APPLICATION
OF
SOIL MOISTURE INFORMATION
FOR
OPERATIONAL WATER MANAGEMENT

UNIVERSITY OF TWENTE.

Michiel Pezij

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DISSERTATION

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the degree of doctor at the University of Twente,
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Prof.dr. T.T.M. Palstra,
on account of the decision of the graduation committee,
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by

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in Almelo, the Netherlands.

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“Soms denk ik uren na en heb ik nog niks op papier,
een andere keer bereik ik precies datzelfde in vijf minuten.”

Herman Finkers

Preface

Na vier jaar en een beetje is mijn proefschrift af. Dit werk beschrijft de toepassing van bodemvochtinformatie voor waterbeheer. Aan de start van dit promotieonderzoek was het gebruik van bodemvochtinformatie in Nederlandse waterbeheer beperkt. Echter, recentelijke ontwikkelingen zoals de droge zomer van 2018 hebben het belang van bodemvochtinformatie benadrukt. Ik hoop dan ook dat ik met dit proefschrift heb bijgedragen om met bodemvochtgegevens waterbeheer robuust voor de toekomst te maken.

Het onderzoek heeft mij op mooie plekken binnen en buiten Nederland gebracht. Zo schrijf ik dit voorwoord in San Francisco, waar ik de AGU-conferentie bezoek. Verder denk ik dan aan zomerscholen op het Italiaanse eiland Capri en in Reading, een workshop in Bonn, en conferenties in Wenen. Mede door deze bezoeken vond ik het een voorrecht om aan een promotieonderzoek te werken. Al staat alleen mijn naam op de voorkant van dit boekwerk, uiteraard heb ik dit onderzoek niet kunnen uitvoeren zonder inbreng van anderen. Dit voorwoord wil ik dan ook graag gebruiken om een aantal personen te bedanken voor hun hulp en steun in de afgelopen jaren.

Denie, hartelijk bedankt voor je begeleiding. Je gaf me altijd veel vrijheid in het onderzoek, maar je was er altijd om de rode draad in zicht te houden. Hoewel ons vaste wekelijkse bespreekmoment niet echt een vast wekelijks bespreekmoment was, had je altijd tijd om bij te praten. Niet alleen hadden we goede inhoudelijke discussies, gelukkig was er ook genoeg ruimte voor humor tijdens deze gesprekken. Dit kon ik altijd erg waarderen. Heel veel succes met je nieuwe baan als opleidingsdirecteur, ik weet zeker dat deze functie goed bij je past.

Dimmie, bedankt voor je inzet en waardevolle input tijdens het onderzoek. Je bood me de kans om als gast bij Deltares aan mijn onderzoek te werken. Voor mij was dit een goede manier om kennis te maken met de manier van werken bij een niet-academische partij.

Ik denk terug aan goede samenwerkingen met je collega's, onder andere met Albrecht en Stef, wat uiteindelijk tot een mooie publicatie heeft geleid. Ook de discussies met verschillende collega's tijdens koffie- en lunchpauzes kon ik erg waarderen. Ik kijk dan ook erg positief terug naar de tijd aan de Princetonlaan en Daltonlaan.

Suzanne, jij bood me in de zomer van 2015 de kans om een promotieonderzoek uit te voeren. Naast inhoudelijke feedback heb je me erg geholpen met de organisatie rond het onderzoek. Daarnaast krijg ik de mogelijkheid om na mijn promotieonderzoek aan de vakgroep verbonden te blijven. Ik hoop dan ook op een goede voortzetting van onze samenwerking in de toekomst.

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Last, but not least wil ik me richten op vrienden en familie. De vele borrels, concerten, Schwalbeweekenden, Schwintersportvakanties, fietsweekenden en andere vakanties boden me goede afleiding. Hopelijk gaan we hier mee door in de toekomst.

In het speciaal, Laura, Thijs, mama en papa, bedankt dat jullie er altijd voor me zijn en dat ik altijd bij jullie terecht kan. Weet dat dit zeer gewaardeerd wordt!

Wat mij rest, is het volgende: ik wens jullie veel plezier bij het lezen van dit werk!

Michiel

Summary

Water in the unsaturated part of the soil subsurface is referred to as soil moisture. Soil moisture and related processes are often considered as key components of the hydrological cycle, affecting hydrological, meteorological, biological, and biogeochemical processes. The dry period in the summer of the year 2018 highlighted the necessity of understanding soil moisture dynamics and integrating related information in water management approaches. However, the application of soil moisture information in operational water resources management is limited. One of the reasons is the lack of measurement data. Recently, the increasing availability of high-resolution soil moisture data retrieved using remote sensing methods has led to new possibilities for utilization in water management.

The research aim of this work was to show the potential use of high-resolution soil moisture information for operational water resources management. We followed a research framework in which the needs of water managers were identified. In addition, we focused on retrieving accurate soil moisture information on both regional and local spatial scales. Furthermore, we discussed several applications to integrate the research findings in operational water management.

Firstly, interviews with operational water management experts illustrated that evidence-based information such as measurement data, system knowledge, meteorological forecasts, hydrological model output, and legislation is used for decision-making in Dutch regional operational water management. It also became clear that the experts considerably depend on experiential information, which leads to opinion-based bypasses in decision-making. In addition, we found that hydrological models play a minor role in decision-making in comparison with other evidence-based information sources. We recommend that decision-makers should focus on the development of structured methodologies for integrating both evidence-based and experiential information in decision sup-

port systems. Such systems should deliver tailor-made information in an understandable format at the right time. Indicators could be used as tools to deliver such information. Also, when investing in new technologies, education of water managers is an important aspect which should be taken into account.

Secondly, we found that the accuracy of root zone soil moisture estimates of a hydrological metamodel can be increased using a data assimilation scheme. Data assimilation schemes allow to merge models with up-to-date observations of current water system conditions. To implement such a scheme for the unsaturated zone metamodel MetaSWAP, we developed a data assimilation tool using the open-source framework OpenDA. A perturbed observations Ensemble Kalman Filter was used to assimilate SMAP satellite L3 Enhanced observations of surface soil moisture. The surface soil moisture observations increased the accuracy of regional root zone soil moisture model estimates in terms of the Root Mean Square Error (RMSE) and bias goodness-of-fit measures. On local scales, the results largely depend on how well the SMAP data reflect field conditions. Notably, we were able to update model estimates of root zone soil moisture using observations of surface soil moisture. This finding increases the value of remote sensing data, as satellite-based soil moisture retrievals generally only provide information about the top part of the unsaturated zone. We expect that the increasing availability of high-resolution remotely sensed soil moisture data and developments in data storage and computational environments will lead to an increase in the application of data assimilation schemes in operational water resources management.

Thirdly, we showed the potential of a novel data-driven method for soil moisture modelling. We found that transfer function-noise (TFN) models can accurately describe soil moisture conditions. Impulse-response functions are used to describe the response of soil moisture to stress series such as precipitation and reference crop evapotranspiration. The TFN models were trained using SMAP satellite L3 Enhanced surface soil moisture data. We found that TFN models produce soil moisture estimates of similar accuracy as the remote sensing data using the RMSE goodness-of-fit measure. However, care should be taken when interpreting TFN modelling results in extreme situations due to the data-driven nature of the method. A sensitivity analysis showed that the TFN training period considerably affects the performance of TFN models in both regular and extreme periods. Furthermore, the parameters of the impulse-response functions describe water system characteristics. However, more research is necessary to relate these parameters to physical phenomena.

Finally, this research provides several recommendations for further research. We recommend to continue to study the relationship between the various spatiotemporal scales covered by soil moisture datasets, to consider additional data assimilation applications for operational water resources management, and to explore TFN modelling. Specifically, we encourage to explore the possibilities of TFN soil moisture modelling for practical applications, such as short term soil moisture predictions using model ensembles, data gap filling, the development of historical soil moisture time series, and satellite validation studies. Additionally, several improvements for water management are proposed, focusing on the development of structured methodologies for integrating new information types. Also, the applicability of indicators to create easy-to-interpret information for water managers is promising. We challenge both researchers and water managers to continue to invest in these approaches, as the call for optimized, consistent, and sustainable water management becomes increasingly important in the future.

Samenvatting

Water in het onverzadigde deel van de bodem wordt bodemvocht genoemd. Bodemvocht en bijbehorende processen zijn belangrijke componenten van de hydrologische cyclus. Bodemvocht beïnvloedt onder andere hydrologische, meteorologische, biologische, en biochemische processen. De droge periode in de zomer van het jaar 2018 toonde aan dat het belangrijk is om bodemvochtdynamiek te begrijpen en dergelijke kennis te integreren in waterbeheer. Echter, het gebruik van bodemvochtinformatie in operationeel waterbeheer is beperkt, onder andere doordat bodemvochtmetingen beperkt beschikbaar zijn. Omdat de beschikbaarheid van bodemvochtgegevens verkregen via satellietobservaties significant stijgt, zijn er nieuwe kansen om bodemvochtinformatie te gebruiken in waterbeheer.

Het onderzoeksdoel van dit werk was om de potentie van hoge resolutie bodemvochtinformatie aan te tonen voor operationeel waterbeheer. We hebben een onderzoekskader gevolgd waarin onder andere de behoeften van waterbeheerders zijn geïdentificeerd. Daarnaast hebben we gefocust op het verkrijgen van bodemvochtinformatie op zowel regionale als lokale ruimtelijke schalen. Verder hebben we verscheidende toepassingen besproken om de onderzoeksresultaten te integreren in operationeel waterbeheer.

Allereerst, uit interviews met operationele waterbeheerexperts blijkt dat informatie zoals meetgegevens, systeemkennis, meteorologische voorspellingen, modelberekeningen en wetgeving wordt gebruikt voor besluitvorming in het Nederlandse regionale operationele waterbeheer. Daarnaast steunen de experts aanzienlijk op ervaringsgerichte kennis, wat kan leiden tot suboptimale beslissingen. Verder blijkt dat hydrologische modellering een relatief kleine rol speelt in besluitvorming vergeleken met andere vormen van informatie. We bevelen aan dat besluitvormers zich moeten richten op het ontwikkelen van gestructureerde methoden om de verschillende informatietypen te integreren in bijvoorbeeld beslissingsondersteunende systemen. Op maat gemaakte informatie kan via dergelijke system in een begrijpelijk formaat aangeleverd worden op het juiste moment. Het gebruik van indicatoren maakt het mogelijk om informatie in een begrijpelijk formaat aan te leveren. Tenslotte moet er aandacht besteed worden aan het overbrengen van nieuwe kennis aan waterbeheerders.

Ten tweede is de nauwkeurigheid van modelsimulaties met betrekking op wortelzonebodemvocht vergroot door gebruik te maken van een data-assimilatiemethode. Data-assimilatiemethoden maken het mogelijk om hydrologische modellen te integreren met up-to-date observaties van watersysteemcondities. Wij hebben een data-assimilatietool ontwikkeld voor het onverzadigd zone metamodel MetaSWAP door gebruik te maken van de open-source OpenDA-software. Het L3 Enhanced oppervlaktebodemvochtproduct afkomstig van de SMAP-satelliet is geassimileerd door het toepassen van een *perturbed observations Ensemble Kalman Filter*. Het integreren van de oppervlaktebodemvochtinformatie zorgt er voor dat de nauwkeurigheid van regionale modelsimulaties van wortelzonebodemvocht verhoogd wordt. De resultaten op lokale schaal hangen sterk af van hoe goed de SMAP-satellietobservaties de lokale schaal representeren. De resultaten laten zien dat het mogelijk is om de nauwkeurigheid van modelsimulaties van diepere bodemlagen te verhogen gebruikmakend van oppervlaktebodemvochtobservaties. Bodemvochtsatellietobservaties leveren over het algemeen informatie over de bovenste paar centimeter van de bodem. De resultaten van dit onderzoek verhogen daardoor de waarde van dergelijke satellietobservaties voor waterbeheertoepassingen. Wij verwachten dat de toenemende beschikbaarheid van bodemvochtsatellietobservaties van hoge resolutie en bijbehorende ontwikkelingen in dataopslag en rekenkracht zullen leiden tot meer implementaties van data-assimilatiemethoden in operationeel waterbeheer.

Ten derde hebben we de potentie van een innovatieve datagedreven modelleermethode voor bodemvochtdynamiek aangetoond. *Transfer function-noise* (TFN) modellen kunnen accuraat bodemvochtcondities beschrijven. De bodemvochtdynamiek wordt beschreven door het combineren van neerslag- en verdampingstijdreeksen en impuls-responsfuncties. De impuls-responsfuncties beschrijven de verandering van bodemvocht door respectievelijk neerslag en verdamping. De parameters van deze functies worden afgeleid uit een optimalisatieprocedure waarbij het SMAP L3 Enhanced oppervlaktebodemvochtproduct gebruikt wordt als trainingsdataset. De TFN-modellen hebben een vergelijkbare nauwkeurigheid als de SMAP-satellietobservaties. Echter dient rekening gehouden te worden met de nauwkeurigheid van de TFN-modellen in extreme situaties door de datagedreven aard van deze aanpak. Een gevoeligheidsanalyse laat zien dat het selecteren van de juiste trainingsperiode een grote invloed heeft op de nauwkeurig van de TFN-modellen in zowel reguliere als extreme situaties. Daarnaast kunnen de impuls-responsfuncties gebruikt worden om watersysteemkarakteristieken af te leiden. Meer onderzoek is nodig om de impuls-responsfuncties te koppelen aan fysische processen en variabelen.

Tot slot volgen er een aantal aanbevelingen uit dit onderzoek voor vervolgonderzoek. We adviseren om de relatie tussen de verschillende ruimtelijke en temporele bodemvochtschalen verder uit te zoeken. Ook raden we aan om aanvullende toepassingen van data-assimilatiemethoden voor operationeel waterbeheer te onderzoeken. Verder raden we aan om de mogelijkheden van TFN-modellering voor bodemvochtsimulaties verder te verkennen. Voorbeelden zijn verschillende toepassingen voor bodemvochtvoorspelling op korte termijnen waarbij ensembletechnieken gebruikt kunnen worden om onzekerheidsschattingen te maken, het vullen van ontbrekende gegevens in tijdseries, het ontwikkelen van historische bodemvochttijdseries en satellietvalidatiestudies. Daarnaast stellen we een aantal mogelijkheden voor waterbeheer voor. Een belangrijk aspect is het ontwikkelen van gestructureerde methoden voor het integreren van nieuwe informatietypen voor besluitvorming. Daarnaast is het aanbieden van indicatoren om de toepasbaarheid van informatie te verhogen interessant om het gat tussen onderzoek en praktijk te overbruggen. We dagen zowel onderzoekers als waterbeheerders uit om te blijven investeren in zowel onderzoek als het toepassen van bovengenoemde methoden, gezien consistent, geoptimaliseerd en duurzaam waterbeheer in toenemende mate belangrijk wordt in de toekomst.

