbom(AER) and Bo Vangso Iversen(BVI) and main supervision of Finn Plauborg(FP). DN developed the model calibration code, performed the simulations and prepared the manuscript with contributions from all co-authors. AER provided the PLAP experiment data of Silstrup, whereas FP provided the corresponding climate data. AER and FP are responsible for the data curation of the experiment.
6 Acknowledgements

The research was funded by Aarhus University. Aarhus University, Department of Agroecology and Geological Survey of Denmark and Greenland, Department of Geochemistry provided all data from the Pesticide Leaching Assessment Programme (PLAP). The data can be requested from Annette E. Rosenbom. email: aer@geus.dk
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Subscripts: DC – Cumulative Drainage [mm], DD – Drainage Dynamics [mm h\(^{-1}\)], BRDD – Br Drainage transport dynamics [kg Br\(^-\) ha\(^{-1}\)h\(^{-1}\)], BRDC – Cumulative Br transport [kg Br\(^-\) ha\(^{-1}\)] [Nagy et al., 2019].

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Table 4. Initial parameters for denitrification, Br\(^-\) uptake, and SOM.

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<td>(3.3)</td>
</tr>
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<td>BRC1</td>
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<td>7.2</td>
<td>(12.4)</td>
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<td>(0.74)</td>
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<td>(27.9)</td>
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<td>DD</td>
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<td>(0.05)</td>
<td>0.04</td>
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<td>MEAN</td>
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<td>(0.43)</td>
<td>1.65</td>
<td>11.89</td>
<td>(17.15)</td>
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Table 6. Calibrated SH/CP parameters. Initial parameter values shown in brackets.

<table>
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<tr>
<th>$\theta_{r,A}$</th>
<th>$\theta_{r,B}$</th>
<th>$\theta_{s,A}$</th>
<th>$\theta_{s,B}$</th>
<th>$\alpha_A$</th>
<th>$n_A$</th>
<th>$n_B$</th>
</tr>
</thead>
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<td>0.39</td>
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<td>(0.38)</td>
<td>(0.051)</td>
<td>(1.186)</td>
<td>(1.201)</td>
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<td>$K_{sat,C}$</td>
<td>$\Psi_{barrier}$</td>
<td>$\rho_{MM3}$</td>
<td>$SOM_{ratio}$</td>
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<td>(0.7)</td>
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<td>$E_{Leaf,FB}$</td>
<td>$E_{SOrg,FB}$</td>
<td>$F_{m,FB}$</td>
<td>$PAR_{ext,FB}$</td>
<td>$Q_{eff,FB}$</td>
<td>$E_{Leaf,SB}$</td>
<td>$PAR_{ext,SB}$</td>
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<td>(0.06)</td>
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<td>$Q_{eff,SB}$</td>
<td>$E_{Leaf,M}$</td>
<td>$E_{Root,M}$</td>
<td>$T_{sum,M}$</td>
<td>$F_{m,M}$</td>
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<td>$Q_{eff,WR}$</td>
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<tr>
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</table>
Impact of drainage conditions on the fate of nitrogen in an agricultural tile-drained silty loam field
Impact of drainage conditions on the fate of nitrogen in an agricultural tile-drained silty loam field

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Abstract Drainage conditions are decisive for percolation of precipitation through the silty loam and hence the degree of flow entering the tile drain system or the groundwater. To evaluate its impact on the fate of nitrogen in such fields, an experiment has been set up on a silty loam field at Tokkerup, Denmark. The field was selected based on it having a poorly-drained part in the North with a groundwater table being close to the soil surface and a well-drained part in the South. Downstream and South of the two parts of the field, the drainage is measured and sampled applying an automatic magnetometer and an automated water sampler installed in a well. Combined with detailed information regarding the climate, agricultural practice, crop rotation and hydrogeological characteristics of both parts of the field, a one-dimensional soil-plant-atmosphere system model was set up to investigate the drainage conditions of the field. The modeling results show that in this silty-loam field, the importance of the drainage depth does not play a significant role in the loss of nitrogen. The direct preferential transport to the drainage dominates the transport of nitrogen with 84% and 90% of the total loss of N. The matrix transport to the drainage, according to the modeling results, acts as an intermediary stage of N as a result of bypass transport of the matrix ended macropores.
1. Introduction
Surplus nitrogen (N) from point and non-point sources are considered one of the leading factors damaging the ecological quality of streams, lakes and estuaries and the degrading quality of groundwater resources [Blann et al., 2009]. Denmark is a low-lying land and covers an area of 42,937 km$^2$, of which approximately 60% is agricultural land in 2018 [Statistics Denmark, 2019] having a net-precipitation somewhere between 50-500 mm y$^{-1}$ depending on location [Scharling and Kern-Hansen, 2002]. Nearly half of the agricultural land has been systematically tile-drained. Drainage in agriculture means, in this case, the artificial removal of excess water from the field, the avoidance of erosion as a result of irrigation, and for the general enhancement of agricultural land-use by improving optimum air and nutrition environment for the plant roots promoting root growth affecting directly plant-available N in the soil [Herzon and Helenius, 2008]. Although drainage has its agronomical benefits, the practice puts the aquatic environment into risk since it facilitates rapid transport pathways to the aquatic environment with decreased possibilities for the reduction of nitrate [Ernstsen et al., 2015]. Although N-losses from the agricultural field can occur in various form depending on the biological transformation within the soil or the applied fertilizers. Significant losses of NO$_3^−$N due to subsurface drainage from mineral soils [Bergstrom, 1995; Kladivko et al., 2004; Gooday et al., 2008; Blann et al., 2009; Ernstsen et al., 2015], as well as preferential flow (PF), has been observed [Ahuja et al., 1993; Larsson and Jarvis, 1999; Kohler et al., 2001; Gooday et al., 2008; Frey et al., 2012; Cheng et al., 2014; Frey et al., 2016]. It has also been reported that controlled drainage systems with adjustable water table depths can significantly reduce NO$_3^−$N losses through subsurface drainage [Wesström et al., 2001; Wesström and Messing, 2007; Wesström et al., 2014]. The total amount of N-loss to the drainage is also dependent on the soil type and the amount of precipitation input. According to Zhao et al. [2016], clay loam soils are more susceptible to larger N-leaching due to the intensive drainage and higher N-loads. Moreover, in the same study, exponentially increasing N-losses were observed with increasing annual precipitation means. Due to this effect of precipitation, the investigation of drainage related N-loss become more critical, since the report of Danish Meteorological Institute prognosis 1.6-6.9 % annual precipitation increase due to the climate change in the area [DMI, 2014].

The studies and findings mentioned delineated the importance of improving the current knowledge on the impact of drainage conditions on the fate of nitrogen in especially loamy tile-drained agricultural fields. Such knowledge is imperative for in the future to be able to conduct N-
differentiated agricultural practices dependent on climate and soil type for the reduction of N-loss to surface waters (drainage) and groundwater. This calls for detailed monitoring studies of the water- and N-balance of fields combined with numerical modeling evaluations.