Contents

List of abbreviations

AHN	Actueel Hoogtebestand Nederland (Elevation Map The Netherlands)
AMSR2	Advanced Microwave Scanning Radiometer 2
AMSR-E	Advanced Microwave Scanning Radiometer for EOS
ARMA	Autoregressive Moving Average
ASCAT	Advanced Scatterometer
BOFEK2012	Bodemfysische Eenhedenkaart (Soil Physical Units Map)
BOS	Beslissingsondersteunend systeem (decision support system)
CEOS	Committee on Earth Observation Satellites
DA	Data assimilation
DINOloket	Data en Informatie van de Nederlandse Ondergrond (Data and information of the Dutch subsurface)
DSS	Decision Support System
EnKF	Ensemble Kalman Filter
ERS	European Remote Sensing
ESA	European Space Agency
ESA CCI	European Space Agency Climate Change Initiative
EVP	Explained Variance Percentage
FDR	Frequency Domain Reflectometry
GEO	Group on Earth Observations
GEWEX	Global Energy and Water Cycle Experiment
HPC	High-Performance Computing
H-SAF	Satellite Application Facility on Support to Operational Hydrology and Water Management

IT	Information technology
IR	Impulse-response
ISMN	International Soil Moisture Network
ITC	Faculty of Geo-Information Science and Earth Observation (International Institute for Geo-Information Science and Earth Observation)
KNMI	Koninklijk Nederlands Meteorologisch Instituut (Royal Dutch Meteorological Institute)
LCW	Landelijke Coördinatiecommissie Waterverdeling (Dutch National Committee for Water Distribution)
LGN	Landelijk Grondgebruik Nederland (National Land Use the Netherlands)
LHM	Landelijk Hydrologisch Model (National Hydrological Model)
MaaS	Model as a Service
NHI	Netherlands Hydrological Instrument
NWO	Netherlands Organisation for Scientific Research
OL	Open loop
OWAS1S	Optimizing Water Availability with Sentinel-1 Satellites
PIRFICT	Predefined Impulse Response Function In Continuous Time
REGIS	Regionaal Geohydrologisch Informatie Systeem (Regional Geohydrological Information System)
RMSE	Root mean square error
uRMSE	Unbiased root mean square error
RQ	Research question
SCA-V	Single Channel Algorithm at V-polarization
SMAP	Soil Moisture Active Passive
SMOS	Soil Moisture and Ocean Salinity
SCI	Storage Capacity Indicator
SVAT	Soil-Vegetation-Atmosphere-Transfer
SWAP	Soil-Water-Atmosphere-Plant
SWDI	Soil Water Deficit Index
TDR	Time Domain Reflectometry
TFN	Transfer function-noise

List of symbols

θ	Volumetric moisture content $[m^3\ m^{-3}]$
w	Water volume in a soil volume $[m^3]$
V	Soil volume $[m^3]$
ψ	Pressure head $[m]$
$\theta(\psi)$	Volumetric moisture content at pressure head ψ $[m^3\ m^{-3}]$
θ_r	Residual soil moisture content $[m^3\ m^{-3}]$
θ_s	Saturated soil moisture content $[m^3\ m^{-3}]$
α_g	Scale parameter $[m^{-1}]$
n_g	Soil pore size distribution parameter $[-]$
K	Hydraulic conductivity $[m/day]$
z	Elevation above a datum $[m]$
t	Time step $[day]$.
$\overline{X}$	Model mean state $[m^3\ m^{-3}]$
P	Model state error covariance matrix $[(m^3\ m^{-3})^2]$
θ_i^obs	Observed soil moisture estimates $[m^3\ m^{-3}]$
θ_i^pred	Predicted soil moisture estimates $[m^3\ m^{-3}]$
N	Number of observations $[-]$
$\overline{\theta^\mathrm{obs}}$	Averaged observed soil moisture estimate $[m^3\ m^{-3}]$
$\overline{\theta^\mathrm{pred}}$	Averaged predicted soil moisture estimate $[m^3\ m^{-3}]$
r	Pearson correlation coefficient $[-]$
h	Observed soil moisture state $[m^3\ m^{-3}]$
N_{stress}	Number of stress series $[-]$
h_i	Change in soil moisture state due to a stress series i $[m^3\ m^{-3}]$

d	Baseline soil moisture state $[m^3\ m^{-3}]$
n_{res}	Residual time series $[m^3\ m^{-3}]$
R_i	Value of a stress series i $[mm]$
Θ_i	Impulse-response transfer function of the corresponding stress series i
s	Step response function $[m^3\ m^{-3}]$
b	Block response function $[m^3\ m^{-3}]$
A	Unit step response of the state variable due to an input stress $[m^3\ m^{-3}]$
a	Decay rate parameter $[day^{-1}]$
n	Shape parameter $[-]$
$\Gamma(n)$	Gamma function of the form $(n-1)!$ $[-]$
v	White noise $[m^3\ m^{-3}]$
α	Decay parameter $[day]$
σ_h^2	Variance of the SMAP soil moisture observations $[(m^3\ m^{-3})^2]$
σ_n^2	Variance of the TFN model residuals $[(m^3\ m^{-3})^2]$
ET_{act}	Actual evapotranspiration $[mm]$
ET_{ref}	Makkink reference crop evapotranspiration $[mm]$
θ_{fc}	Soil moisture content at field capacity $[m^3\ m^{-3}]$
θ_{aws}	Available water storage $[m^3\ m^{-3}]$
θ_{wp}	Soil moisture content at wilting point $[m^3\ m^{-3}]$

CHAPTER 1

Introduction

1.1 Soil moisture information for water management

Water systems all over the world are affected by climate variability and increasing socio-economic developments. Historically, water management practices in the Netherlands have been strongly driven by flood events (for example in 1993 and 1995), drought events (for example in 1976 and 2003), and socio-economic trends (for example the introduction of Building with Nature concepts) (Haasnoot and Middelkoop, 2012; PBL, 2012; De Vriend et al., 2014; Whelchel et al., 2018). The recent drought caused by the 2018 European heatwave had considerable impacts on water management, agriculture, and nature reserve protection (Vogel et al., 2019; Arcadis, 2019). Figure 1.1 and Figure 1.2 show surface water systems in the eastern part of the Netherlands which ran dry in the summer periods of 2018 and 2019. The drought period activated governmental institutions and water authorities in the Netherlands to re-evaluate management policies. Hence, the grand challenge for national and regional water managers is to optimize water availability for different functions according to users' demands. Among others, reliable and up-to-date information on the current hydrological conditions is essential for skilful management of water systems.

Soil moisture is a central component of the hydrological cycle (Vereecken et al., 2008; Seneviratne et al., 2010; Petropoulos et al., 2015; Zhuo and Han, 2016). Soil moisture is the water in the unsaturated soil above the groundwater table. Although only accounting for approximately 0.01 – 0.05% of global freshwater resources (UNESCO, 1971; Shiklomanov, 1993; Dingman, 2002), soil moisture affects hydrological, meteorological, biological, and biogeochemical processes and interacts with the atmosphere, vegetation, surface water and deeper groundwater layers. For example, the availability of soil moisture affects evapotranspiration rates, which influence atmospheric processes. Also, vegetation growth depends on root water uptake, which is related to the water availability near root systems. Moreover, the soil saturation degree controls the amount of overland flow due to severe precipitation events. Furthermore, soil moisture conditions determine the recharge rate of groundwater aquifers.

Soil moisture is often considered as the missing link in available hydrological data. While data on discharges, surface water levels, groundwater levels, precipitation, and evapotranspiration are more or less integrated into operational water resources management, the application of soil moisture data is limited. A main reason is the limited availability of soil moisture field observations (Cassiani et al., 2006). It has long been recognized that remote sensing data can provide estimates of environmental variables and fluxes

Figure 1.1: A stream in the Netherlands (the Schipbeek) that has run dry during the 2018 European heat wave. Source: RTV Oost/Jan Colijn.

Figure 1.2: Also in 2019 many streams ran dry in the Netherlands, like the Hooge Laarsleiding in the Eastern part of the Netherlands. Photo was taken on September 21 2019 by the author.

(Moradkhani, 2008; Reichle, 2008; Ma et al., 2015; STOWA, 2016; Zhuo and Han, 2016; Sadeghi et al., 2018). For many years, water managers have been interested in remote sensing as a source of high-resolution spatially distributed data. While several initiatives have been employed to utilize remotely sensed soil moisture products (e.g. Crow and Ryu, 2009; Drusch et al., 2009; De Rosnay et al., 2013; Wanders et al., 2014b), operational application is still limited in water resources management. Recently, the emergence of high-resolution remotely sensed soil moisture products has lead to new opportunities for integrating soil moisture information in water management approaches. We define soil moisture products as soil moisture data retrieved from satellite observations. Sentinel-1 and SMAP are examples of satellites providing high-resolution soil moisture data (Entekhabi et al., 2010; Hornacek et al., 2012; Petropoulos et al., 2015; Benninga et al., 2019). This research focused on the integration of high-resolution soil moisture information obtained from remote sensing products in operational water resources management. We studied how to integrate soil moisture information in operational water resources management using both qualitative and quantitative methods.

This chapter provides contextual information on soil moisture (Section 1.2), the relevance of this study (Section 1.3), the problem statement (Section 1.4), the general research aim and questions (Section 1.5), and the research methodology (Section 1.6). Section 1.7 gives an outline for the dissertation.

1.2 Context

1.2.1 Subsurface processes

First, we give an overview of soil subsurface processes. Several zones can be distinguished for hydrological applications. Figure 1.3 shows a schematization of the soil subsurface. Generally, a distinction is made between the unsaturated and saturated zones (Freeze and Cherry, 1979). The unsaturated zone, also known as the vadose zone, is the part of the subsurface where soil pores are not entirely filled with water. Water is retained in the pores by negative pressure heads. The less negative the pressure head, the more saturated the soil is. Water in the unsaturated zone is referred to as soil moisture. Various non-linear processes related to precipitation, evapotranspiration, capillary forces, and infiltration to deeper layers control soil moisture dynamics. Often, soil moisture is expressed as a volumetric moisture content (θ), which is the dimensionless ratio

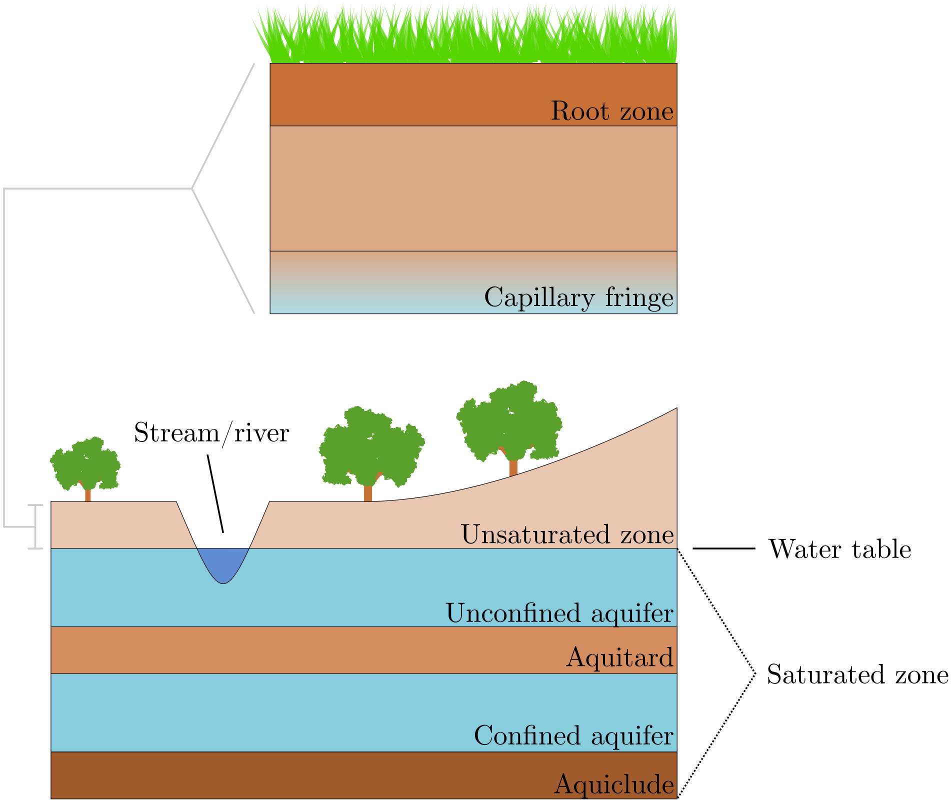

Figure 1.3: Schematization of the soil subsurface. The various zones often distinguished in hydrological applications are shown.

of moisture volume to soil volume:

$$\theta = \frac{w}{V}, \tag{1.1}$$

where w is the water volume in a soil volume $[m^3]$ and V is the soil volume $[m^3]$. The soil moisture content can also be described using pressure heads. The relationship between pressure head and volumetric moisture content is characterized by water retention curves, also known as pF curves. These curves can be described using the relation defined by Van Genuchten (1980):

$$\theta(\psi) = \theta_r + \frac{\theta_s - \theta_r}{[1 + (\alpha|\psi|)^{n_g}]^{1-1/n_g}}, \tag{1.2}$$

where ψ is the pressure head $[m]$, $\theta(\psi)$ is the volumetric moisture content at pressure head ψ $[m^3\ m^{-3}]$, θ_r is the residual soil moisture content $[m^3\ m^{-3}]$, θ_s is the saturated soil moisture content $[m^3\ m^{-3}]$, α_g is a scale parameter inversely proportional to the air entry value $[m^{-1}]$, and n_g is a parameter related to the pore size distribution $[-]$. These parameters are soil-specific. The Staring series provides the parameters for the soil types found in the Netherlands (Wösten et al., 2001). The dataset *BOFEK2012* provides the spatial distribution of the Staring series in the Netherlands (Wösten et al., 2013).

Furthermore, Figure 1.3 shows the capillary fringe and root zone within the unsaturated zone. The capillary fringe forms the transition of the unsaturated zone into the saturated zone. In this zone, capillary tension causes soil pores to almost completely fill with water. The root zone is the part of the unsaturated zone in which vegetation roots can be found. The depth of the root zone depends on both vegetation and soil type. Root zone soil moisture is defined as the amount of moisture in the root zone. The root zone and related processes such as root water uptake and evapotranspiration are vital for hydrological and agricultural applications. The soil porosity, field capacity, and wilting point limits are often associated with the root zone. During a precipitation event, the soil pores start filling due to infiltration of water from the surface. The soil porosity is the maximum amount of soil volume (or pores) that can be filled by water. If the soil moisture content is equal to the soil porosity, the soil is saturated. During and after a precipitation event, water will drain to deeper layers. After both precipitation and gravitational drainage have stopped, the soil is at field capacity. This situation describes the maximum amount of water available for vegetation. The soil moisture content at which vegetation starts to wither is the wilting point. Generally, the soil still contains water at wilting point, although roots are not able to extract the water.

The saturated zone is the part of the subsurface where soil pores are fully filled with water. Water in the saturated zone is referred to as groundwater. The saturated zone can be divided into permeable and impermeable layers. Permeable layers are known as aquifers and typically consist of sand and gravel. An unconfined or phreatic aquifer is connected to the unsaturated zone and allows water to seep from the soil surface to deeper layers directly. A confined aquifer is generally bounded by an impermeable layer which prevents water from seeping into the aquifer. Layers where groundwater flow is limited due to soil properties are referred to as aquitards. The soil of aquitards typically consists of a mix of sand, clay, and silt. A completely impermeable layer is known as an aquiclude and typically consists of clay. The boundary of the unsaturated and saturated zones is defined by the (ground)water table (or level) in case of an unconfined aquifer.