_Hansen and Jensen_ [2013] conducted a research on the relation between drainage condition and cereal yields (winter wheat and spring barley). The experiment was set up in Tokkerup, south-eastern Denmark. They placed seven different plots in 2012 to assess the effect of drainage condition on crop yield throughout the field. They identified a significant yield reduction (up to 25%) in spring barley between a “well-drained(WD)” and “poorly drained(PD)” part of the field. Possible causes for the observed yield differences were considered to be drainage effects on the root development, the soil temperature, the timing of field operations, and on the N availability [Hansen and Jensen, 2013]. _Gyldengren_ [2016] continued the experiment and used the collected dry matter yield and N-yield of the crops with their continuation up to 2016. He simulated the groundwater dynamics and crop yield of dry matter and N from the PD and WD part of the field by the soil-water-atmosphere-crop model, DAISY. He identified that the harvested winter wheat dry matter yield (2.5 Mg ha$^{-1}$) at PD is significantly different (35%) from the harvested dry matter yield (1.8 Mg DM ha$^{-1}$) at WD in 2015-2016. By analyzing the grain N-yield of the seasons 2013-2015 in conjunction of season 2015-2016, he showed that at WD the grain N-yield was 33% higher than at the PD part of the field. Using the DAISY model he was able to simulate the N-uptake differences and suggested that besides the drainage condition there could be an another factor involved in the reduction of N. In a follow-up study, _Holbak_ [2017] conducted a pedological investigation of the field at the PD area, to identify the hydraulic condition of the area analyzing soil samples for water retention and air permeability at depth 50 cm and 100 cm. She took the samples horizontally and vertically from the horizons in order to show the anisotropy of the hydraulic conductivity in terms of representing PF-transport. She also used the DAISY model for simulating the measured groundwater table, by using the retention models of Burdine - van Genuchten (BvG) and Mualem - van Genuchten (MvG) derived from the laboratory data. The attempt of Hansen and Jensen [2013], Gyldengren [2016] and Holbak [2017] to simulate and describe the water and solute transport in the PD and WD part of the field by describing the groundwater fluctuation as a representation of the soil water content yielded satisfactory results. Although the groundwater levels were matched alone, they could not verify the transport via drainage due to lack of measurements.
This study focuses on improving the current model-description of the N-transport through the PD and WD part of this field by obtaining monitoring data on drainage and its chemical characteristics. For this purpose, the modeling and parametrization methodology of Nagy et al. [2019a] and Nagy et al. [2019b] and DAISY dual permeability approach is applied. This enables an evaluation of the drainage conditions impact of the N-fate, including preferential N-transport and denitrification.

2. Material and methods

2.1. Field description and instrumentation

![Field Diagram]

**Figure 1.** The instrumentation and topography of the Tokkerup field with the division of the poorly-drained (PD) and well-drained (WD) part.

The field is located at Tokkerup, Denmark (55°17’16.63”N, 12°8’24.59”E). The topography range from 22 to 23 m above sea level (a.s.l.) with an area of 3.93 ha. The western part of the field is terminated by the Vivide Mølleå stream, which is also the recipient of the effluent including drainage from the field. The tile-drain network is designed as a herringbone system. It consists of parallel tile laterals that enter the main drain at a varying angle. The central drain is located at 120
cm depth at the western end of the field, whereas at the eastern part of the field the drain depth increases to 60 cm due to the slope of 2%, which is a minimum requirement in regard to tile-drain systems [Aslyng, 1980]. The field is divided into a poorly-drained silty loam part (PD) and well-drained sandy loam part (WD), which was delineated by Hansen and Jensen [2013] having an area of 1.28 ha and 2.65 ha, respectively (Fig.1). In order to monitor the drainage of both parts of the field, two drainage wells were installed with an electromagnetic flowmeter (Pmag, from SGM LEKTRA). One well is installed downstream of the main drain next to the stream, wherefrom the drainage of the whole field is monitored, and the other well is installed in the middle of the northeastern part of the field, wherefrom the drainage of the approximately 1.28 ha PD part is monitored. Automatic flow proportional ISCO samplers (Teledyne ISCO, Lincoln, NE, USA) were used to collect drainage samples flow-proportional 100 ml via both wells for every 12000 L (0.3 mm ha⁻¹) bypassing water. All the collected samples are pooled weekly, from which a sample is analyzed for N, the sampler is reset, and sampling is hereafter restarted with an empty canister. During the plot-experiment study of Hansen and Jensen [2013], automatic hourly measurements of the groundwater table (GWT) via piezometers were initiated. The location of the wells related to the plot-experiment study was GWT_PD denoted as “plot 6” and GWT_WD denoted as “plot 2” (Fig.1) [Hansen and Jensen, 2013; Gyldengren, 2016; Holbak, 2017]. The GWT monitoring data is available at http://www.hydroinform.dk/Afvanding.html. Besides the drainage and GWT monitoring, a weather station has been deployed at the southwestern corner of the field. The weather data includes wind [ms⁻¹], global radiation [Wm⁻²], air temperature [°C] and vapor pressure [Pa] in order to calculate the evaporative demand using the Penman-Monteith Reference Evaporation equation [Allen et al., 1998]. The wind speed measurements at 10 m height were scaled to 2 m, assuming logarithmic wind profile and neutral atmosphere [Allen et al., 1998]. Hourly precipitation [mm] was monitored with a tipping bucket gauge (Lambrecht meteo GmbH, Göttingen, Germany; Fig.1).

The field was surveyed with a DUALEM21 ground conductivity meter (GCM). The processing and inversion of GCM data were done by Aarhus Workbench using the Aarhus Inv inversion code [Auken et al., 2015]. The apparent resistivity maps reveal that the top 40 cm of soil was relatively conductive with highly resistive spots indicating some sandy area in the plow layer. With depth, it becomes more homogeneous and electric conductive indicating a clayey subsoil (Fig.2). This is in accordance with the findings of Holbak [2017]’s pedological survey of PD. She identified that the
soil horizons below the plow layer consist of 19-20% of clay with the bulk density of 1.87-1.93 g cm$^{-3}$.

**Figure 2.** Apparent resistivity measurement of the Tokkerup field.

According to the USDA (United States Department of Agriculture) bulk densities, that are higher than 1.8 g cm$^{-3}$, are restricting root growth. As Table 1 shows, both depths have also a very low porosity, which also indicates high compaction with little space for water and gas.
Table 1. Soil texture analysis from the pedological profiles from the study of Holbak [2017] (Hr – Horizon, OM – Organic Matter, BD – Bulk Density).

<table>
<thead>
<tr>
<th>Hr</th>
<th>Depth [cm]</th>
<th>Clay &lt;2µm [%]</th>
<th>Silt 2-20µm [%]</th>
<th>Fine sand 20-200µm [%]</th>
<th>Coarse sand 200-2000µm [%]</th>
<th>OM [%]</th>
<th>BD [g cm(^{-3})]</th>
<th>Porosity [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>50</td>
<td>20</td>
<td>19</td>
<td>39</td>
<td>22</td>
<td>0.77</td>
<td>1.87</td>
<td>29.45</td>
</tr>
<tr>
<td></td>
<td>SD (0.9)</td>
<td>(1.3)</td>
<td>(3.2)</td>
<td>(0.2)</td>
<td>(0.06)</td>
<td></td>
<td>(0.01)</td>
<td>(0.4)</td>
</tr>
<tr>
<td>C2</td>
<td>100</td>
<td>19</td>
<td>19</td>
<td>40</td>
<td>22</td>
<td>0.75</td>
<td>1.93</td>
<td>27.29</td>
</tr>
<tr>
<td></td>
<td>SD (3.4)</td>
<td>(0.8)</td>
<td>(0.6)</td>
<td>(0.3)</td>
<td>(0.04)</td>
<td></td>
<td>(0.01)</td>
<td>(0.3)</td>
</tr>
</tbody>
</table>

In the study of Holbak [2017], the presence of vertical macropores was also measured at the soil surface and at 50, 100 and 135 cm depth, with three replicates at each depth. Macropores is defined as visible pores (≈>0.2 mm) and divided as either fine pores <1 mm or coarse pores >1 mm. The macropores counts were converted to the distribution of one square meter. In the plow layer, no fine pores were present, and no sign of earthworm activity was observed. Coarse pores were present down to 1 m depth, which indicates preferential connectivity to the level of the tile drain present at 60 cm depth (Table 2).

Table 2. Vertical macropore counts and the coherent standard deviation (SD) at a depth of 0, 50, 100, and 135 cm in 10x10 cm\(^2\) areas in the PD part (Holbak [2017]).

<table>
<thead>
<tr>
<th>Depth [cm]</th>
<th>Fine pores [m(^2)]</th>
<th>SD [m(^2)]</th>
<th>Coarse pores [m(^2)]</th>
<th>SD [m(^2)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-</td>
<td>-</td>
<td>800</td>
<td>150</td>
</tr>
<tr>
<td>50</td>
<td>1000</td>
<td>250</td>
<td>850</td>
<td>100</td>
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<td>100</td>
<td>650</td>
<td>150</td>
<td>550</td>
<td>50</td>
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<tr>
<td>135</td>
<td>200</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
Hansen and Jensen [2013] also conducted a pedological survey of the two parts of the field (PD and WD), where only WD-survey was included in this study since Holbak [2017] included a much more extensive survey of the PD part. The survey of the two-part reveals a much more diverse horizon division of WD with lower clay content and bulk density, which correspondence to the resistivity map. The pedological WD-survey included two C2 horizon, due to the observable differences on the walls of the excavated trench (Table 3).