The various meteorological and hydrological processes associated with the subsurface can be described using the hydrological cycle (Freeze and Cherry, 1979). The hydrological cycle describes the circulation of water. Figure 1.4 shows a schematization of the terrestrial part of the hydrological cycle. Water enters the terrestrial part in the form of precipitation. Precipitation is intercepted by vegetation cover or temporarily stored on the surface. Water in the surface storage will either evaporate, infiltrate in the soil, or end up as standing water and overland flow to surface water if the soil infiltration capacity is exceeded. The term evapotranspiration describes both transpiration from vegetation cover and evaporation from bare soil. Transpiration from the saturated zone occurs in areas where vegetation roots tap in groundwater, for example, in wetlands (Balugani et al., 2017). Evapotranspiration rates depend, among others, on the availability of soil moisture. Evapotranspiration reduction can occur in dry periods, which is a mechanism which reduces evapotranspiration when only low amounts of moisture are available. The flow of water from the unsaturated to the saturated zone is known as percolation or recharge. Vice versa, the flow of water from the saturated to the unsaturated zone is known as capillary rise, which can supply water to the unsaturated zone from deeper layers. Interflow and drainage describe lateral unsaturated and saturated flow to surface water, respectively. As interflow does hardly occur in flat regions like the Netherlands, modelling approaches for these regions often neglect this lateral process to allow one-dimensional vertical unsaturated flow assumptions (De Laat, 1980; Van Walsum and Groenendijk, 2008).

1.2.2 Estimating soil moisture states

The limited availability of soil moisture data is a major reason that soil moisture information is not frequently used in water management. A particular challenge is that the direct observation of soil moisture is challenging (Cassiani et al., 2006). A standard technique of directly observing soil moisture is the gravimetric method, in which a soil sample of a known volume and weight is dried in an oven at 105 °C (Walker et al., 2004). The soil moisture content can be derived from the difference in soil weight before and after drying. However, this method is time-consuming, has to be performed in a laboratory, and destroys the soil sample (Dobriyal et al., 2012). The latter implies that the gravimetric method cannot be used for continuous measurements at the same location. As a consequence, indirect non-destructive methods using converting algorithms have to be applied. Therefore, we will use the term *estimate* rather than *measure* or *observe* in the following sections.

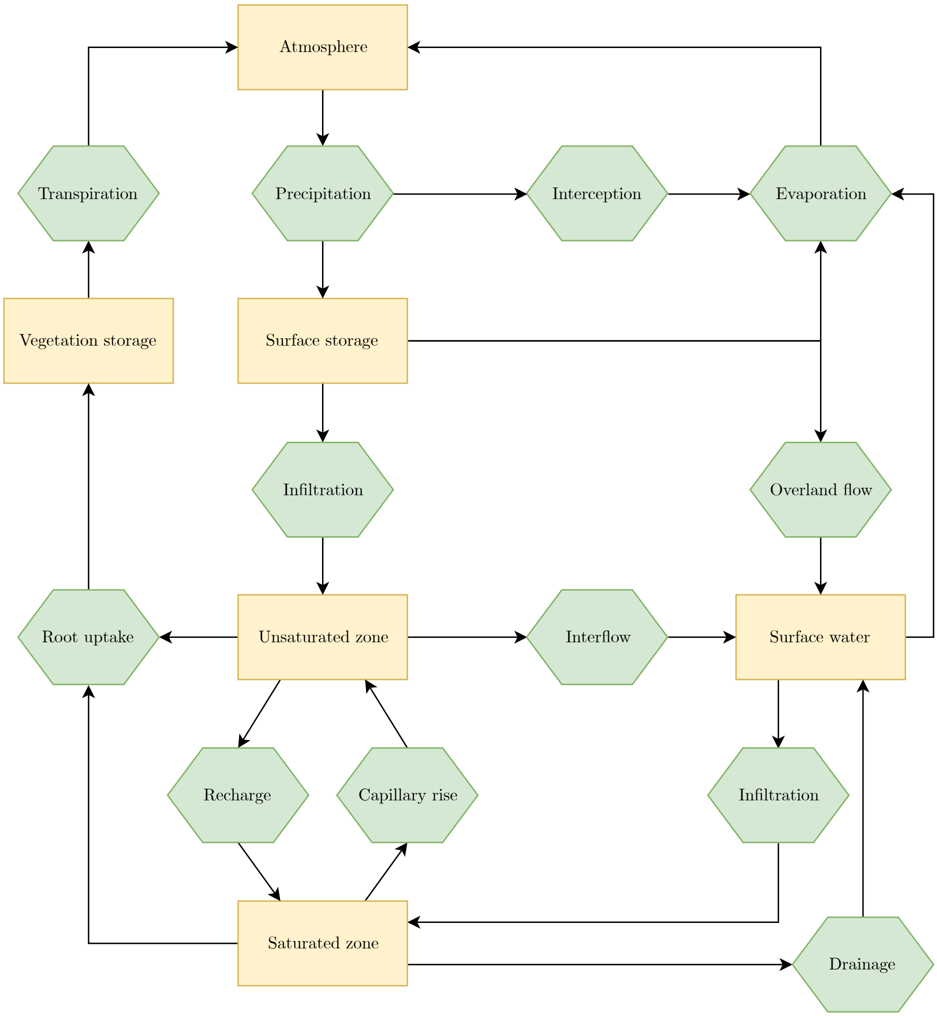

Figure 1.4: System representation of the terrestrial part of the hydrological cycle based on Freeze and Cherry (1979). The rectangles indicate storage reservoirs, while the hexagons indicate fluxes.

Alternatively, three indirect methods exist for estimating soil moisture states on various spatiotemporal scales: in situ (Robinson et al., 2008; Dobriyal et al., 2012), remote sensing (Petropoulos et al., 2015; Srivastava, 2017) and hydrological modelling (Šimůnek et al., 2003; Ochsner et al., 2013; Vereecken et al., 2008). Generally, in situ methods provide information on point scales, while remote sensing and modelling methods are applicable on larger scales. Robinson et al. (2008) and Ochsner et al. (2013) define point estimates on a spatial scale of $\leq 1\ m^2$, while larger-scale estimates have spatial scales of $> 1\ m^2$. The next sections elaborate on the strengths and limitations of the three methods.

In situ

Soil moisture can be estimated by installing sensors in soils at various depths. Electromagnetic techniques such as Time Domain Reflectometry (TDR) and Frequency Domain Reflectometry (FDR) are widely used. The moisture content can also be estimated using neutron probes, cosmic-ray neutron detectors, heat pulse sensors, and tensiometers. We refer to Walker et al. (2004), Robinson et al. (2008), Dorigo et al. (2011), and Susha Lekshmi et al. (2014) for an overview of in situ estimation techniques.

Generally, in situ soil moisture estimates are considered accurate, as the sensors can be calibrated using soil-specific calibration procedures (e.g. by applying the gravimetric method). Furthermore, the estimates can have a high temporal resolution if the sensors are autonomously monitoring. Also, because the sensors can be installed at various depths, a higher vertical spatial resolution can be obtained. However, due to the nature of in situ techniques, the horizontal spatial coverage is typically limited. A dense spatial coverage of point-based in situ estimates is practically impossible due to budget and other practical limitations. Therefore, the application of in situ techniques for continuous monitoring of soil moisture on catchment scales is regarded as impractical. This limitation poses a serious challenge, since in situ estimates are generally used for the validation of remotely sensed soil moisture products, which cover much larger spatial footprints than the in situ sensors.

A well known hub for accessing in situ soil moisture data is the International Soil Moisture Network (ISMN) (Dorigo et al., 2011). The ISMN is a cooperation of the Global Energy and Water Cycle Experiment (GEWEX), the Group on Earth Observations (GEO), the Committee on Earth Observation Satellites (CEOS), and the European Space Agency (ESA). The ISMN can be accessed at `https://ismn.geo.tuwien.ac.at/en`. Examples in the Netherlands are the Twente (Dente et al., 2012; Van der Velde, 2018; Van der Velde et al., 2019) and the Raam (Benninga et al., 2018) soil moisture and tem-

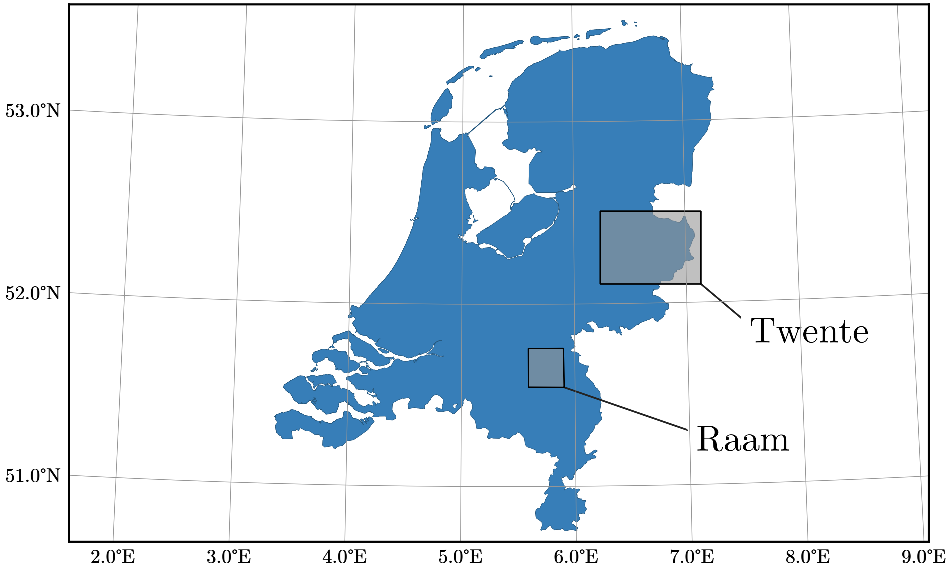

Figure 1.5: Location of the Twente and Raam in situ soil moisture and temperature monitoring networks in the Netherlands.

perature monitoring networks. The networks are maintained by the ITC faculty of the University of Twente and Wageningen University & Research. Figure 1.5 shows the location of the two networks in the Netherlands.

Remote sensing

Remote sensing provides a means to get spatially distributed information. Soil moisture information can be retrieved using both multispectral and microwave sensors. However, multispectral methods show weak relationships to soil moisture in the presence of vegetation covers (Petropoulos et al., 2015). Also, cloud cover significantly impacts multispectral soil moisture retrievals. Therefore, multispectral sensors are limitedly used for soil moisture retrievals. Alternatively, both active and passive microwave sensors are suitable to capture soil moisture dynamics. Microwave sensors show sensitivity to soil moisture, particularly in the low frequency range (1–5 GHz) (Du et al., 2000). Active sensors emit a microwave signal and detect the corresponding backscatter, while passive sensors observe reflected or emitted microwave signals from the soil surface. Examples of satellite sensors providing active soil moisture microwave retrievals are ERS (Naeimi et al., 2009), ASCAT (Wagner et al., 2013), and Sentinel-1 (Wagner et al., 2009; Benninga et al., 2019). Examples of satellite sensors providing passive soil moisture microwave retrievals are AMSR-E, (Njoku et al., 2003; Mladenova et al., 2014), AMSR2 (Imaoka et al., 2010), SMOS (Kerr et al., 2001), and SMAP (Entekhabi et al., 2010).

Generally, soil moisture estimates from remote sensing sensors represent the upper part of the unsaturated zone (up to a couple of centimetres depth), because microwave signals have limited soil penetration depths. Therefore, remote sensing estimates are often referred to as surface soil moisture. We refer to Petropoulos et al. (2015) for an overview of surface soil moisture retrievals from remote sensing. The relationship between surface soil moisture and soil moisture at greater depth is complex, especially in dry periods (Carranza et al., 2018). Extrapolating surface soil moisture to root zone soil moisture information is not trivial, as complex non-linear processes concerning dry-down and hysteresis have to be considered. Currently, no universal method exists for translating surface to root zone soil moisture information. Several studies show that statistical methods (e.g. Albergel et al., 2008; Carranza et al., 2018) or hydrological modelling (e.g. Sabater et al., 2007; Renzullo et al., 2014; Dumedah et al., 2015; Blyverket et al., 2019) can help in extrapolating surface soil information to deeper layers.

Hydrological modelling

Hydrological modelling can be used to estimate soil moisture conditions on various spatial and temporal scales, ranging from local field scale estimates to global soil water storage analyses. Various process-based models exist for describing soil water flow. Typically, they are based on physical laws for mass conservation and energy balances. Many soil water flow models apply the Richards equation to describe water movement in unsaturated soils (Šimůnek et al., 2003; Vereecken et al., 2016). The transient form of the one-dimensional Richards equation, formulated for a time step of one day, is:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial \psi}{\partial z} + 1\right)\right] \tag{1.3}$$

where K is the hydraulic conductivity of the soil $[m/day]$, ψ is the pressure head $[m]$, z is an elevation above a datum $[m]$, and t is the time step $[day]$. As the Richards equation is highly non-linear, it can be challenging to find stable numerical solutions (Vereecken et al., 2016; Zha et al., 2019).

Generally, soil water flow models are forced by meteorological data, such as precipitation and evapotranspiration. On scales larger than field scales, these measurements are obtained by remote sensing methods or interpolation of point measurements. The complex structure of the subsurface is implemented using various parametrizations of surface elevation, soil type, land use, vegetation type, and other characteristics. Parameter values are generally obtained by applying calibration approaches using training data. Typically, these parameter sets are fixed in time. However, hydrological conditions are non-stationary and vary considerably over time , which means that the optimal parameter set of a hydrological model differs over time (Thirel et al., 2015; Beven, 2016). Furthermore, the spatial discretization (e.g. model grid size and the resolution of input data) determines the spatial resolution of the model output. These aspects introduce uncertainties due to the parametrization of soil physical and land use characteristics.

A distinct advantage of hydrological modelling is that models can offer information on similar spatial scales as remote sensing, however on a wider range of temporal scales. While the temporal scale of remote sensing is related to satellite overpasses, models can be run using hourly, daily, and other time steps. Furthermore, hydrological models have the ability to simulate historical and future situations. Additionally, they can be used to estimate the effects of water management measures on hydrological conditions. Therefore, hydrological modelling is suitable for application in operational settings.

The Netherlands Hydrological Instrument (NHI) is an example of an operational tool for water management in the Netherlands. NHI is an integrated process-based modelling instrument for unsaturated water flow, groundwater flow, surface water flow, and surface water distribution (De Lange et al., 2014). The instrument is used for decision-making in operational water management and scenario analyses in the Netherlands. Due to the operational setting, this instrument is particularly suitable for the research presented in this dissertation. The NHI model codes and input data are freely available and can be downloaded at `www.nhi.nu`. Chapter 3 provides a detailed description of NHI.

1.3 Relevance

1.3.1 Impact

Soil moisture significantly impacts other hydrological processes (Vereecken et al., 2008; Seneviratne et al., 2010). For example, soil moisture governs the partitioning of precipitation into infiltration and surface runoff, which affects groundwater recharge and streamflow (Brocca et al., 2010, 2017). Capturing soil moisture dynamics leads to a better understanding of drought, flood and heatwave events (McColl et al., 2017). Spinoni et al. (2014) estimate that more than two billion people have been affected by droughts during the 20th century, causing eleven million deaths globally. Furthermore, Grillakis (2019) states that understanding the role of soil moisture dynamics in the water cycle, including the effect of climate change on soil moisture, is essential to project and mitigate potential impacts on agriculture. Also, soil moisture variability can lead to increased CO_2 emissions from soils (Kechavarzi et al., 2010) and land subsidence in clayey areas, wetlands and peatlands (Querner et al., 2012; Pritchard et al., 2015), which can lead to the destabilization of soils containing construction foundations (Hawkins, 2013).