Table 3. Soil texture analysis from the pedological profiles of the WD part (Hr – Horizon, OM – Organic Matter, BD – Bulk Density) (Hansen and Jensen [2013]).

<table>
<thead>
<tr>
<th>Hr.</th>
<th>Depth [cm]</th>
<th>Clay &lt; 2μm [%]</th>
<th>Silt 2 - 20μm [%]</th>
<th>Fine sand 20 - 200μm [%]</th>
<th>Coarse sand 200 - 2000μm [%]</th>
<th>OM [%]</th>
<th>BD [g cm⁻³]</th>
<th>Porosity [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ap</td>
<td>30</td>
<td>18</td>
<td>14</td>
<td>38</td>
<td>27.2</td>
<td>2.8</td>
<td>1.484</td>
<td></td>
</tr>
<tr>
<td>C1</td>
<td>60</td>
<td>8</td>
<td>20</td>
<td>52</td>
<td>19.5</td>
<td>0.5</td>
<td>1.83</td>
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<tr>
<td>C2.1</td>
<td>125</td>
<td>13</td>
<td>41</td>
<td>36</td>
<td>9.5</td>
<td>0.5</td>
<td>1.725</td>
<td></td>
</tr>
<tr>
<td>C2.2</td>
<td>170</td>
<td>13</td>
<td>41</td>
<td>36</td>
<td>9.5</td>
<td>0.5</td>
<td>1.725</td>
<td></td>
</tr>
<tr>
<td>C3</td>
<td>190</td>
<td>5</td>
<td>9</td>
<td>63</td>
<td>22.5</td>
<td>0.5</td>
<td>1.725</td>
<td></td>
</tr>
<tr>
<td>C4</td>
<td>250</td>
<td>13</td>
<td>41</td>
<td>36</td>
<td>9.5</td>
<td>0.5</td>
<td>1.725</td>
<td></td>
</tr>
</tbody>
</table>

2.2. Soil hydraulics parameter uncertainties

As mentioned earlier, Holbak [2017] measured the soil water retention (SWR) at pF 2 on all samples. As all samples were drained to pF 2, the air permeability was measured. Afterward, samples were rewetted and drained to pF 0.6, 1, 1.7, 2.3, 2.7, 3 and 4.2, respectively. Due to the samples were measured in batches, there were no coherent measurements on one sample (Fig. 3).
Figure 3. Soil water retention and unsaturated conductivity uncertainty range of the C₁ and C₂ horizon for vertical (V) and horizontal (H) direction based on the soil retention and saturated conductivity measurement at PD from Holbak [2017] by fitting the van Genuchten – Mualem soil water retention and conductivity model.

Therefore, all measured retention point were paired up with all possible combination in respect of depth and sampling plane (horizontal-vertical) (~10^5) and selected 2000. To the acquired 8000 combinations, the vG SWR model was fitted. By doing that, parameter ranges were acquired for model calibration. Using the transformed air permeability to saturated hydraulic conductivity [Holbak, 2017] (Kₛ) all Kₛ pair up with the fitted vG model and calculated vGM SWR – conductivity model to represent the uncertainty boundaries within for the C1 and C2 horizon.
Due to the fact that only soil texture analysis excited for the WD-part, SWR model-fitting approach was not a viable option. Therefore pedotransfer functions (PTF) were used to identify the hydraulic properties of the given horizons (Fig. 4). PTFs are functions where unknown soil parameters are estimated based on known soil parameters [Wösten et al., 1999; Wösten and Nemes, 2004]. PTFs are primarily used to estimate soil hydraulic properties because these are difficult, expensive, and time-consuming to analyze [Wösten et al., 1999]. For the WD-part, three different PTF were used. The most well-known HYPRES [Wöst et al., 1999] for European soils, the new PTFs were recently developed by Tóth et al. [2015] called EUPTF, and the updated version of ROSETTA (ROSETTA3) developed by Zhang and Schaap [2017].

Using the above-mentioned approaches, the following parameter ranges have been identified and used for the sensitivity and calibration procedure (Table 4-5).
**Table 4.** Uncertainty range of vGM parameters at PD of C\textsubscript{1} and C\textsubscript{2} horizon for vertical (V) and horizontal (H) direction and the established parameter (PM) range for the calibration.

<table>
<thead>
<tr>
<th>vGM pm</th>
<th>C1</th>
<th></th>
<th></th>
<th></th>
<th>C2</th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td></td>
<td>0\textsubscript{sat}</td>
<td>0\textsubscript{res}</td>
<td>A</td>
<td>n</td>
<td>K\textsubscript{sat}</td>
<td>0\textsubscript{sat}</td>
<td>0\textsubscript{res}</td>
</tr>
<tr>
<td>V</td>
<td>Min</td>
<td>0.31</td>
<td>0.10</td>
<td>0.013</td>
<td>1.131</td>
<td>0.32</td>
<td>0.27</td>
</tr>
<tr>
<td>Max</td>
<td>0.34</td>
<td>0.10</td>
<td>0.116</td>
<td>1.220</td>
<td>4.24</td>
<td>0.32</td>
<td>0.10</td>
</tr>
<tr>
<td>H</td>
<td>Min</td>
<td>0.29</td>
<td>0.10</td>
<td>0.009</td>
<td>1.087</td>
<td>0.29</td>
<td>0.27</td>
</tr>
<tr>
<td>Max</td>
<td>0.37</td>
<td>0.10</td>
<td>0.203</td>
<td>1.225</td>
<td>2.93</td>
<td>0.32</td>
<td>0.10</td>
</tr>
<tr>
<td>PM range</td>
<td>Min</td>
<td>0.29</td>
<td>0.10</td>
<td>0.009</td>
<td>1.087</td>
<td>0.29</td>
<td>0.27</td>
</tr>
<tr>
<td>Max</td>
<td>0.37</td>
<td>0.10</td>
<td>0.203</td>
<td>1.225</td>
<td>4.24</td>
<td>0.32</td>
<td>0.10</td>
</tr>
<tr>
<td>Initial</td>
<td>0.33</td>
<td>0.10</td>
<td>0.106</td>
<td>1.156</td>
<td>2.26</td>
<td>0.29</td>
<td>0.05</td>
</tr>
</tbody>
</table>

The parameter range of vGM for PD is not profoundly diverse, although it seems in Fig. 3, that the SWR based on horizontally sampled retention point, C\textsubscript{1} and C\textsubscript{2} horizon are more variable then SWR based on the vertically collected samples (Table 4). In order to include the variability of both direction, the minimum and the maximum were selected in respect of vGM parameters from both horizons. The I parameter from the Mualem hydraulic conductivity equation was set in a range of –3 to 3 since no direct measurements were available on the unsaturated hydraulic conductivity.

The parameter range of WD was estimated following the same principle, that was used for PD. All horizon seems to have a similar range of SWR with the \(\theta_{sat}\) around 0.4 cm\textsuperscript{3}cm\textsuperscript{-3}, as well as similar shape parameters (a, n), except in C3 horizon, where the ROSETTA3 PTF predicted a much steeper retention curve (Table 5).
Table 5. Parameter range of vGM parameters at WD of Ap, C1, C2, C2.2, C3, and C4 horizon for the calibration.

<table>
<thead>
<tr>
<th>vGM pm</th>
<th>$\theta_{sat}$</th>
<th>$\theta_{res}$</th>
<th>$\alpha$</th>
<th>$n$</th>
<th>l</th>
<th>$K_{sat}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[cm$^3$cm$^{-3}$]</td>
<td>[cm$^3$cm$^{-3}$]</td>
<td>[-]</td>
<td>[-]</td>
<td>[-]</td>
<td>[cm h$^{-1}$]</td>
</tr>
<tr>
<td>Ap</td>
<td>Min</td>
<td>0.40</td>
<td>0.00</td>
<td>0.009</td>
<td>1.191</td>
<td>-4.30</td>
</tr>
<tr>
<td></td>
<td>Max</td>
<td>0.44</td>
<td>0.13</td>
<td>0.043</td>
<td>1.267</td>
<td>5.00</td>
</tr>
<tr>
<td></td>
<td>Initial</td>
<td>0.42</td>
<td>0.06</td>
<td>0.026</td>
<td>1.229</td>
<td>0.35</td>
</tr>
<tr>
<td>C1</td>
<td>Min</td>
<td>0.31</td>
<td>0.00</td>
<td>0.007</td>
<td>1.170</td>
<td>-5.00</td>
</tr>
<tr>
<td></td>
<td>Max</td>
<td>0.40</td>
<td>0.11</td>
<td>0.012</td>
<td>1.308</td>
<td>5.00</td>
</tr>
<tr>
<td></td>
<td>Initial</td>
<td>0.37</td>
<td>0.07</td>
<td>0.020</td>
<td>1.206</td>
<td>0.00</td>
</tr>
<tr>
<td>C2</td>
<td>Min</td>
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<td>0.00</td>
<td>0.005</td>
<td>1.219</td>
<td>-3.32</td>
</tr>
<tr>
<td></td>
<td>Max</td>
<td>0.40</td>
<td>0.11</td>
<td>0.012</td>
<td>1.308</td>
<td>5.00</td>
</tr>
<tr>
<td></td>
<td>Initial</td>
<td>0.37</td>
<td>0.05</td>
<td>0.009</td>
<td>1.263</td>
<td>0.84</td>
</tr>
<tr>
<td>C2.2</td>
<td>Min</td>
<td>0.34</td>
<td>0.00</td>
<td>0.005</td>
<td>1.219</td>
<td>-3.32</td>
</tr>
<tr>
<td></td>
<td>Max</td>
<td>0.40</td>
<td>0.11</td>
<td>0.012</td>
<td>1.308</td>
<td>5.00</td>
</tr>
<tr>
<td></td>
<td>Initial</td>
<td>0.37</td>
<td>0.05</td>
<td>0.009</td>
<td>1.263</td>
<td>0.84</td>
</tr>
<tr>
<td>C3</td>
<td>Min</td>
<td>0.34</td>
<td>0.00</td>
<td>0.008</td>
<td>1.197</td>
<td>-3.73</td>
</tr>
<tr>
<td></td>
<td>Max</td>
<td>0.42</td>
<td>0.14</td>
<td>0.068</td>
<td>1.332</td>
<td>5.00</td>
</tr>
<tr>
<td></td>
<td>Initial</td>
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<td>0.07</td>
<td>0.038</td>
<td>1.264</td>
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<tr>
<td>C4</td>
<td>Min</td>
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<td>0.00</td>
<td>0.005</td>
<td>1.219</td>
<td>-3.32</td>
</tr>
<tr>
<td></td>
<td>Max</td>
<td>0.40</td>
<td>0.11</td>
<td>0.012</td>
<td>1.308</td>
<td>5.00</td>
</tr>
<tr>
<td></td>
<td>Initial</td>
<td>0.37</td>
<td>0.05</td>
<td>0.009</td>
<td>1.263</td>
<td>0.84</td>
</tr>
</tbody>
</table>

2.3. Model and conceptualization

DAISY is a one-dimensional, mechanistic, and deterministic soil-plant-atmosphere system model simulating water and solutes transport, carbon and nitrogen turnover driven by daily or hourly weather and management data [Hansen et al., 2012b]. The model simulates the water flow using the Richards equation [Richards, 1931] and solute transport using the convection – dispersion equation (ADE) in the soil matrix and a macropore model [Hansen et al., 2010a; Mollerup, 2010; Hansen et al., 2012a] to account for preferential N-transport. The model describes the soil hydrology based on measured precipitation and reference evapotranspiration using the Penman-Monteith equation [Allen et al., 1998]. Turnover of organic N from litter and roots, organic fertilizer, and soil organic matter (SOM) is calculated from the actual amount of N in these pools using their carbon-to-nitrogen (C/N) ratio. Net N-mineralization (or immobilization) is driven by the overall N-balance. Additional information regarding the DAISY model can be found at DAISY.
website ([https://daisy.ku.dk/](https://daisy.ku.dk/)) or the following DAISY publications [Hansen et al., 1990; Hansen, 2002; Hansen et al., 2010b; Hansen et al., 2010a; Hansen et al., 2012b].

Figure 5 shows the used division of the soil horizons in the part of the field. PD and WD have been divided according to the pedological profiling, to A_p, C_1, and C_2, and A_p, C_1,C_2,C_2.2, C_3, and C_4, respectively. The macropore settings were based on the macropore count at PD, and macropore count on Nielsen et al. [2010] at WD, due to no macropore description is available at the WD part of the field. Nielsen et al. [2010] counted the macropore distribution on a field with similar characteristics at Taastrup, Denmark, ~56 km away from the location of this study.

**Figure 5.** The model conceptualization of PD and WD. The depth [cm] is given as height above soil surface: The models include the division of the horizon of PD and WD, respectively. The macropore settings include surface connected and buried macropores: ending in the tile drain (DM), and ending in the matrix (MM). The bottom features denoted with A_q represent the fictive aquitard used in the Hooghout Drain Theory.

The macropore setting described is similar to the one applied in Nagy et al. [2019a], using tile drain connected and matrix ended macropore, described by diameter, density, and start – end position. The hydromechanics of the PF is driven by the Poiseuille's equation from the surface and between
the matrix and macropore media is described by the water movement in a confined aquifer, towards a well, where the well is the macropore [Hansen et al., 2010a; Mollerup, 2010; Hansen et al., 2012a]. The macropore flow was initiated by predefined pressure parameters (\(\Psi_{\text{init/term}}, \Psi_{\text{barrier}}\)).

The macropore settings of PD include tile drain connected macropore (DM1 and DM2) and matrix ended macropore (MM2 and MM3). Both types of macropore include surface connected and buried macropores since there was an increase of macropore count in relation to soil depth (Table 2). The macropore description shows that there is no appearance of fine pores in the plow layer (Table 2). In contrast, the description of Nielsen et al. [2010] shows fine macropores in the plow layer. Therefore a surface connected matrix ended macropore (MM1) is included in the WD macropore settings ended in the bottom of the plow layer.

Table 6 shows the used distribution and diameter parameter ranges used for sensitivity and calibration. The average distribution of MM2 and MM3 are 500 m\(^2\) (Table 2), whereas the DM macropore considered to be 10% of the MM macropores. MM1 was set to 100. In order to take into the variation of the horizon depth account, 10 cm variation (min, max), have been added to the identified horizon depth [Holbak, 2017] at PD, and 5% uncertainty range at WD in both up and downward.

**Table 6.** The established parameter range for the macropore setting and horizon division for PD and WD part of the field (Nielsen et al. [2010]; Holbak [2017]; Nagy et al. [2019a]).
2.4. Lower boundary and denitrification model

The drainage in DAISY is described by the widely used Hooghoudt equation [Hooghoudt, 1940]. Originally, the Hooghoudt drainage theory was made for the drainage of land with an impermeable layer below the tile drains. For PD and WD model, an aquitard is set as a boundary condition with a user-defined, constant hydraulic conductivity corresponding to always saturated conductivity, thickness, and the aquifer pressure potential just below the aquitard bottom (Table 7). The parameter range is arbitrarily chosen for the thickness and conductivity of the aquitard. The aquifer pressure potential is assumed to be closely related to the water level in the nearby stream (Vivide Mølleå; Fig. 1).