Drought issues

We can classify droughts in several stages to understand the role of soil moisture in drought issues (Tallaksen and Van Lanen, 2004). The first stage of drought is *meteorological drought*, which is characterized by precipitation deficits. Precipitation deficits arise when evapotranspiration rates are larger than precipitation rates. A meteorological drought can act as a signal value for the other drought stages. One speaks of *agricultural drought* if the precipitation deficit significantly affects crop growth and vegetation in nature areas. Soil moisture conditions play a vital role during agricultural droughts, as crop growth is directly related to the water availability in the unsaturated zone. We refer to a *hydrological drought* if the drought keeps increasing to an extent that surface water and groundwater levels are impacted. Soil moisture also plays an important role in hydrological droughts, as a decrease in soil moisture also leads to decreasing groundwater recharge rates and surface water supply. Eventually, a *socio-economic drought* occurs when the drought is significantly impacting economic activities and leads to reduced water availability for functions like cooling facilities for energy producers and drinking water extractions.

Each drought stage is influenced by the propagation of the drought in the previous stage. Figure 1.6 reflects the time scales on which the various stages of a drought play a role. The dashed lines show the propagation of a drought anomaly, starting from a precipitation deficit to the effect on groundwater levels. Van Loon (2015) refers to the pathways shown in Figure 1.6 with the term *drought propagation*. The pathways show that drought periods in terms of soil moisture may have an substantial impact on groundwater dynamics on longer time scales. Thus, the effect of an agricultural (or soil moisture) drought is not directly tangible when monitoring groundwater observations. Water managers will have to understand both the effects of the different drought stages as well as the drought propagation rate through the hydrological cycle to mitigate drought impacts.

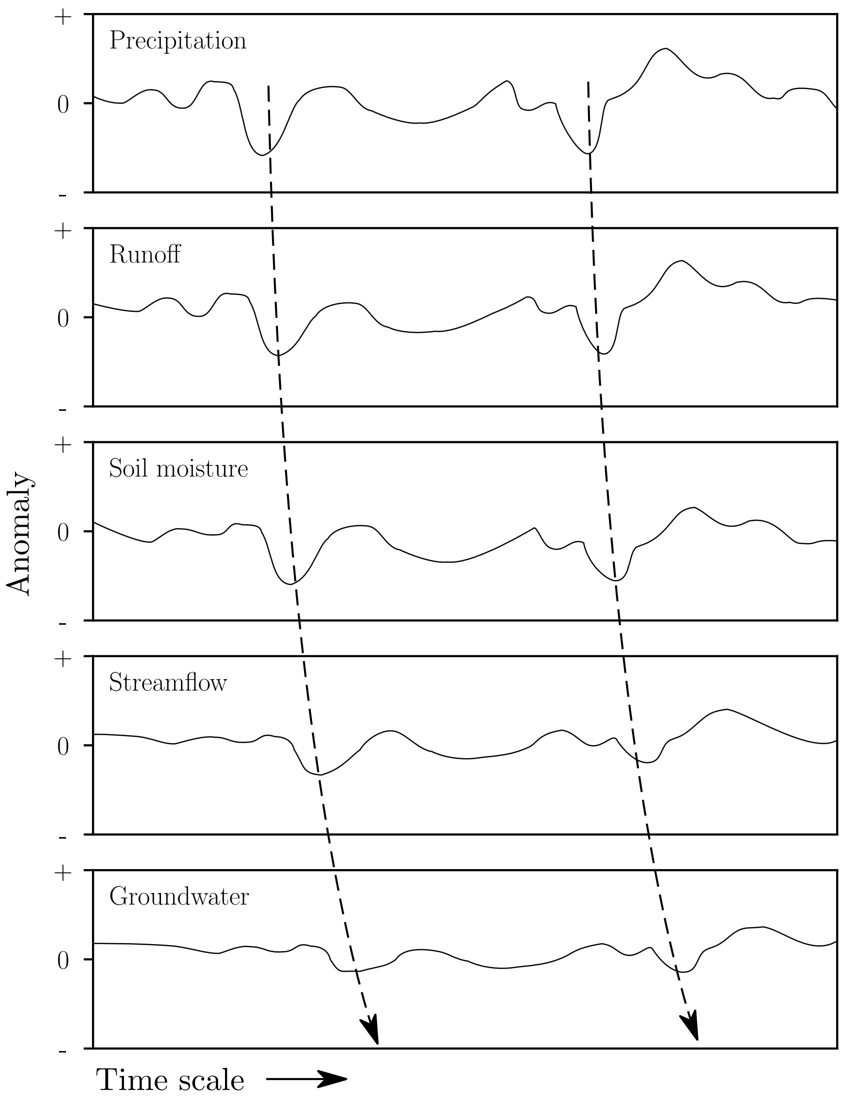

Figure 1.6: Propagation of a drought anomaly through the terrestrial part of the hydrological cycle. The figure is adapted from Changnon Jr (1987) and Van Loon (2015).

Excess water issues

Soil moisture is also an important indicator in excess water situations. The soil moisture content, the soil porosity, and infiltration rates control how much water can be stored in soils during extreme precipitation events. Pre-storm soil moisture conditions partly determine whether precipitation will either infiltrate to deeper soil layers or lead to standing water or overland flow. The accuracy of (flash) flood forecasting systems greatly benefit if up-to-date information on soil moisture is included (Crow and Ryu, 2009; Brocca et al., 2009, 2010; Tramblay et al., 2010; Sutanudjaja et al., 2014; Naz et al., 2019). In particular, soil moisture information improves the understanding of flood peak heights (Wanders et al., 2014b).

1.3.2 Implications for water management

Several studies have investigated the implementation of soil moisture information in operational water resources management (Wanders et al., 2014b; Kurtz et al., 2017; Deng et al., 2019; He et al., 2019), meteorological forecasting (Drusch et al., 2009; De Rosnay et al., 2013), and irrigation management (Brocca et al., 2018). Since soil moisture provides valuable information for drought and flood events as described in Section 1.3.1, information on soil moisture dynamics is a valuable asset for water managers. For example, the recent dry period in the summer of 2018 had an enormous impact on water systems in the Netherlands, as Figure 1.1 and Figure 1.2 illustrate. Figure 1.7 shows the spatially averaged daily soil moisture content for the years 2016–2018 based on data from the in situ Twente soil moisture monitoring network (Dente et al., 2012; Van der Velde, 2018; Van der Velde et al., 2019); see Figure 1.5 for the location of the network. The 2018 time series clearly shows the impact of the 2018 summer heatwave in the months July–August. The soil moisture content drops to the lowest levels observed in recent years. However, it is remarkable that the soil was relatively wet in the spring of 2018 in comparison with 2016 and 2017. So, the soil moisture conditions at the beginning of a year are not necessarily appropriate indicators for the soil moisture conditions in the remainder of a year. Other explanatory variables, like meteorological conditions, are essential to take into account for forecasting purposes.

This example highlights that water managers have to understand historical, present, and soil moisture conditions. However, the application of soil moisture information in operational water resources management is limited. Bastiaanssen et al. (2001) state that although the possibilities of soil moisture remote sensing methods have progressed, accessing, applying, and understanding such information is a challenge for water man-

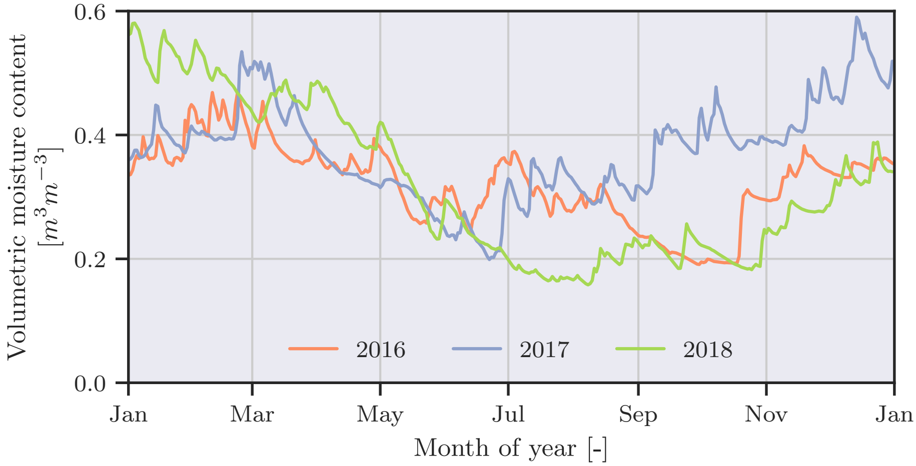

Figure 1.7: Spatial average of daily in situ soil moisture over the Twente region at 20 cm soil depth for the years 2016, 2017, and 2018. Data are retrieved from the Twente soil moisture monitoring network maintained by ITC (Dente et al., 2012; Van der Velde, 2018; Van der Velde et al., 2019).

agers in the Netherlands. During the drought period of 2018, it became clear that Dutch water managers still focus on drought indicators based on precipitation deficit, surface water and groundwater levels, and discharge rates rather than soil moisture conditions. However, evaluations of the 2018 drought period show the importance of incorporating soil moisture information in operational water management (Arcadis, 2019; STOWA, 2019). Several water authorities in the Netherlands are starting studies on how to include such information in their daily operational management. Recently, several initiatives have been launched to study how to integrate soil moisture information in operational applications, such as the European projects EarthH_2Observe (`http://www.earth2observe.eu`) and IMPREX (`http://www.imprex.eu`), OWAS1S by the University of Twente and Wageningen University & Research (`http://www.owas1s.nl`), OWASIS-NL by HydroLogic (`https://business.esa.int/projects/owasis-nl`), and the deployment of various high-resolution soil moisture products by VanderSat (`https://www.vandersat.com`).

1.4 Problem statement

Based on Sections 1.2 and 1.3, we formulate a problem statement. First, we elaborate on the issues and challenges of integrating new information in operational water management. Next, we discuss the discrepancies between spatiotemporal scales of soil moisture estimates. These issues lead to the introduction of a research framework in section 1.6.

Incorporation of new information in water management

Several studies state that the emphasis of information producers should shift from producing large amounts of data towards tailor-made information (Seager, 2001; Timmerman, 2015; STOWA, 2016). Because the perspectives of scientists and water managers (or decision-makers) can be very different for various problems, the needs of water managers should be identified (Acreman, 2005; Timmerman, 2015). Due to this science-policy gap, decision-makers still need to have extensive knowledge for interpretation. The knowledge centre for Dutch regional water managers (*Stichting Toegepast Onderzoek Waterbeheer, STOWA*) identified the science-policy gap as one of the main threats for the application of remote sensing products in operational water management (STOWA, 2016). It is unknown to what extent water managers depend on their experiential (implicit) knowledge in comparison with evidence-based information. Furthermore, to support robust operational water management, it is essential to have reliable hydrological models which can evaluate water management optimization measures as well as provide accurate information on the historical, present and future state of water systems. Water authorities invest considerably in the development of hydrological models. Reinhard and Folmer (2009) state that the application of hydrological models in Dutch water management is widely accepted. However, the extent to which hydrological models are applied for decision-making in operational water resources management is unknown and might not be common practice (Borowski and Hare, 2006; Serrat-Capdevila et al., 2011; Leskens et al., 2014). Therefore, we want to identify the current role of evidence-based information, in particular hydrological models, in operational water management.

Relating soil moisture estimates on various spatiotemporal scales

Figure 1.8 visualizes the spatial and temporal scales covered by the soil moisture estimation methods described in Section 1.2.2. In situ methods cover both small and large temporal scales. However, they lack support for large horizontal spatial scales. Remote sensing methods cover these large horizontal spatial scales. However, the temporal scale of remote sensing is limited. Hydrological modelling covers both small and large spatial and temporal scales. Additionally, considerable variability in soil moisture is found on vertical scales. In situ measurements cover a limited soil volume at specific soil depths.

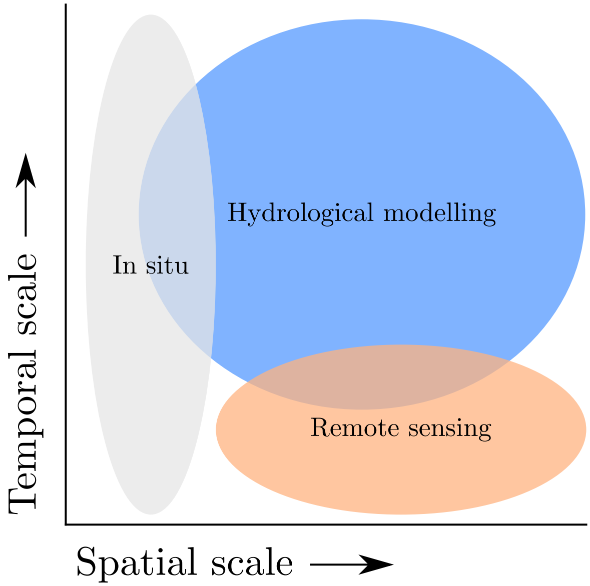

Figure 1.8: The three main soil moisture estimation methods cover different spatial and temporal scales.

Remote sensing products typically capture the upper part of the soil. Hydrological models are often discretized as volume elements of specific surface area and depth as the different soil layers, shown in Figure 1.3, have to be conceptualized.

Operational water management needs consistent and reliable soil moisture information. As the distinct advantages and limitations of the three main estimation methods partly overlap, as shown in Figure 1.8, it is possible to relate the three methods (Houser et al., 1998; Vischel et al., 2008; Rebel et al., 2012; Zhuo and Han, 2016; Brocca et al., 2017; Ford and Quiring, 2019). In situ soil moisture data are often applied in validation studies, in which the in situ data act as ground truth for remote sensing and modelling estimates (e.g. Jackson et al., 2010; Crow et al., 2012; Van der Velde et al., 2019).

A valuable way of merging different soil moisture data sources can be found in the field of data assimilation. Data assimilation methods are promising tools to continuously update process-based models, data-driven models and metamodels with new observations. Sequential data assimilation methods can be used to update model states or parameters at various time steps, which limits model error propagation. Moreover, such methods can handle multiple sources of uncertainties. Several studies show the applicability of data assimilation methods for soil moisture modelling (Houser et al., 1998; Moradkhani, 2008; Reichle, 2008; Liu et al., 2012). Still, the application of sequential soil moisture data assimilation in operational settings is limited. Furthermore, it is unclear how the assimilation of soil moisture affects simulations of other hydrological variables, such as groundwater levels, in integrated hydrological modelling (Brocca et al., 2017).

Innovative modelling approaches

Process-based unsaturated zone models require considerable computational power. Also, the parametrization of the subsurface in the model is often a rough assumption, since many parameters cannot be observed directly. Furthermore, it can be challenging to find stable numerical solutions for process-based soil water flow models (Vereecken et al., 2016; Zha et al., 2019), as was discussed in Section 1.2.2. The availability of new high-resolution remote sensing data enables exploring new data-driven and metamodelling approaches as a replacement of process-based modelling approaches.

1.5 General research aim and questions

The overall aim of this research is to show the potential use of soil moisture information as part of operational water resources management systems, in particular hydrological models, using high-resolution remote sensing data. The following research questions (RQs) are formulated:

RQ1 To what degree are hydrological models currently applied in operational water management and how can their applicability be increased for operational water management?

RQ2 To what extent can the assimilation of a high-resolution remotely sensed surface soil moisture product increase the accuracy of an unsaturated zone hydrological metamodel?

RQ3 To what extent can data-driven modelling, based on high-resolution remote sensing data, be used to provide up-to-date soil moisture information for operational water management?