The denitrification model in DAISY is described by the potential denitrification derived from the CO2 evolution scaled by the anaerobic denitrification constant ($\alpha_d^*$) and the empirical proportionality factor ($K_d$). The potential denitrification is modified by abiotic reduction factors, such as temperature or water content. In this study, the water reduction factor is parametrized by starting relative saturation ($S_t$) and a power function($w$). The denitrification model adjustment follows the study of Nagy et al. [2019b], where they modified the denitrification process of the slow and fast SOM pool as well as the $SOM_{ratio}$ (Table 7).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>PD &amp; WD</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_{MM2}$ [mm]</td>
<td>1 1 3</td>
<td>1 1 3</td>
</tr>
<tr>
<td>$d_{MM3}$ [mm]</td>
<td>1 1 3</td>
<td>1 1 3</td>
</tr>
</tbody>
</table>

Table 7. Parameter range of the DAISY denitrification model and the fictive aquitard at PD and WD.
3. Sensitivity and Calibration methodology

The sensitivity and calibration protocol is adopted from Nagy et al. [2019a] and Nagy et al. [2019b]. The sensitivity analysis is based on the Morris One-At-the-Time (OAT) sensitivity screening [Morris, 1991] by calculating of the Elementary Effect (EE) of each input variable on the output variable, resulting the $\mu^*$ (absolute value of the $\mu(EE)$ proposed by Campolongo et al. [2007]), which represent the absolute importance or additive effects and $\sigma$ (standard deviation), represents the non-linearity or parameter interaction. The sensitivity screening output is ranked by the Morris distance ($\varepsilon$), the euclidean distance from the origo on the $\mu^*$-$\sigma$ coordinate system. For an unbiased selection of sensitive parameters, Nagy et al. [2019b] used a K-means clustering for classifying Low, Medium, and High sensitivity groups.

For calibration, differential evolution (DE) optimization is used developed by Storn and Price [1997] and adapted in the R package by Mullen et al. [2011] and Ardia D. [2016]. DE is commonly known as metaheuristic method as it makes few or no assumptions about the problem, which is being optimized. DE optimizes a problem by keeping a parameter set of a candidate solutions and generating new candidate solutions by incorporating existing parameters in accordance with its formulae, then keeping the parameter set, which has the best fitness to the optimization problem. For further information of the used methods see the cited publication in this section.

The multi-objective function includes the fitting of the GWT - simulated Groundwater Table (cm), $ND$ - transport dynamics (kg N ha$^{-1}$h$^{-1}$), $NC$ - Cumulative N transport (kg N ha$^{-1}$), $DD$ - Drainage Dynamics (mm h$^{-1}$) and $DC$ - Cumulative Drainage (mm) to their measured counterpart from PD and WD for period from 01 May 2017 to 01 May 2018. The sensitivity of the parameters are screened against each sub-objective function separately ($GWT, ND, NC, DD, DC$). The sensitivity screening and calibration are based on nMAE (normalized Mean Absolute Error), and the evaluation of the calibration is based on nMAE, nRMSE (normalized Root Mean Squared Error) and the Kling–Gupta Efficiency measure (KGE). For detailed information on the performance, further information can be found in Krause et al. [2005], Moriasi [2007], Gupta et al. [2009] and Muleta [2011].
4. Results and discussion

4.1. The drainage monitoring of the Tokkerup field

Drainage was measured since 9 November 2016 (Fig. 6). Nitrogen concentration measured in the drainage was initiated 2 January 2017. During the growing season 2017, spring barley was cultivated, but due to the wet autumn, there was no winter crop sown in the fall of 2017. It was, however, decided to add 100 kg of ammonium nitrate (50:50) to evaluate on the drainage N-flux obtained via the N-concentration of the flow-proportional weekly sampled drainage from the two drainage wells representing PD part and the whole field (WD+PD).

Figure 6 shows data from the Tokkerup field in associated drainage periods from well of the PD part and the whole field, respectively. The difference in the drainage was for the entire period less than 30 mm, although the monthly difference during the drainage period is approximately 8.9 mm. The difference occurred in a short-term period in the first half of February 2018. The difference is probably realistic, but can also be zero-point operation for the flow meter in the well representing the PD part, as it measured a drainage event of 22L 10 min^-1 during the summer period, where no other observations from the field could confirm such an event. This zero-point error has been corrected during the summer period of 2018. Drainage during the period 1 January to the end of March was corrected. From 1 December 2017 to 21 April 2018 monitoring results show that the amount of drainage is almost twice the amount of precipitation in the same period. This seems to be caused by the soil profile being close to saturated at the initiation of the period, which is much earlier than normal. The total N-mass transported via drainage in the period was approximately 95 kg N ha^-1 for PD-part and approximately 72.5 kg N ha^-1 for the whole field, which means that N-mass from the WD-part was only 62 kg N ha^-1. This can probably be explained by the higher position of the drain at PD, and thus the much shorter flow path for water and nitrogen for the tile drains.
Figure 6. a) Measured air temperature and precipitation, b) Measured cumulative drainage, c) Measured groundwater table and d) Measured N-concentration and cumulative N-mass at PD and WD during the period of 1 May 2017 – 1 May 2018.
4.2. Sensitive parameters of PD and WD

The sensitivity screening allows identifying the dominant processes in regards to the sub-objectives. Figure 7 shows that in terms of ND to the drainage, the saturated hydraulic conductivity of the horizon C₂ is the most influential at WD part from the matrix parameters, whereas the for the rest of the sub-objectives surprisingly the most sensitive to the residual water content ($\theta_{res}$) of C₄ horizon. Although some other parameter such as $\alpha$, mostly describing the shape of the SWR close to the entry pressure, and saturated hydraulic conductivity ($K_{sat}$) show some sensitivity, it clearly shows that the matrix is not the dominant domain where the transport of water and solute seem to occur. In contrast at PD the Aₚ and C₁ horizon clearly dominant to the water and solute transport, especially C₁, which is to be expected, since the drain is located in this particular horizon in this part of the field. C₂ horizon of PD is not involved in a significant manner of the soil hydraulic as only its saturated hydraulic conductivity shows Medium sensitivity.

In regard to PF, both models show Medium/High sensitive to the same macropore types such as DM₁, DM₂, and MM₂. Nonetheless, Figure 7 shows that due to the higher position of the tile drains at PD, DM₁ as a surface connected macropore more sensitive to DD, ND, and NC. Due to the dual permeability model, the $\Psi_{init/term}$ and $\Psi_{barrier}$ are expected to be sensitive, since they are one of the main drivers of this hydraulic model. The horizon depth of WD shows no sensitivity to any of the sub-objectives. This could mean that the variability of the horizon might not play any role in the hydraulics in a large extent at this part of the field. The SOM ratio surprisingly is only Medium sensitive at PD and WD towards ND and NC. In contrast, the denitrification shows High sensitivity in both slow and fast pool towards NC and Medium to ND.
Figure 7. Result of the Morris sensitivity screening of PD and WD model in regards to DD, DC, ND, NC, and GWT sub-objectives. The results are grouped in matrix, macropore, denitrification, aquitard, horizon, and macropore parameters. The parameter sensitivity is classified as Low, Medium, or High. Chosen calibration parameters are colored black.

4.3. Calibration results of PD and WD model

The calibration of both models resulted in satisfactory results, in at least one, two, or three efficiency measure (nMAE, nRMSE, KGE), in respect of all sub-objectives. As Table 7 shows, the PD-model was able to perform less than SD/2 of the observation, in the case of nMAE and nRMSE,
except in \textit{DD-nRMSE(\%)} and \textit{GWT-KGE}. In respect of WD-model, the performance measures disagree in case of \textit{DD, ND, and GWT}, nMAE, and nRMSE(\%) declare that the \textit{GWT} simulation is not satisfactory, whereas KGE evaluates as a good approximation of the reality.

\textbf{Table 7}. Calibrated sub-objectives and the normalized standard deviation (SD) of the measurements for the model representing the PD and WD part of the field. nMAE – normalized mean absolute error, nSD\textsubscript{MAE} – SD normalized by mean observation, nRMSE(\%) – normalized root mean squared error, nSD(\%) – SD normalized by the maximum deviation of the observation, KGE Kling-Gupta Efficiency.