1.6 Research methodology

We developed a research framework to tackle the challenges identified in Section 1.4, see Figure 1.9. The framework focuses on three aspects: identification, accuracy and

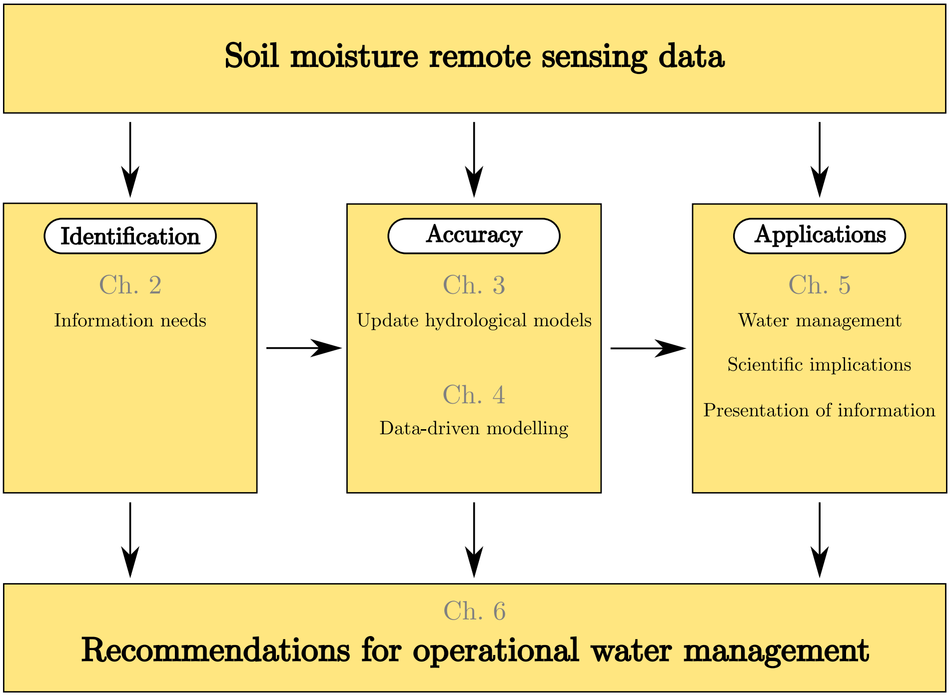

Figure 1.9: Flowchart showing the research framework and the relation between the research steps.

applications. Firstly, RQ1 is studied in Chapter 2, where we identified the information needs of operational water managers. Next, RQ2 and RQ3 focused on retrieving accurate soil moisture information on several spatial and temporal scales. RQ2 is studied in Chapter 3, which focuses on the updating of a process-based hydrological model using a data assimilation scheme and high-resolution remote sensing soil moisture data. RQ3 is studied in Chapter 4, which focuses on data-driven soil moisture modelling. Last, several potential applications of the findings of Chapters 2, 3 and 4 are discussed in Chapter 5, focusing on both scientific and water management implications.

1.6.1 RQ1

We first have to understand which information is currently used and which information is currently requested to integrate new soil moisture information in operational water management. We identified the various types of information used in regional operational water management using interviews with operational water management experts at Dutch regional water authorities. Furthermore, we used the interviews to quantify the extent to which operational decisions are based on available information sources, which we identified as either evidence-based or experiential information. Specifically, we used these results to identify challenges and propose improvements to increase the application of various information types in operational water resources management, based on a literature study.

1.6.2 RQ2

The accuracy of hydrological models partly depends on the training dataset used for model calibration. Data assimilation is a means to incorporate up-to-date information in the model simulations. We developed an open-source data assimilation tool based on the OpenDA framework for the unsaturated zone metamodel MetaSWAP as part of the Netherlands Hydrological Instrument (NHI). The framework is applied to update hydrological metamodel simulations by assimilating remotely sensed surface soil moisture observations obtained from the SMAP satellite. We used a perturbed observations Ensemble Kalman filter. A particular strength of the applied data assimilation scheme is the opportunity to update root zone soil moisture estimates using surface soil moisture observations by defining an appropriate error model. In situ soil moisture measurements were used to validate the results on both regional and local spatial scales.

1.6.3 RQ3

RQ3 focuses on the application of a data-driven method for soil moisture modelling. We applied transfer function-noise (TFN) modelling using remotely sensed surface soil moisture observations for retrieving soil moisture conditions. TFN modelling is a statistical time series modelling method to relate observed time series to input stresses using a linear transformation of impulse-response functions. A distinct advantage of such a method is that no prior assumptions of system processes are needed. Furthermore, TFN modelling is much faster than commonly-used process-based modelling tools for unsaturated zone dynamics. Again, surface soil moisture observations from the SMAP satellite were used to train the TFN models and in situ soil moisture measurements were used to validate the model results.

1.7 Dissertation outline

The structure of the thesis is as follows: Chapter 2 focuses on the current information use in regional operational water resources management in the Netherlands. Chapter 3 describes a method for integrating remotely sensed surface soil moisture observations and an integrated process-based hydrological metamodel using a data assimilation scheme. Chapter 4 elaborates on TFN modelling: a fast and easy-to-construct method for describing soil moisture dynamics based on remote sensing data. Chapter 5 discusses the results of the thesis and focuses on the operational application of the various methods studied in this research. Last, conclusions and recommendations are given in Chapter 6.

CHAPTER 2

The role of evidence-based information in regional operational water management in the Netherlands

This chapter is published as:

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Abstract

The integration of evidence-based information in operational water management is essential for robust decision-making. We investigated the current use of experiential and evidence-based information in Dutch regional operational water management. Interviews with operational water managers at regional water authorities in the Netherlands reveal that they use both evidence-based and experiential information for decision-making. While operational water management is shifting towards an evidence-based approach, experiential information is still important for decision-making. To fulfil the current information need, the operational water managers indicate they would like to have access to high-resolution spatial data, value-added products, and tools for communication to stakeholders. We argue that hydrological models are suitable tools to support these needs. However, while several evidence-based information types are used by operational water managers, hydrological models are limitedly applied. Hydrological models are regarded as inaccurate for operational water management at desired spatial scales. Also, operational water managers often struggle to correctly interpret hydrological model output. We propose several means to overcome these problems, including educating operational water managers to interpret hydrological model output and selecting suitable indicators for evidence-based decision-making.

2.1 Introduction

Densely populated regions like the Netherlands need well-designed operational water management for coping with varying water availabilities and demands (Haasnoot and Middelkoop, 2012). Operational water management requires decision-making within limited time intervals and involve multiple criteria related to for example flood risk, water supply, and navigability (Xu and Tung, 2008). These complex settings are characterized by large uncertainties (Ascough et al., 2008). It is challenging to take robust water management decisions as one has to quantify and assess these uncertainties (Walker et al., 2003; Warmink et al., 2017). Also, water managers have to operate under regulatory, institutional, political, resources, and other constraints, which limit their capacity to use new information (Morss et al., 2005).

Water managers generally use several information types for decision-making (Polanyi, 1966; Raymond et al., 2010), e.g. experiential and evidence-based information. According to Raymond et al. (2010), the classification of information is arbitrary, which means that there are multiple and overlapping ways of defining experiential and evidence-based information. Experiential information is linked to personal perspectives, intuition, emotions, beliefs, know-how, experiences, and values which are not easily articulated and shared (Timmerman, 2015). Evidence-based information can be described, communicated, written down and documented (Nonaka and Takeuchi, 1995). Evidence-based decision-making can help to ensure that untested practices are not widely adopted, because they have been used previously (Sutherland et al., 2004).

Although evidence-based information can significantly contribute to decision-making in operational water management (Timmerman and Langaas, 2005), several studies state that the science-practice gap limits the use of evidence-based information (Ward et al., 1986; Brown et al., 2015). In other words, evidence-based information does not always match the needs of operational water managers. Instead, managers rely on experiential information for decision-making (Pullin et al., 2004). For example, Boogerd et al. (1997) found that decision-making at regional water authorities in the Netherlands is mainly based on personal expertise. Although the amount of available evidence-based information has greatly increased in recent years, the dissemination of relevant information for decision-making remains a challenge (OECD, 2014). The science-practice gap has to be bridged to improve evidence-based decision-making in operational water management (Cosgrove and Loucks, 2015; Timmerman, 2015). In this study, we investigated the present application of experiential and evidence-based information in the Netherlands and its impact on decision-making in operational water management.

Brown et al. (2015) show that the adoption of a scientific framework by operational water managers will improve the credibility of evidence-based decision-making. Decision support systems (DSSs) are designed as supporting frameworks to guide evidence-based decision-making in operational water management. Hydrological models are often an integral part of DSSs (Kersten and Mikolajuk, 1999; Zhang et al., 2013). In this chapter, when we refer to hydrological models, we refer to the application of models in a DSS. Several studies have shown the potential of hydrological models for decision-making in operational water management. Hydrological modelling can help in increasing the understanding of a problem and in defining solution objectives (Guswa et al., 2014), in developing and evaluating promising control measures (Beven and Alcock, 2012), and in providing confidence in the solutions proposed (Kurtz et al., 2017). Not only can hydrological models be used to manage and optimize water systems, model output can also be used to create understanding among stakeholders (Hanington et al., 2017).

However, hydrological model output does not always comply with the needs of decision-makers. Although approaches such as participatory modelling and indicator-based modelling are developed to decrease the science-practice gap, the application of hydrological models by operational water managers is not common practice (Borowski and Hare, 2006; Leskens et al., 2014; Serrat-Capdevila et al., 2011). In contrast, Reinhard and Folmer (2009) state that the use of hydrological models in Dutch water management is widely accepted. It is unknown how hydrological models contribute to decision-making in present-day regional operational water management in the Netherlands.

The aim of this study is to investigate the current role of experiential and evidence-based information, in particular hydrological models, for decision-making in regional operational water management in the Netherlands. We used expert interviews to study the perspective of regional water managers, similar to the studies of Warmink et al. (2011) and Höllermann and Evers (2017). A step-wise approach is applied; first, we studied how experiential and evidence-based decision-making is integrated in Dutch regional operational water management. Secondly, we assessed the integration of hydrological models in evidence-based operational water management.

This chapter is organised as follows: Section 2.2 describes the decision-making framework applied in this study. Section 2.3 introduces the research methodology for the interviews. Results are presented in section 2.4, and are discussed in section 2.5. Finally, conclusions are drawn in section 2.6.

2.2 Decision-making framework

We set up a decision-making framework based on Dicks et al. (2014), see Figure 2.1. This framework is used to analyse interviews with operational water managers to determine which information they use in the decision-making process. The framework is based on the following assumptions:

1. Water managers have to evaluate a water system condition.
2. Water managers collect both evidence-based and/or experiential information concerning this condition.
3. Water managers will assess the water system condition using all available information.
4. Taking a decision will lead to new water system conditions, which again have to be evaluated in time.

Dicks et al. (2014) present two bypass routes that, in this case, operational water man-

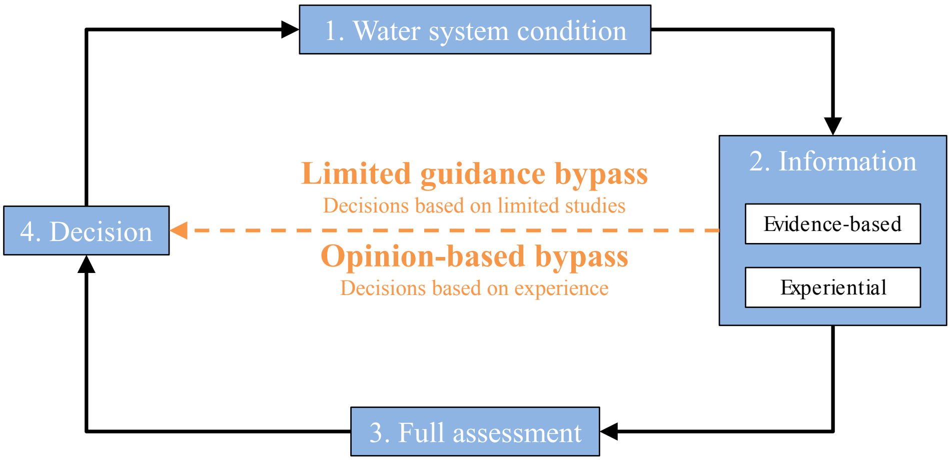

Figure 2.1: Decision-making framework and typical bypasses, adapted from Dicks et al. (2014).

agers can take in decision-making. Firstly, water managers who base their decisions on experiential rather than evidence-based information use the opinion-based bypass. Pullin et al. (2004) described the opinion-based bypass as "relying on the status quo of continuing with an established but unevaluated practice". Secondly, water managers who do not incorporate all available evidence-based information in decision-making use the limited guidance bypass. Water managers are bound to time and other constraints, which limits the ability to take all available information into account. These bypasses may lead to sub-optimal water management decisions. For example, small-scale solutions, such as locally adapting water levels by raising weir levels, may not have the desired effect on catchment-wide scales.

We categorize the decisions as defined in the framework using two aspects that characterize operational water management. These aspects are the situation type and the situation urgency. Firstly, decisions are made for dry or wet situations. Secondly, the decision urgency is a reflection of the severity of the situation. We identify regular day-to-day decisions and calamity decisions concerning extreme events. This leads to four decision-making situations:

- Regular-Dry
- Regular-Wet
- Calamity-Dry
- Calamity-Wet

Typically, decisions concerning dry periods are considered over a time span of weeks. Dry periods often occur during summer. Operational water managers have to monitor and maintain the supply of both surface water and groundwater resources. In regular situations, operational water managers can deal with droughts by controlling a system of pumps and weirs to optimize water supply. During calamity situations, water managers focus on limiting water use by prioritizing important functions like drinking water supply above functions like agriculture, which is a general tendency across the European Union (Kampragou et al., 2011).

Decisions concerning wet situations are generally taken over a time span of hours to days. For example, the supply of water regularly exceeds water demand in winter periods. Decreasing evapotranspiration rates lead to wet soils and shallow groundwater levels. Often, soils cannot adequately cope with heavy precipitation events during such periods, which lead to inundations. Operational water managers can control soil water storage to an extent by adapting surface water levels. Calamity situations like the imminent flooding of streams and rivers can cause severe damage. Controlling the discharge capacity of water infrastructure plays a large role during calamities.

2.3 Methodology

We set up a case study for investigating the use of experiential and evidence-based information for decision-making in regional operational water management.

2.3.1 Study area

We selected six regional water authorities out of a total of twenty-two to incorporate various water management approaches in the Netherlands. Table 2.1 shows their main characteristics and Figure 2.2 shows their management areas within the Netherlands. Aa en Maas and Vechtstromen represent areas within the Netherlands situated above sea level. These areas mainly consist of sandy soils and are generally free-draining, which limit the ability to take control measures. Delfland and Zuiderzeeland represent the low-lying areas within the Netherlands. Most of their management areas lies below sea level and soils are mainly clayey and peaty. Since the water system of the latter authorities is well regulated, water managers have several options for control measures. De Stichtse Rijnlanden and Drents Overijsselse Delta have sandy, clayey, and peaty soils.

Table 2.1: Selected regional water authorities. Statistics are obtained from Unie van Waterschappen (2014).