<table>
<thead>
<tr>
<th>PD/WD</th>
<th>Sub-objectives</th>
<th>nMAE</th>
<th>nSD\textsubscript{MAE}</th>
<th>nRMSE(%)</th>
<th>nSD\textsubscript{RMSE}(%)</th>
<th>KGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>PD</td>
<td>\textit{DD}</td>
<td>0.38</td>
<td>1.25</td>
<td>9.4</td>
<td>17</td>
<td>0.64</td>
</tr>
<tr>
<td></td>
<td>\textit{DC}</td>
<td>0.27</td>
<td>0.95</td>
<td>13.9</td>
<td>35.7</td>
<td>0.63</td>
</tr>
<tr>
<td></td>
<td>\textit{ND}</td>
<td>0.36</td>
<td>1.39</td>
<td>6.8</td>
<td>14.5</td>
<td>0.79</td>
</tr>
<tr>
<td></td>
<td>\textit{NC}</td>
<td>0.05</td>
<td>0.95</td>
<td>3.3</td>
<td>39</td>
<td>0.94</td>
</tr>
<tr>
<td></td>
<td>\textit{GWT}</td>
<td>0.35</td>
<td>0.91</td>
<td>16.2</td>
<td>33.6</td>
<td>0.59</td>
</tr>
<tr>
<td>WD</td>
<td>\textit{DD}</td>
<td>0.4</td>
<td>1.59</td>
<td>7.8</td>
<td>14.9</td>
<td>0.65</td>
</tr>
<tr>
<td></td>
<td>\textit{DC}</td>
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<td>7.7</td>
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</tr>
<tr>
<td></td>
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<td>12.4</td>
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</tr>
<tr>
<td></td>
<td>\textit{NC}</td>
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<td>0.96</td>
<td>7.5</td>
<td>38.9</td>
<td>0.82</td>
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<tr>
<td></td>
<td>\textit{GWT}</td>
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<td>0.29</td>
<td>12.8</td>
<td>20.2</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Figure 8 shows that 62\% and 70\% of the water was transported to the tile drain via the macropore domain, 38\% and 30\% by the matrix medium in the model representing the PD and WD part of the field, respectively. Even though 62\% drainage originated from macropores, 84\% of the N-mass is transported within this water amount in the PD-model, whereas in 70\% drainage from macropore responsible of the transport of 90\% of leached N in WD-model. Macropore type DM1 and DM2 transported 25\% and 38\% of the total amount of drainage, whereas 36\% and 48\% of the total amount of leached N in the PD-model. In contrast, the WD-model predicted that the majority of the drainage(50\%) and N(50\%) was transported via DM2. Although both models show some discrepancies of the drainage mainly after January 2018. This discrepancy can be traced back to the problem of the drainage not yet corrected for the zero-point operation as mentioned earlier.

The simulated GWT matches well the descent measured GWT during May – September 2017 as simulated by the PD-model, whereas the WD-model underpredicts the GWT by \textasciitilde20 cm gradually during the same period. The PD-model shows no dynamics of the GWT after September 2017, where the GWT rises up to the drain level (\textasciitilde66 cm) for about two weeks, but there was no drainage recorded.
Figure 8. Calibration results of model PD and WD: a) separated simulated drainage against measured, b) separated simulated N-mass against measured and c) simulated GWT against measured GWT with the applied aquifer pressure head. All sub-objective presented accordingly with the performance measure nMAE, nRMSE(%) and KGE.

It could be explained that the installed piezometer might not be measuring the actual GWT, but rather a fast transport of water, which is ending up in the piezometric tube by PF. Due to the high compaction of the PD-part, the water could be retained for a more extended period of time in the piezometer, which could result in the slow descent after these rapid rising. The WD-model is able
to capture the dynamics of the winter period 2017-2018, although the ~20 cm mismatch is maintained. The rapid rising at the PD part of the field can be further supported by the low fraction of water transport from the matrix to the drainage, which could be the result of the hindered lateral water flow to the drain by the low conductivity of the surrounding matrix.

The denitrification has remained around the 20 kg N ha\(^{-1}\), which indicate that at the PD part of the field additional 20 kg N ha\(^{-1}\) was mineralized from the soil organic N.

Overall, it can be inferred that the direct connection of PF to the drainage is a significant transport feature of this field. As Figure 9 shows the indirect connection of PF through the top layer, the GWT is also essential. MM2 macropores in both models show a bypass feature by supplying the groundwater table with NO\(_3\)-N from the top part and bottom part of the A\(_p\) layer in the model representing the PD and WD part of the field, respectively. Both model show consistency with the findings of Shipitalo [2004], Frey et al. [2012] and Nagy et al. [2019b] that NO\(_3\)-N is susceptible to leaching through preferential pathway due to the water build-up causing higher pressure potential above a more compacted layer.

The earlier modeling attempts of Holbak [2017] and Gyldengren [2016] were assessed in terms of the sub-objectives of this modeling study. The results and the assessment can be found in the supporting information. All calibrated parameters and model descriptions are available in the supporting information as well.
Figure 9. The summarized NO3-N solute inflow (+) and solute outflow (-) by depth below the surface for the model representing the PD and WD part of the field. The macropore types were separated to show only DM types and MM types.

5. Perspective
This study only includes one season monitoring data from the loamy tile-drained field, Tokkerup. Nonetheless, the findings clearly show the impact of PF and denitrification need to be addressed when assessing the N-fate in such fields. Otherwise, denitrification could be a reason for substantial N-loss, although this modeling study proves the opposite. In order to identify the responsible processes for the nitrogen loss, plot 2 (PD) and 6 (WD), which are located between two side drains, have been selected for further studies. For each plot/location, TDR probes and redox probes have been installed at three different depths at 0.3, 0.6 and 0.9 meters, perpendicular to the side drains at distances 0.5, 4.25 and 8 meters. Six piezometer tubes were placed at only two depths of 0.6 and 0.9 m but at the same distances. With additional bromide tracer experiment, better flow separation can be investigated by assessing the deep percolation and deep leaching of solute to the groundwater.

6. Conclusion
This study was able to prove under no crop condition, that NO3-N can be leached out dramatically faster by PF than it is expected. Macropore transport directly and indirectly involved with the N
loss to the drainage. Buried deep macropore can transport NO$_3$-N to the top layer of the groundwater, which behaves as a rapid intermediary before its transporting further to the tile drain system. In regards to drainage condition, the depth difference does not play a major role in the N loss at the field, since a large majority of the NO$_3$-N is transported by PF, as a result of a highly compacted soil with low conductivity.

Denitrification, in the presence of preferential flow, can be significantly lower as it was expected before, due to the short residence time of the N. Further study needed to understand denitrification and its velocity in macroporous soil.

7. Acknowledgment

The authors would like to express their special thanks of gratitude to members of University of Copenhagen (Kasper S. Jensen, Maja Holbak, Merete Styczen, Per Abrahamsen) for providing the data of the previous model studies, to the members of Agrohydrologerne Aps (Robert Nøddebo Poulsen, Svend Poulsen) for field data collection and to Maja Hørning Skjødt for her terrific data management work.
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Supporting Information for

[Impact of drainage conditions on the fate of nitrogen in an agricultural tile-drained silty loam field.]

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Comparison of earlier studies

In order to see the improvement of the current model, it was intended to compare the model with the previous simulation attempts of the field. Holbak [2017]’s PD model (HPD) and Gyldengren [2016]’s WD model (GWD) were selected, due to they are an improvement on the original study of Hansen and Jensen [2013]. Both models are a single-porosity model, which does not account for PF. According to the efficiency measures, the HPD model is failed to prove satisfactory results in terms of the DD, DC, ND, and NC. However, GWT shows better agreement than in this study. The reason could that the wetting front in this model is much slower than in the PD model, due to the lack of PF.

Table S1. The sub-objectives and the normalized standard deviation (SD) of the measurements of the original model PD [Holbak, 2017] and WD [Gyldengren, 2016]. nMAE – normalized mean absolute error, nSD\textsubscript{MAE} – SD normalized by mean observation, nRMSE(\%) – normalized root mean squared error, nSD\textsubscript{RMSE}(\%) – SD normalized by the maximum deviation of the observation, KGE Kling-Gupta Efficiency. Additionally, ND and NC of the original PD and WD model with the calibrated denitrification model (New D).

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<th>PD/WD</th>
<th>Sub-objectives</th>
<th>nMAE</th>
<th>nSD\textsubscript{MAE}</th>
<th>nRMSE(%)</th>
<th>nSD\textsubscript{RMSE}(%)</th>
<th>KGE</th>
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<tr>
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<tr>
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On the other hand, the GWD model shows better performance towards DD, DC, and ND. It was able to capture the drainage dynamics better as well as resulted in a satisfactory GWT simulation. Nevertheless, both models were unable to capture the quantity of the leached N. Gyldengren [2016] suggested, that it might be the reason for the denitrification model. Therefore, both models were combined with the currently calibrated denitrification model. However, as Table S1 shows, no significant improvement was achieved. In Figure S1, both models (HPD, GWP) outcome is presented. It is also interesting to see in the HPD model, even though the simulated GWT is above the drainage level constantly from October 2017 to March 2018, only a fraction of drainage is simulated. Thereby it can be concluded that these model’s conceptual approach failed to prove their adequacy for this field.
Figure S1. The results of the original models of PD [Holbak, 2017] and WD [Gyldengren, 2016]: a) simulated drainage against measured, b) simulated N leaching against measured and c) simulated GWT against measured GWT with the applied aquifer pressure head. All sub-objective presented accordingly with the performance measure nMAE, nRMSE(%) and KGE.
Figure S2. Simulated N leaching to the drain against measured of the original models of PD[Holbak, 2017] and WD[Gyldengren, 2016] with the calibrated denitrification model. All sub-objective presented accordingly with the performance measure nMAE, nRMSE(%) and KGE.
Table S2. All used parameter for sensitivity screening and calibration of PD and WD. Sensitive parameters are denoted as bold. HPD[Holbak, 2017] and GWD[Gyldengren, 2016] model parameters added for comparison.

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<td>0.021</td>
<td>0.021</td>
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DAISY PD SOIL COLUMN MODEL CODE

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;; Defining soil horizons of plot2

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  0.665101991098054 0)
  (hydraulic_M_VG
    (Theta_res 0.064465)
    (Theta_sat 0.42292378)
    (alpha -0.0349582813409281)
    (n 1.22887216)
    (l 0.35000634)
    (K_sat 4.2895345552366 [cm/h])))

(defhorizon "C1" ISSS4
  (dry_bulk_density 1.830 [g/cm^3])
  (clay 0.08 []) (silt 0.20 [])
  (fine_sand 0.52 [])
  (coarse_sand 0.195 [])
  (humus 0.005 [])
(hydraulic M_vG
(Theta_res 0.06779)
(Theta_sat 0.359498272)
(alpha 0.0333506332592252)
(n 1.205613395)
(l 0)
(K_sat 0.357340078816296 [cm/h]))
)

(defhorizon "C2" ISSS4
 (dry_bulk_density 1.725 [g/cm^3])
 (clay 0.13 [])
 (silt 0.41 [])
 (fine_sand 0.36 [])
 (coarse_sand 0.095 [])
 (humus 0.005 [])

(hydraulic M_vG
(Theta_res 0.052645)
(Theta_sat 0.372584941)
(alpha 0.0111842952656236)
(n 1.2209612599062)
(l 0.83766121)
(K_sat 0.0770274797133575 [cm/h]))
)

(defhorizon "C22" ISSS4
 (dry Bulk Density 1.725 [g/cm^3])
 (clay 0.13 [])
 (silt 0.41 [])
 (fine_sand 0.36 [])
 (coarse_sand 0.095 [])
 (humus 0.005 [])

(hydraulic M_vG
(Theta_res 0.0339921925219481)
(Theta_sat 0.381310173114928)
(alpha 0.00851996)
(n 1.26326391)
(l 0.83766121)
(K_sat 0.96689976 [cm/h]))
)

(defhorizon "C3" ISSS4
 (dry Bulk Density 1.725 [g/cm^3])
 (clay 0.05 [])
 (silt 0.09 [])
 (fine_sand 0.63 [])
 (coarse_sand 0.225 [])
 (humus 0.005 [])

(hydraulic M_vG
(Theta_res 0.071645)
(Theta_sat 0.37673057)
(alpha 0.038211175)
(n 1.264234635)
)
(l 0.63606326)
(K_sat 1.53575195 [cm/h])
)

(defhorizon "C4" ISSS4
  (dry_bulk_density 1.725 [g/cm^3])
  (clay 0.13 [])
  (silt 0.41 [])
  (fine_sand 0.36 [])
  (coarse_sand 0.095 [])
  (humus 0.005 [])

(hydraulic M_vG
  (Theta_res 0.084898747527099)
  (Theta_sat 0.372584941)
  (alpha 0.00851996)
  (n 1.26326391)
  (l 0.83766121)
  (K_sat 0.39188461911724 [cm/h]))
)

(defbiopore common matrix
  (K_wall_relative 1 [%])
  (allow_upward_flow false))

(defbiopore "matrix_1" ;; plough layer
  (common
    (height_start 0 [cm])
    (height_end -30 [cm])
    (diameter 1 [mm])
    (density 5.5 [m^-2])))

(defbiopore "matrix_2" ;; surface connected
  (common
    (height_start 0 [cm])
    (height_end -130 [cm])
    (diameter 1 [mm])
    (density 2.4953023624964 [m^-2])))

(defbiopore "matrix_3" ;; below plough layer
  (common
    (height_start -30 [cm])
    (height_end -130 [cm])
    (diameter 1 [mm])
    (density 10 [m^-2])))

(defbiopore "drain_1" ;; surface connected
  (drain
    (height_start 0 [cm])
    (height_end -30 [cm])
    (diameter 1 [mm])
    (pipe_position -120 [cm])
    (density 7.0868219777476 [m^-2])))

(defbiopore "drain_2" ;; below plough layer
(drain (height_start -30 [cm])
  (height_end -120 [cm])
  (diameter 1 [mm])
  (pipe_position -120 [cm])
  (density 8.6925406048571 [m^-2])))

;; Silstrup Soil Column
(defcolumn TOKK_P2 default
  (Bioclimate default (pet FAO_PM))
  (Chemistry Tokkerup)
  (Surface (EpFactor 0.6 [[]]));; 0.6 under danish condition
  (Soil (MaxRootingDepth 150 [cm])); was 150cm
  (border -110 [cm] -120 [cm] -130 [cm] -140 [cm] -150 [cm])
  (horizons ( -30 [cm] "Ap"
    ( -60 [cm] "C1"
      ( -125 [cm] "C2"
        ( -170 [cm] "C22"
          ( -190 [cm] "C3"
            ( -250 [cm] "C4")
          )
        )
      )
    )
  )
  (Movement vertical
    (Tertiary
      (biopores
        (pressure_initiate -14.9376938446522 [cm]);; Pressure needed to activate biopore flow. clear cut
        (pressure_end -14.9376938446522 [cm]);; Pressure below which biopore flow is deactivated. It should 10
        (pond_max 0.05 [cm]);; Maximum height of ponding before spilling into biopores. After macropores are activated pond will have this height.
        (classes ("matrix_1"
          ("matrix_2"
            ("matrix_3"
              ("drain_1"
                ("drain_2")
            )
          )
        )
        (pressure_barrier 14.9939071753799 [cm]);; Pressure barrier between matrix and biopore domain.
      )
    )
  )
)(drain lateral
  (pipe_position -120 [cm])
  (L 16 [m])
  (x 8 [m]));; needs to be clarified
)(Groundwater aquitard ;;"gwtobsP2.dai"
  (pressure_table file "AquiferP2.txt"
    (Z_aquitard 2 [m])(K_aquitard 0.00828312840484828 [cm/h]))
)(OrganicMatter OM_JG
  (init (input 5385 [kg C/ha/y])
    (bioinc 1502 [kg C/ha/y])
    (root 1123 [kg C/ha/y])
    (end -30 [cm])))