Water authority	Inhabitants [capita]	Surface area [ha]	Characteristics
Aa en Maas	743,842	161,007	Elevated sandy soils
Delfland	1,200,000	40,547	Clayey polders
De Stichtse Rijnlanden	750,000	83,021	Elevated sandy soils and peaty polders
Drents Overijsselse Delta	600,000	255,500	Elevated sandy soils and clayey polders
Vechtstromen	800,000	227,045	Elevated sandy soils
Zuiderzeeland	400,000	150,000	Clayey polders

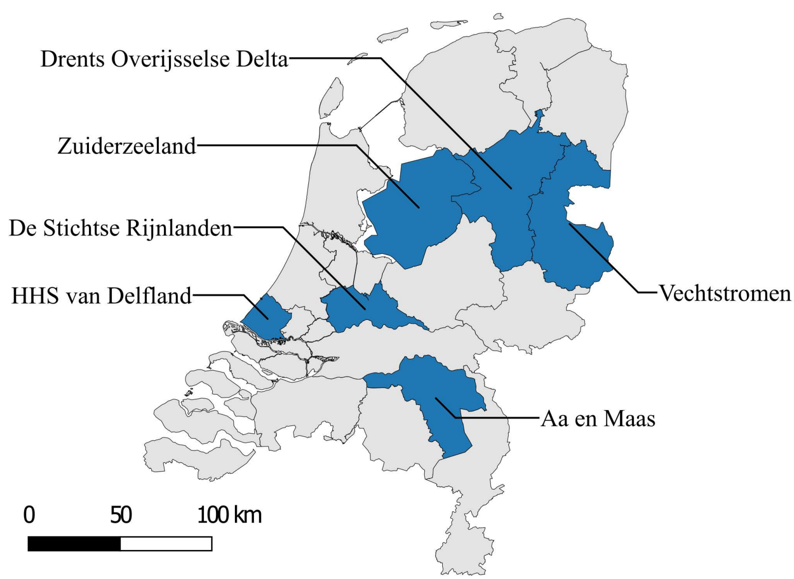

Figure 2.2: Management area of selected regional water authorities in the Netherlands.

Table 2.2: Overview of interview respondents.

	Work experience		
Water authority	<10 years	≥ 10 years	Total
Aa en Maas	1	2	3
Delfland	1	1	2
De Stichtse Rijnlanden	1	1	2
Drents Overijsselse Delta	2	1	3
Vechtstromen	1	1	2
Zuiderzeeland	1	1	2
Total experts	**7**	**7**	**14**

2.3.2 Expert interviews

We interviewed operational water managers at the selected regional water authorities. The daily tasks of these water managers, in this paper also referred to as experts, mainly focus on surface water quantity management. Generally, the regional operational water managers are responsible for a sub-catchment of the water authorities' management area. The limited size of these sub-catchments enables them to develop a good understanding of catchment dynamics and possible measures. At least one experienced and one inexperienced operational water manager was interviewed at each authority. We assume that operational water managers are experienced if they have at least 10 years of work experience, similar to Warmink et al. (2011). In total 14 experts were individually interviewed, see Table 2.2. To limit researcher bias, supervisors at the regional water authorities selected the experts. The interviews were set-up using a semi-structured approach. The interview questions were developed using a literature review and a test interview at regional water authority Vechtstromen. Section 2.7 contains an overview of the interview questions. The interview length was approximately one hour.

Using the decision-making framework (Figure 2.1), we wanted to identify three key aspects in the interviews: the conditions, problems and decisions which regional operational water managers have to cope with, which information water managers use for these decisions, and how the various types of information are used for decision-making. The experts were asked to indicate what type of information they use for decision-making. Since the operational water managers did not use the same terminology, we categorized their answers in information type groups. These information types are split in experiential and evidence-based types according to the decision-making framework defined in section 2.2. Furthermore, we asked the experts to indicate the importance of each information type in the four decision-making situations defined in section 2.2.

The experts had to fill in a Microsoft Excel spreadsheet. A pie chart was updated to directly show the experts the result of their input. The experts were allowed to adapt their input until the results visualized in the pie chart fitted their opinion. This method enabled the experts to reflect on their input. The results were used to study to what extent the experts apply experiential and/or evidence-based information for decision-making. Also, these results indicate whether the experts use all available information for decision-making, or if they use the limited guidance or opinion-bases bypasses as defined in the decision-making framework. Next, the experts were asked to elaborate on their opinion of the current application of hydrological models for decision-making in regional operational water management. They were encouraged to comment on both positive and negative aspects of hydrological model application. This resulted in the identification of improvement points for both model developers and operational water managers. Last, the interview ended with an open question about the information which operational water managers are currently missing for decision-making. We tried to activate experts to not only talk about possible technological developments, but also about social, institutional, and other developments.

2.4 Results

2.4.1 Information types

Operational water managers use a broad spectrum of information types. We identified six information types which are typically applied. These types are listed in Table 2.3.

Firstly, water managers typically use measurement data such as precipitation, runoff in streams, groundwater levels in wells, etc. Next, water managers can use system knowledge such as surface elevation, land use, and soil type. Furthermore, meteorological

Table 2.3: Identified information types.

Information type	Examples
Measurement data	Monitoring of discharge and groundwater levels
System knowledge	Surface elevation, land use and soil type data
Meteorological forecasts	Precipitation and temperature forecasts
Experience	Prior experiences with an encountered situation, such as the lowering of a weir during wet conditions based on intuition
Hydrological model (output)	Assessment of different water management scenarios
Legislation	Water level decrees and other laws

forecasts of precipitation and temperature are valuable to make predictions of future water system states. Also, operational water managers use their expertise and experience to take decisions. For example, a water manager can take a decision based on prior experiences with an encountered problem. Such a decision can lead to the opinion-based bypass (Figure 2.1). In addition, hydrological models are used for decision-making. While the experts do not directly operate models, they often have access to hydrological model output in a DSS. Hydrological models typically provide forecasts of hydrological variables for a specific spatial domain, based on meteorological forecasts and other input data. Last, operational water managers are bound to legislation and institutional policies. For free-draining areas such as the more elevated sandy areas of Aa en Maas, De Stichtse Rijnlanden, Drents Overijsselse Delta and Vechtstromen, water managers have to take into account water level bounds that are pre-described in policy documents. However, water managers are allowed to diverge from this pre-defined set in extreme situations. Polder areas in the management area of De Stichtse Rijnlanden, Drents Overijsselse Delta and Zuiderzeeland have much stricter defined water level rules which are described in water level decrees. Water managers are not allowed to diverge from these decrees. The bound and decrees are defined in cooperation with local stakeholders.

2.4.2 Importance of information types

Every expert agrees that they take decisions based on at least several information types. Figure 2.3 shows the importance of each information type described in Section 2.4.1 in the four decision-making situations (Regular-Dry, Regular-Wet, Calamity-Dry, and Calamity-Wet). The vertical axis in the figure represents the importance of an information type in each decision-making situation. The importance is defined as the contribution of an individual information type in a specific decision-making situation expressed as a percentage. The error bars represent the sample spread by means of the unbiased standard deviation. The variability between the experts is limited, indicating conformity between expert opinions at different regional water authorities.

Operational water managers depend in all decision-making situations mainly on measurement data, system knowledge, meteorological forecasts, and experience. These information types contribute for more than eighty percent to decision-making. Hydrological models and legislation each account for approximately three to eleven percent in all decision-making situations. Experience is the most important information type in every situation. Hydrological models form the least important information type, except for the Calamity-Wet situation, for which legislation is least important.

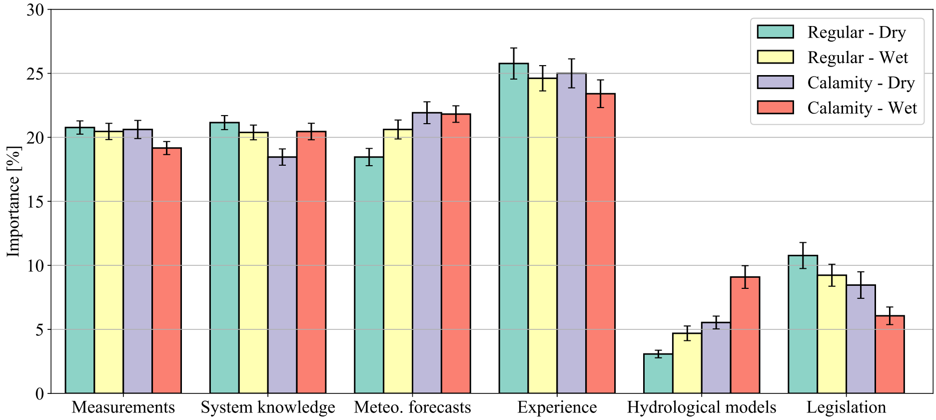

Figure 2.3: Information types used by operational water managers in the four decision-making situations. the error bars represent the unbiased standard deviation.

The importance of each information type slightly differs per decision-making situation. Experience is the most import in all situations, especially in the Regular-Dry situation. The importance of measurement data is similar in the Regular-Dry, Regular-Wet, and Calamity-Dry situations. However, measurement data become slightly less important in the Calamity-Wet situation. Contrarily, the experts attach less value to system knowledge in the Calamity-Dry situation than in the other situations. During dry calamities, the experts state that groundwater level measurement data become more relevant relative to system knowledge. Next, while the importance of meteorological conditions is similar in Calamity-Dry and Calamity-Wet situations, the importance in less in Regular-Dry and Regular-Wet situations. The contribution of hydrological models is relatively small, although models become more important in Calamity-Wet situations. The experts indicate that in those situations models are applied for discharge forecasts. Striking is the relatively small contribution of legislation. The experts see this information type as a boundary condition rather than an information source for decision-making. Legislation is least important in the Calamity-Wet situation, likely because the aim of water management is to get rid of as much water as possible in such a situation. Legislation tends to become a more important information source in Regular-Dry situations, as the water management aim then shift towards maintaining water level bounds and decrees.

2.4.3 Application of hydrological models

Figure 2.3 shows that hydrological models are less used for decision-making in regional operational water management than other information types. Although most experts see the potential of such tools, they give two reasons why hydrological models are limitedly used. Firstly, the experts consider hydrological model output to be too inaccurate and uncertain for their applications. Especially for local scale problems, model estimates often do not comply with observations in their opinion. Secondly, several experts have difficulties interpreting hydrological model output. The interpretation of such data requires understanding of the processes on which the model is based. The experts often do not know on which assumptions, input data and forcing hydrological models are based. Therefore, regional operational water managers tend to ignore model output for decision-making.

2.4.4 Information needs

The experts suggested various improvements for the provision of information. We identified three categories:

- Improved understanding of current water system conditions

The experts want access to up-to-date high-resolution spatial information about current water system conditions. However, they struggle to get a system-wide understanding of these conditions. For example, they find it hard to integrate measurement data to larger spatial scales. Although the application of remote sensing data and hydrological models is promising, such data are currently integrated insufficiently in decision-making.

- Value-added products and triggers

Valuable information should be presented in an adequate way to water managers. According to the experts, information is not always presented to them in the way they want to. For example, operational water managers are generally not directly interested in groundwater level or soil moisture data; they rather want to know what the remaining soil storage capacity is in a wet situation. Also, the experts sometimes have difficulties interpreting the information provided.

- Tools for communication to stakeholders

Operational water managers have to be able to motivate their decisions to stakeholders. However, the experts struggle with communicating their decisions to stakeholders like nature conservation organizations, farmers, industry, etc. These stakeholders can have limited knowledge of water management or fail to overlook the "big picture". The provision of proper information should not only contribute to decision-making itself, but should also play a role in convincing stakeholders to accept decisions.

2.5 Discussion

2.5.1 Experiential versus evidence-based decision-making

Based on the definition in Section 2.1, we classify measurement data, system knowledge, meteorological forecasts, hydrological model output, and legislation as evidence-based information. Experience is classified as experiential information. Figure 2.3 shows that, in their perception, experts depend for approximately 75% on evidence-based information and for 25% on experiential information. So, while Boogerd et al. (1997) stated that regional water management in the Netherlands should increase the integration of evidence-based information, this study shows that operational water management at the selected regional water management authorities is based on both experiential and evidence-based information.

Regional operational water managers considerably depend on experiential information for decision-making. Since there is often no structured way to process the available evidence-based information, the interpretation and expertise of operational water managers remain important for decision-making. Because the hydrological system includes many inherent uncertainties, decision-making will probably always partly depend on experiential information. It is important to note that the interpretation of evidence-based information can differ per water manager.

One could argue that during regular conditions, operational water management functions sufficiently using the currently applied information. However, the application of experiential information may lead to the opinion-based bypass (Figure 2.1) and consequently to sub-optimal decisions. Water managers are not able to validate the effectiveness of measures beforehand. Furthermore, if their decision has the desired effect, no incentive will exist to check whether the decision could be optimized. In addition, the lack of evidence limits posterior evaluation of experiential-based decisions. Finally, experiential information is limited to individual operational water managers. This information will be lost if these managers stop working at the regional water authority. So, there is a need to capture tacit knowledge as evidence-based information.

Therefore, efforts should continue to integrate evidence-based with experiential information for decision-making in regional operational water management in the Netherlands. Similar advice is given for water management in e.g. Japan (Nakanishi and Black, 2018), South Africa and Canada, (Wolfe, 2009) and South Korea (Nam and Choi, 2014). Special focus should be given to the development of structured methodologies for interpreting evidence-based information. The continuing integration of hydrological models in DSSs is suitable for structured decision-making and should therefore be encouraged.

2.5.2 Application of hydrological models for operational water management

The results indicate that the importance of hydrological models for decision-making in regional operational water management is substantially smaller than other evidence-based information types. However, we consider hydrological models as suitable tools which can help improving the three aspects identified in Section 2.4.4. Firstly, hydrological models can provide up-to-date high-resolution spatial information about current water system conditions (Wood et al., 2011). Secondly, spatial information from hydrological models can be used to retrieve value-added products interpretable for operational water managers (Guswa et al., 2014; Kurtz et al., 2017). Thirdly, hydrological models are suitable tools for deriving information in the form of indicators, which can be used in the communication with stakeholders (Eden et al., 2016; Hanington et al., 2017).

Unfortunately, a gap exists between what hydrological model developers think models should provide and what decision-makers demand from models. This gap has both a social and a technical aspect (Leskens et al., 2014). The social gap concerns the fact that model users do not see models as determinant tools for decision-making. Figure 2.3 indicates that the experts consider hydrological models less important than other information types. Decision-makers simply do not have the means or knowledge to investigate all possible measures. This is represented as the limited guidance bypass in the decision-making framework. Also, Section 2.4.3 discusses that the experts often do not have sufficient knowledge to apply hydrological model output in decision-making. Therefore, one should not underestimate the need to sufficiently educate decision-makers and other stakeholders on the use and understanding of hydrological model output.

The technical gap relates to the discrepancy between the information deliverd by hydrological models and the information decision-makers need. The experts think that model output generally contains large uncertainties and therefore hydrological models are inaccurate and unreliable. Although hydrological models should indeed not be seen as perfect representations of reality, they can be applied to identify and quantify uncertainties concerning water management decisions (Refsgaard et al., 2007; Todini, 2007; Warmink et al., 2010).

Furthermore, the experts indicate that they have a need for a better representation of information. Focusing on hydrological models, they state that model output is often difficult to comprehend for implementation in water management. Several studies affirm this statement. Colosimo and Kim (2016) state that decision-makers do not have the time needed to review which information is available and needed for decision-making, while Leskens et al. (2014) found that decision-makers tend to discard information which seems to increase the complexity they already have to deal with. Hanger et al. (2013) found that decision-makers generally do not have a lack of information, but a need for better filtered and accessible information. Therefore, scientists who wish to aid decision-making must generally not offer scientific knowledge, but rather develop information that clearly applies to specific decision–making settings (Maiello et al., 2015).

One way of properly representing evidence-based information is the selection of suitable indicators. Indicators help operational water managers to retrieve system-wide information on historical, current and future time scales. Indicators have already been developed for water resources management (Ioris et al., 2008; Juwana et al., 2012), river management (Richter et al., 1996, 1997; De Girolamo et al., 2017), coastal zone management (Diedrich et al., 2010), climate change adaptation (Hanger et al., 2013; Spiller, 2016), ecosystem management (Guswa et al., 2014), forest management (Carvalho-Santos et al., 2014), hydropower management (Kumar and Katoch, 2014), urban water system management (Dizdaroglu, 2015; Spiller, 2016), and agricultural management (Wang et al., 2015). If suitable indicators are selected, model output can be made more understandable for operational water management. Furthermore, easy-to-interpret model output can be used for communication with stakeholders. Future studies should focus on the validation of suitable indicators for regional operational water management.