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DAISY WD SOIL COLUMN MODEL CODE

(defchemistry Tokkerup multi
  (combine (N
    (reaction nitrification
      (denitrification
        (K 0.020833)
        (K_fast 0.020833)
        (alpha_fast 0.050346063)
        (alpha 0.1)
        (water_factor_fast (0.837349216 0) (0.847349216 2.85412962596007e-07) (0.857349216 1.2077190490195e-05) (0.867349216 0.000107994807435034)
        (water_factor (0.77000272 0) (0.78000272 0.0434787750533398)
        (dry_bulk_density 1.484 [g/cm^3]) (clay 0.18 []) (silt 0.14 []) (fine_sand 0.38 []) (coarse_sand 0.272 [])
        (humus 2.8 [%]) (C_per_N 9.0 [g C/g N]) (SOM_fractions 0.334898009 0.665101991)
      )
      (hydraulic M_VG
        (Theta_res 0.064465)
        (Theta_sat 0.42292378)
        (alpha 0.034958281)
        (n 1.22887216)
        (l 0.35000634)
        (K_sat 4.289534555 [cm/h])
      )
    )
    (reaction denitrification
      (K 0.020833)
      (K_fast 0.020833)
      (alpha_fast 0.050346063)
      (alpha 0.1)
      (water_factor_fast (0.837349216 0) (0.847349216 2.85412962596007e-07) (0.857349216 1.2077190490195e-05) (0.867349216 0.000107994807435034)
      (water_factor (0.77000272 0) (0.78000272 0.0434787750533398)
      (dry_bulk_density 1.830 [g/cm^3]) (clay 0.06 []) (silt 0.20 []) (fine_sand 0.52 []) (coarse_sand 0.195 []) (humus 0.005 []))
  )))

;; Defining soil horizons of plot2

(defhorizon "Ap" ISSS4
  "Data from Hansen og Jensen 2012"
  (dry_bulk_density 1.484 [g/cm^3]) (clay 0.18 []) (silt 0.14 []) (fine_sand 0.38 []) (coarse_sand 0.272 [])
  (humus 2.8 [%]) (C_per_N 9.0 [g C/g N]) (SOM_fractions 0.334898009 0.665101991)
  (hydraulic M_VG
    (Theta_res 0.064465)
    (Theta_sat 0.42292378)
    (alpha 0.034958281)
    (n 1.22887216)
    (l 0.35000634)
    (K_sat 4.289534555 [cm/h])
  )

(defhorizon "C1" ISSS4
  (dry_bulk_density 1.830 [g/cm^3])
  (clay 0.06 [])
  (silt 0.20 [])
  (fine_sand 0.52 [])
  (coarse_sand 0.195 [])
  (humus 0.005 []))
(hydraulic M_vG
 Theta_res 0.06779)
(Theta_sat 0.359498272)
(alpha 0.033350633)
(n 1.205613395)
(l 0)
(K_sat 0.357340079 [cm/h]))
)

defhorizon "C2" ISSS4
(dry_bulk_density 1.725 [g/cm^3])
(clay 0.13 [])
(silt 0.41 [])
(fine_sand 0.36 [])
(coarse_sand 0.095 [])
(humus 0.005 [])

(hydraulic M_vG
 Theta_res 0.052645)
(Theta_sat 0.372584941)
(alpha 0.011184295)
(n 1.22096126)
(l 0.83766121)
(K_sat 0.07702748 [cm/h]))
)

defhorizon "C22" ISSS4
(dry_bulk_density 1.725 [g/cm^3])
(clay 0.13 [])
(silt 0.41 [])
(fine_sand 0.36 [])
(coarse_sand 0.095 [])
(humus 0.005 [])

(hydraulic M_vG
 Theta_res 0.033992193)
(Theta_sat 0.381310173)
(alpha 0.00851996)
(n 1.26326391)
(l 0.83766121)
(K_sat 0.96689976 [cm/h]))
)

defhorizon "C3" ISSS4
(dry_bulk_density 1.725 [g/cm^3])
(clay 0.05 [])
(silt 0.09 [])
(fine_sand 0.63 [])
(coarse_sand 0.225 [])
(humus 0.005 [])

(hydraulic M_vG
 Theta_res 0.071645)
(Theta_sat 0.37673057)
(alpha 0.038211175)
(n 1.264234635)
(l 0.63606326)
(K_sat 1.535575195 [cm/h])

(defhorizon "C4" ISSS4
  (dry_bulk_density 1.725 [g/cm^3])
  (clay 0.13 [])
  (silt 0.41 [])
  (fine_sand 0.36 [])
  (coarse_sand 0.095 [])
  (humus 0.005 [])

(hydraulic M_vG
  (Theta_res 0.084898748)
  (Theta_sat 0.372584941)
  (alpha 0.00851996)
  (n 1.26326391)
  (l 0.83766121)
  (K_sat 0.391884619 [cm/h])
)

(defbiopore common matrix
  (K_wall_relative 1 [%])
  (allow_upward_flow false))

(defbiopore "matrix_1" ;;plough layer
  (common (height_start 0 [cm])
            (height_end -30 [cm])
            (diameter 1 [mm])
            (density 5.5 [m^-2])))

(defbiopore "matrix_2" ;;surface connected
  (common
    (height_start 0 [cm])
    (height_end -130 [cm])
    (diameter 1 [mm])
    (density 2.495302362 [m^-2])))

(defbiopore "matrix_3" ;;below plough layer
  (common
    (height_start -30 [cm])
    (height_end -130 [cm])
    (diameter 1 [mm])
    (density 10 [m^-2])))

(defbiopore "drain_1" ;; surface connected
  (drain
    (height_start 0 [cm])
    (height_end -30 [cm])
    (diameter 1 [mm])
    (pipe_position -120 [cm])
    (density 7.086821978 [m^-2])))

(defbiopore "drain_2" ;;below plough layer
  (drain (height_start -30 [cm])
  }
(height_end -120 [cm])
(diameter 1 [mm])
(pipe_position -120 [cm])
(density 8.68925406 [m^-2]))

Silstrup Soil Column
(defcolumn TOKK_P2 default
(Bioclimate default (pet FAO_PM))
(Chemistry Tokkerup)
(Surface (EpFactor 0.6 []) ;; 0.6 under danish condition
(Soil (MaxRootingDepth 150 [cm]); was 150cm
(bbox -110 [cm] -120 [cm] -130 [cm] -140 [cm] -150 [cm])
(horizons (-30 [cm] "Ap"
(-60 [cm] "C1"
(-125 [cm] "C2"
(-170 [cm] "C22"
(-190 [cm] "C3"
(-250 [cm] "C4"))

(Movement vertical
(Tertiary (biopores
(pressure_initiate -14.93769384 [cm]); Pressure needed to activate biopore flow. clear cut
(pressure_end -14.93769384 [cm]); Pressure below which biopore flow is deactivated. It should 10
(pond_max 0.05 [cm]); Maximum height of ponding before spilling into biopores. After macropores are activated pond will have this height;
(classes "matrix_1"
("matrix_2"
("matrix_3"
("drain_1"
("drain_2"

(pressure_barrier 14.99390718 [cm]); Pressure barrier between matrix and biopore domain.
))
)

(Drain lateral
(pipe_position -120 [cm])
(L 16 [m])
(x 8 [m])); needs to be clarified
(Groundwater aquitard ;;"gwtobsP2.dai"
(pressure_table file "AquiferP2.txt"
(Z_aquitard 2 [m]) (K_aquitard 0.008283128 [cm/h]))

(OrganicMatter OM_JG
(init (input 5385 [kg C/ha/y])
(bioinc 1502 [kg C/ha/y])
(root 1123 [kg C/ha/y])
(end -30 [cm])))

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Holbak, M. (2017), Hydraulic properties of calcareous subsoils - An investigation of water retention, permeability, and water table dynamics in a drained agricultural field on a young calcareous moraine soil, 119 pp, University of Copenhagen Faculty of Science, Copenhagen.