2.6 Conclusion

Regional operational water management in the Netherlands depends on both experiential and evidence-based information for decision-making. We identified by means of interviews with regional operational water managers that these experts typically use six information types for decision-making. Measurement data, system knowledge, meteorological forecasts, hydrological models, and legislation are evidence-based information types, while the experience of water managers is experiential information. While the experts largely depend on evidence-based information for decision-making, the experts also depend considerably on experiential information. This may lead to opinion-based bypasses and subsequently to sub-optimal decisions. Operational water managers can improve the decision-making process by continuing efforts to integrate evidence-based information in structured methodologies.

Regional operational water managers depend significantly less on hydrological models than other evidence-based information types for decision-making. Although hydrological models can help in improving the understanding of historic, current, and future water system conditions, can help in deriving interpretable information, and can be used as tools for communication with stakeholders, hydrological models are considered as unreliable for decision-making. Also, operational water managers often have limited knowledge to correctly interpret hydrological model output. We have proposed several means to overcome these issues, for example by increasing efforts to educate decision-makers and other stakeholders, and the selection of suitable indicators for evidence-based decision-making.

Acknowledgments

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2.7 Appendix A

This appendix shows the questions of the semi-structured interviews performed in this chapter.

1. Do you wish to remain anonymous?
2. What is your function at the regional water authority?
3. How long are you working as [*function*] at the regional water authority?
4. What are the problems which you have to deal with?

5. What are the decisions which you have to make?
6. Who else is involved in taking these decisions?
7. Which information do you use in decision-making?
8. Why do you use this information for decision-making?
9. What do you think of the application of hydrological models in regional operational water management?
10. Which information do you want to have for decision-making?

CHAPTER 3

State updating of root zone soil moisture estimates of an unsaturated zone metamodel for operational water resources management

This chapter is published as:

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Abstract

Combining metamodels with data assimilation schemes allows the incorporation of up-to-date information in metamodels, offering new opportunities for operational water resources management. We developed a data assimilation scheme for the unsaturated zone metamodel MetaSWAP using OpenDA, which is an open-source data assimilation framework. A twin experiment showed the feasibility of applying an Ensemble Kalman Filter as a data assimilation method for updating metamodels. Furthermore, we assessed the accuracy of root zone soil moisture model estimates when assimilating the regional SMAP L3 Enhanced surface soil moisture product. The model accuracy is assessed using in situ soil moisture measurements collected at 12 locations in the Twente region, the Netherlands. Although the accuracy of the model estimates does not improve in terms of correlation coefficient, the accuracy does improve in terms of Root Mean Square Error and bias. Therefore, the assimilation of surface soil moisture observations has value for updating root zone soil moisture model estimates. In addition, the accuracy of the model estimates improves on both regional and local spatial scales. The increasing availability of remotely sensed soil moisture data will lead to new possibilities for integrating metamodelling and data assimilation in operational water resources management. However, we expect that significant investments in computational capacities are necessary for effective implementation in decision-making.

3.1 Introduction

The application of integrated physically-based hydrological models is increasing in water resources management (Guswa et al., 2014; Kurtz et al., 2017). Such modelling tools are used for water resources management on various spatial and temporal scales. Water managers can use model output for decision-making while taking into account uncertainties of, among others, input data, boundary and initial conditions, and model structure (Beven and Alcock, 2012). To reduce the uncertainties inherent to integrated physically-based hydrological modelling, data assimilation schemes are often applied (Liu et al., 2012; Weerts et al., 2014). Data assimilation aims to find an optimal combination of merging hydrological model state estimates with observations. Several studies have shown the value of data assimilation schemes for integrated surface-subsurface modelling (Camporese et al., 2009a,b; Zhang et al., 2016; Botto et al., 2018; Zhao and Yang, 2018), some specifically focusing on operational applications (Hendricks Franssen et al., 2011; De Rosnay et al., 2013; Kurtz et al., 2017; He et al., 2019).

Combining integrated physically-based modelling with data assimilation schemes often need considerable computational capacities, which limit the application of data assimilation schemes in operational water resources management. Several studies propose metamodelling as a tool to significantly decrease computation times (Van Walsum and Groenendijk, 2008; Ratto et al., 2012; Razavi et al., 2012; Fraser et al., 2013; Berends et al., 2018). Haberlandt (2010) defines a metamodel as "a substitute for a complex simulation model consisting of simplified, but often non-linear and dynamic relationships. Metamodels can be trained using results from simulation experiments with available process models, expert knowledge and observations if available". The decrease in computational time is a trade-off, since metamodels generally have lower accuracies than the models from which they are derived (Fraser et al., 2013). Metamodels are usually based on models which are calibrated using training datasets. Such datasets consist of a specific period of hydrological observations. Since physically-based models typically include parameters which are difficult to obtain for large spatial domains (Yilmaz et al., 2010), calibration is an important aspect of hydrological model development (Beven and Binley, 1992). However, it is practically impossible to monitor hydrological variables in situ on catchment scales due to time and budget constraints. Remote sensing data provide a means for monitoring across large spatial domains.

A recent development is the emergence of high-resolution satellite-based surface soil moisture observations (Petropoulos et al., 2015; Balsamo et al., 2018). Soil moisture is a key variable in integrated hydrological modelling, since the unsaturated zone relates atmospheric, land surface and subsurface processes (Brocca et al., 2017). Satellite-based soil moisture products provide valuable information for hydrological models if they are used in combination with data assimilation schemes (Houser et al., 1998; Moradkhani, 2008; Reichle, 2008; Liu et al., 2012). Several studies investigated the applicability of remotely sensed soil moisture data for data assimilation by using data products from satellites such as AMSR-E (Sahoo et al., 2013; Wanders et al., 2014a,b), ASCAT (Gruber et al., 2015; Loizu et al., 2018), SMOS (Lievens et al., 2015; Srivastava et al., 2015), H-SAF (Laiolo et al., 2015), SMAP (Koster et al., 2018; Blyverket et al., 2019), a combination of AMSR-2 and SMOS (Gevaert et al., 2018) and a combination of Sentinel-1 and SMAP (Lievens et al., 2017).

Ratto et al. (2012) state that integrating metamodelling with data assimilation schemes could significantly contribute to the operational use of metamodels and remotely sensed soil moisture products for decision-making in operational water resources management. In this study, we use the Netherlands Hydrological Instrument (NHI), a tool used for decision-making in operational water resources management in the Netherlands. NHI is an integrated physically-based modelling framework developed for hydrological simulations on several spatial scales (De Lange et al., 2014). A few studies focus on the combination of the unsaturated zone metamodel MetaSWAP as part of NHI and the assimilation of actual evapotranspiration estimates (Schuurmans et al., 2011; Hartanto et al., 2017), however not on assimilating soil moisture observations. The goal of this study is to evaluate the applicability of a data assimilation scheme for updating root zone soil moisture estimates of a metamodel using a regional surface soil moisture product based on SMAP satellite data (Chan et al., 2018). The main research question is: to what extent can we increase the accuracy of root zone soil moisture estimates of a metamodel by assimilating satellite-based regional surface soil moisture observations?

Section 3.2 gives a description of the data assimilation framework, the metamodel, the data, and the research methodology. Results are shown in section 3.3 and discussed in section 3.4. Conclusions are drawn in section 3.5. A list of abbreviations can be found in section 3.6. Finally, the data assimilation theory is found in section 3.7.

3.2 Methodology

3.2.1 Data assimilation framework

We apply a sequential data assimilation scheme that applies statistical uncertainty measures for assigning weights to both model estimates and observations. Sequential data assimilation improves the accuracy of model estimates in two ways. Firstly, these methods update model states, which lead to more accurate model estimates at the update step. Secondly, the updated model state estimates are used as input for the next modelling time step, which reduces model error propagation. Sequential data assimilation schemes require calculation of the model mean state $\overline{X}$ and corresponding model state error covariance matrix P. Due to the size of P in hydrological model calculations, it is generally not feasible to explicitly calculate P. An alternative approach is the Ensemble Kalman Filter (EnKF), which is a sequential data assimilation scheme suitable for high-dimensional systems (Evensen, 1994). The EnKF is a Monte Carlo implementation of Kalman filtering for non-linear problems. The EnKF uses a sample of evolved model states to estimate the covariance matrix P. This ensemble of model runs is created by perturbing model forcing, parameters and/or states. The model perturbations should represent total model uncertainty and require the development of an error model. Among others, Reichle et al. (2002) and Crow and Wood (2003) showed the potential of applying an EnKF in soil moisture modelling. We refer to 3.7 for a description of EnKF data assimilation theory.

We implemented an EnKF scheme using OpenDA, which is an open-source framework for implementing data assimilation schemes in hydrological modelling (`www.openda.org`). Applications of OpenDA can be found in Ridler et al. (2014) and Van Velzen et al. (2016). OpenDA is a relatively easy-to-implement solution for coupling hydrological models and data assimilation schemes. We coupled this framework with the unsaturated zone metamodel MetaSWAP (described in section 3.2.2) by means of the OpenDA black-box wrapper. Implementation of the black-box wrapper does not require changes in model code and allows for reading and editing of model input and output files. The source code of OpenDA, including the MetaSWAP black-box wrapper, is freely accessible at: `https://github.com/OpenDA-Association/OpenDA`. For the remainder of this chapter, we refer to this coupling as MetaSWAP-OpenDA.

3.2.2 Model description

The NHI modelling framework consists of coupled hydrological models for unsaturated flow, saturated flow, and surface water flow and distribution (De Lange et al., 2014). Figure 3.1 shows a schematic overview of the models and the coupling between them. The models are coupled in a modular way, which means that individual models can run independently. In this research, we use the subsurface part of the Landelijk Hydrologisch Model (LHM), which is the Dutch national application of NHI. The subsurface part consists of two coupled hydrological models: the metamodel MetaSWAP (Van Walsum and Groenendijk, 2008) represents unsaturated zone dynamics and MODFLOW-2005 (Harbaugh et al., 2017) represents saturated zone dynamics. The subsurface part of LHM is schematized on a rectangular grid with a spatial resolution of 250 m by 250 m and a simulation time step of one day.

MetaSWAP

The Soil-Vegetation-Atmosphere-Transfer (SVAT) model MetaSWAP computes the vertical transfer of water in a one-dimensional column between the atmosphere and the saturated zone (Van Walsum and Groenendijk, 2008). MetaSWAP is a metamodel based on the open-source SWAP model (Van Dam et al., 2008). SWAP solves unsaturated soil water flow on field scales by applying the Richards equation. MetaSWAP applies a simplified approach in which the one-dimensional partial differential Richards equation is replaced by two ordinary differential equations: an equation for vertical variations as-

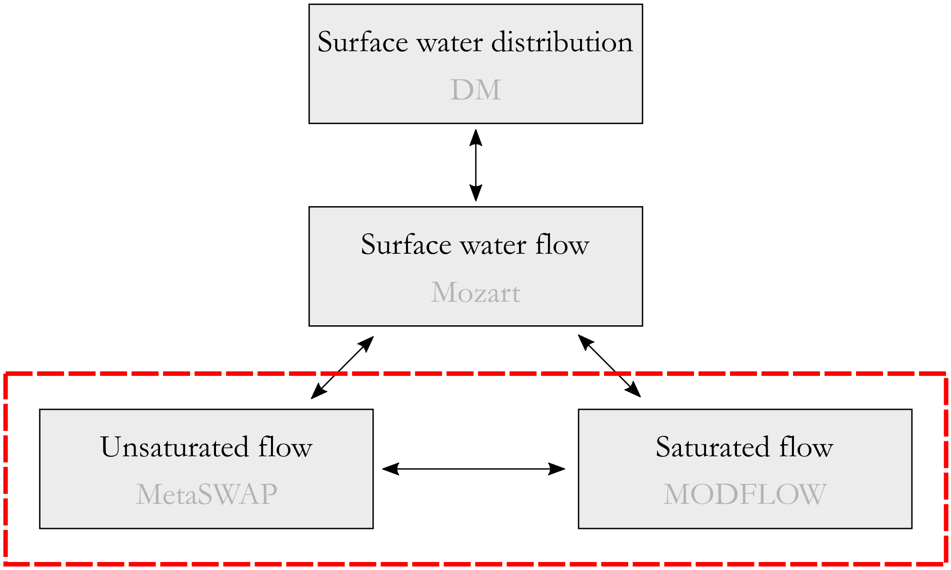

Figure 3.1: Software codes covering the various hydrological domains within the Netherlands Hydrological Instrument (NHI) (De Lange et al., 2014). The red dashed box indicates the subsurface part applied in this study.

suming steady state flow and an equation accounting for variations in time. Steady state solutions are stored in a database of pre-computed soil saturation profiles at discrete intervals of soil moisture conditions and groundwater depths. The unsaturated zone is discretized into up to 18 vertical aggregation boxes, starting with the root zone and ending with a box extending into the saturated zone. These boxes are linked as reservoirs. The soil saturation degree of each box is retrieved from the pre-computed database during each time step.

MetaSWAP needs several spatial datasets as input. The Actueel Hoogtebestand Nederland (AHN) is used as a digital elevation model (Actueel Hoogtebestand Nederland, 2019). The Landelijk Grondgebruik Nederland (LGN) dataset supplies land cover data (Hazeu, 2014). Precipitation and Makkink reference evapotranspiration rasters obtained from KNMI data are used as model forcing (KNMI, 2018b,a). The BOFEK2012 dataset supplies soil physical parameters for 72 soil units in the Netherlands (Wösten et al., 2013). Van Walsum and Van der Bolt (2013) verified the MetaSWAP meta-approach for these soil units by comparing transpiration output of MetaSWAP with transpiration output of the SWAP model. The meta-approach leads to faster calculation times in comparison with SWAP, while the transpiration output of MetaSWAP did not deviate more than 5%

from the SWAP output.

The metamodelling concept of MetaSWAP has implications for applying data assimilation procedures. Firstly, vegetation dynamics are parametrized using a pre-defined root zone depth growth pattern. As the root zone depth varies in the growing season, also the depth of the first aggregation box of MetaSWAP varies. Data assimilation results are therefore only comparable for periods with similar root zone depths, like summer or winter periods. Secondly, the data assimilation procedure requires a model restart after each update step. The use of a single precision format in the model restart files introduces small differences in the restarted model run (Van Walsum, 2017). Section 3.4.1 discusses the effect of the model restart on model accuracy.

MODFLOW

MODFLOW-2005 is a software package for simulating 3D groundwater flow (Harbaugh et al., 2017). The schematization of MODFLOW in LHM consists of seven layers. These seven aquifers and aquitards represent the hydrogeological layers distinguished in the Dutch national hydrogeological database REGIS (De Lange et al., 2014). MODFLOW is coupled to MetaSWAP using a shared state variable (Van Walsum and Veldhuizen, 2011), phreatic groundwater head for MODFLOW and groundwater level for MetaSWAP respectively. During each time step, groundwater levels are determined by iteration of MODFLOW and MetaSWAP. The iteration stops when the difference in groundwater head of MODFLOW and MetaSWAP is within a pre-defined limit.

Data assimilation for MetaSWAP-MODFLOW models

The potential of data assimilation for coupled MetaSWAP-MODFLOW models has been studied before. Schuurmans et al. (2011) assimilated satellite-based actual evapotranspiration data using a constant gain Kalman filter to update actual evapotranspiration model estimates. Furthermore, Hartanto et al. (2017) used satellite-based actual evapotranspiration data in combination with a Particle Filter to improve discharge simulations. Due to the availability of high-resolution soil moisture observations, we extend the findings of Schuurmans et al. (2011) and Hartanto et al. (2017) by assessing the applicability of soil moisture observations to update soil moisture states of MetaSWAP.

In the aforementioned studies, the MetaSWAP grid was scaled with a single factor per time step, therefore not accounting for the spatial distribution of the observations. The OpenDA framework enables assimilation of multiple observations at various locations.

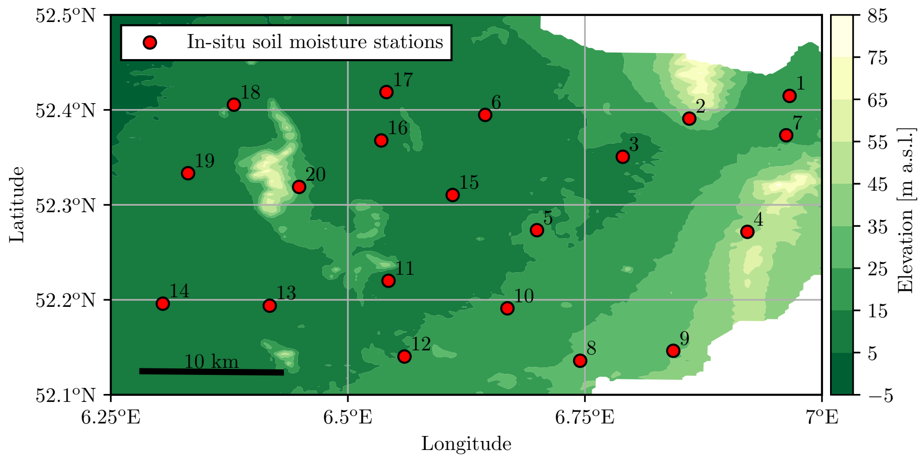

Figure 3.2: Overview of the Twente region in the Netherlands. Elevation data are based on the AHN elevation dataset. Also, the stations of the Twente soil moisture monitoring network are shown.

3.2.3 Study area

The study area is the Twente region in the east of the Netherlands, see Figure 3.2. The region includes part of the Dinkel and Regge catchments and is situated in a temperate marine climate zone (Hendriks et al., 2014). Annual precipitation rates vary between 800 and 850 *mm* (Kaandorp et al., 2018). The region is relatively flat with an elevation between 3 to 85 $m.a.s.l.$ and has a size of approximately 40 *km* by 50 *km*. Glacial ridges form elevated features in the landscape. The main soil types are sand and loamy sand, while the main land use is agriculture. The water system is free-draining and water management is mainly performed by operating a system of weirs and pumps.

3.2.4 Data

We use the SMAP (Soil Moisture Active Passive) L3 Enhanced Radiometer-only daily gridded soil moisture product for the data assimilation scheme (Entekhabi et al., 2010; Chan et al., 2018; O'Neill et al., 2018). The value of SMAP data for hydrological data assimilation has been shown in several studies (Kolassa et al., 2017; Lievens et al., 2017; Koster et al., 2018; Blyverket et al., 2019). The delivery of the enhanced SMAP soil moisture products was motivated by the gap that emerged after failure of the SMAP radar (Chan et al., 2018; Das et al., 2018). The 9 km resolution of the enhanced data products is achieved through an optimal interpolation technique applied to the antenna temperature from which the brightness temperature T_b is calculated. Subsequently, the same soil moisture retrieval procedure is followed as is applied to the native T_b data. We use the baseline SMAP L3 Enhanced product, which relies on the Single Channel Algorithm at V-polarization (SCA-V). The SMAP L3 Enhanced product is available approximately every 2 to 3 days for the Twente region. Colliander et al. (2017) found that SMAP soil moisture products generally perform well in the Twente region. Chan et al. (2018) assessed the accuracy of the enhanced SMAP L3 products in the Twente region using in situ soil moisture measurements at 5 cm soil depth from the Twente network (see next section) for the period April 2015 – October 2016 and found an unbiased root mean square error (uRMSE) of 0.056 $m^3\ m^{-3}$. For this study, we used the soil moisture retrievals from the morning satellite overpasses. During the morning, the moisture and temperature profiles across the soil-vegetation system are more uniform, which is one of the assumptions underlying retrieval algorithms. Indeed, Chan et al. (2018) found more reliable soil moisture estimates for data collected in the morning compared to the data collected in the afternoon.

Furthermore, we use in situ soil moisture measurements from a monitoring network operating since 2009. The network is maintained by the faculty of ITC of the University of Twente. The network consists of 20 stations equipped with Decagon Em50 data loggers and probes for measuring both soil moisture and soil temperature (Dente et al., 2012). Decagon EC-TM probes were installed when the network was first developed. Gradually, the probes were replaced by the 5TM probes. Soil type specific calibration functions have been developed for both sensors. The expected accuracies are 0.023 $m^3\ m^{-3}$ for the EC-TM probes and 0.027 $m^3\ m^{-3}$ for the 5TM probes respectively. The station locations are shown in Figure 3.2. The sensors are installed in agricultural fields, except station 20, which is installed in a forest area. The stations provide a reading every 15 minutes since July 2009 at nominal soil depths of 5, 10, 20, 40 and 80 cm. Installation of the monitoring network is similar to the installation of the Raam soil moisture monitoring network described in Benninga et al. (2018). The in situ measurements are used to validate the assimilation results.

3.2.5 Error model: noise definition

We perturb the MetaSWAP ensemble members for the EnKF scheme by adding noise to the model forcing. Syed et al. (2004) show that precipitation and potential evaporation are the most dominant forcing terms for the hydrological cycle. In addition, uncertainties in precipitation measurements dominate errors in subsurface and runoff predictions

(McMillan et al., 2011). Tian et al. (2013) show that a multiplicative error model outperforms an additive error model for daily precipitation measurements. We perturb input rasters of daily precipitation and daily Makkink reference evapotranspiration with Gaussian white multiplicative noise. The noise is described using the distribution mean and standard deviation. We assume that the errors in the input data are not systematic and therefore, in the case of multiplicative noise, the distribution mean is set equal to one. The standard deviation of the precipitation error distribution function is often arbitrarily set ranging from 15% (Weerts and El Serafy, 2006) up to 50% (Pauwels and De Lannoy, 2006) of the nominal precipitation value. We found that the model ensemble does not collapse when using a standard deviation defined as 25% of the maximum daily precipitation rate. The average annual maximum daily precipitation rate in the Twente area is close to 30 mm for the years between 1961 to 2014 (Rahimpour Golroudbary et al., 2017; KNMI, 2018b). Correspondingly, we assume that the error distribution of the precipitation input has a standard deviation of 7.5 mm. In a similar way, we assume a standard deviation of 2 mm for the reference evapotranspiration input (KNMI, 2018a). Furthermore, using the KNMI precipitation and reference evapotranspiration datasets, we found that the correlation length of precipitation and reference evapotranspiration is larger than our region of interest (approximately 40 km by 50 km). Therefore, we assume a spatial correlation length of 50 km for the noise in every direction, which means that the spatial anisotropy of precipitation fields is not considered.

In addition, the SMAP observations are perturbed with Gaussian white additive noise. For data assimilation applications, Drusch et al. (2009) and De Rosnay et al. (2013) defined the soil moisture satellite observational error as a standard deviation with a value of 0.010 $m^3\ m^{-3}$. We use a standard deviation of 0.056 $m^3\ m^{-3}$ for defining the satellite observation error. This error was found by Chan et al. (2018), which focuses on the SMAP product and the Twente region.

3.2.6 Experimental setup

We set up two experiments to assess the applicability of the EnKF for updating soil moisture estimates of the metamodel MetaSWAP. First, we test the MetaSWAP-OpenDA data assimilation implementation by performing a synthetic experiment often referred to as a twin experiment. Then, we evaluate data assimilation in a real-world application on regional and local spatial scales using the SMAP satellite data. The flowcharts visualized in Figure 3.3 show the research steps for the two experiments.

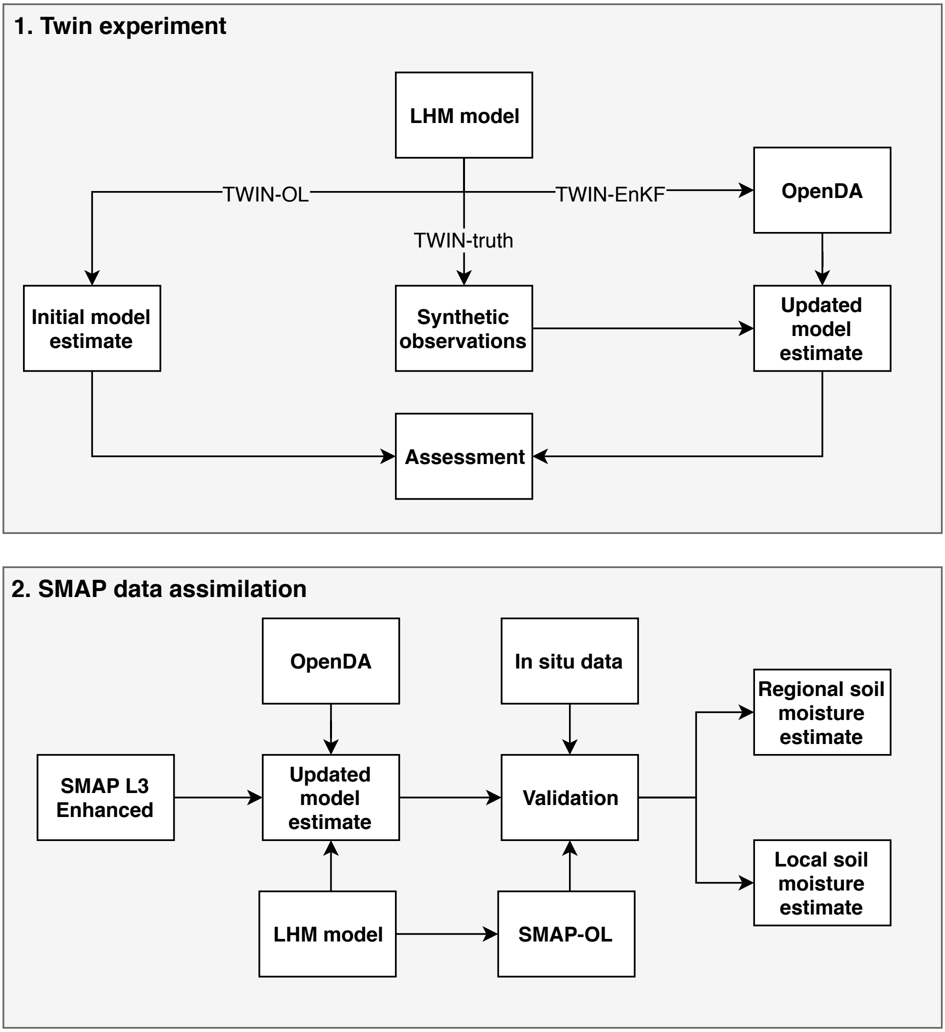

Figure 3.3: Flowcharts visualizing experimental setup: (1) Synthetic twin experiment and (2) SMAP data assimilation experiment.

Twin experiment

A twin experiment allows testing of a data assimilation implementation in an idealized situation (Remy et al., 2002; Robinson and Lermusiaux, 2002; Irrgang et al., 2017). The goal is to assess whether the EnKF scheme improves the accuracy of soil moisture model estimates when all error statistics are known. The twin experiment is performed for the in situ station locations and for a period of two months: May 1 2015 to July 1 2015. The twin experiment consists of three model runs:

TWIN-truth: This run represents the true state of root zone soil moisture in the period May 1 2015 to July 1 2015. The run produces synthetic soil moisture observations which are assimilated in the TWIN-EnKF run. The synthetic observations are assumed to be perfectly accurate.

TWIN-OL: This run represents a reference simulation without data assimilation, also known as an open loop (OL) run. To resemble an imperfect model, we perturbed the forcing data of this run. White multiplicative noise with a nominal value of 2% is added to the forcing data to resemble model uncertainty.

TWIN-EnKF: This run applies the EnKF using the MetaSWAP-OpenDA framework to correct root zone soil moisture by assimilating the synthetic soil moisture observations from the TWIN-truth run. The run contains the same uncertainty as the TWIN-OL run by using the same perturbed forcing data.

In general, increasing the ensemble size will lead to a better representation of model uncertainty (Zhang et al., 2016). However, due to computational limitations, one has to find a balance between computational costs and appropriate ensemble size (He et al., 2019). To determine the number of ensemble members, we varied the ensemble size (8, 16, 32, and 64 members) and assessed the corresponding Root Mean Square Error (RMSE) of the TWIN-EnKF run. We found that at least 32 ensemble members are needed to get a good representation of model uncertainty, see Figure 3.5.

The twin experiment is successful if the accuracy of the TWIN-EnKF soil moisture estimates increases with respect to the soil moisture estimates of the TWIN-OL run. The accuracy is assessed using three performance indicators: the RMSE for the absolute deviation, the model bias for the systematic deviation, and the Pearson correlation coefficient

r for the dynamics. The RMSE is defined as:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} \left(\theta_i^{\text{obs}} - \theta_i^{\text{pred}}\right)^2}{N}}, \tag{3.1}$$

in which θ_i^{obs} are the observed soil moisture estimates (in this case the synthetic observations from the TWIN-truth run), θ_i^{pred} are the predicted soil moisture estimates (from the TWIN-OL and TWIN-EnKF runs), and N is the number of observations. The closer the RMSE is to zero, the more accurate the model predictions are.

Next, the model bias is defined as:

$$Bias = \frac{\sum_{i=1}^{N} \left(\theta_i^{\text{obs}} - \theta_i^{\text{pred}}\right)}{N}. \tag{3.2}$$

Again, the closer the bias is to zero, the less biased the model predictions are.

Last, the Pearson correlation coefficient r is defined as:

$$r = \frac{\sum_{i=1}^{N} \left(\theta^{\text{obs}} - \overline{\theta^{\text{obs}}}\right)\left(\theta^{\text{pred}} - \overline{\theta^{\text{pred}}}\right)}{\sqrt{\sum_{i=1}^{N} \left(\theta^{\text{obs}} - \overline{\theta^{\text{obs}}}\right)^2}\sqrt{\sum_{i=1}^{N} \left(\theta^{\text{pred}} - \overline{\theta^{\text{pred}}}\right)^2}} \tag{3.3}$$

in which $\overline{\theta^{\text{obs}}}$ and $\overline{\theta^{\text{pred}}}$ are the averaged observed and predicted soil moisture estimates. The correlation coefficient r can range between -1 and 1. A value of 1 (-1) indicates a perfect positive (negative) linear relationship between θ^{obs} and θ^{pred}.

Assimilation of SMAP observations

Next, we performed an EnKF data assimilation run with the SMAP L3 Enhanced observations. An EnKF run is performed for the full year 2016 to capture soil moisture variability in both wet and dry periods. 32 ensemble members are used to resemble model uncertainty. The ensemble members are initialized with a spin-up period between January 1 2014 and January 1 2016. Furthermore, a deterministic model run without data assimilation is performed. We refer to this run as SMAP-OL to distinguish between this run and the TWIN-OL run. The updated soil moisture model estimates and the open loop run are validated by evaluating the RMSE, model bias, and correlation coefficient *r* performance indicators using the in situ soil moisture measurements. The in situ measurements are daily averaged.

Both satellite soil moisture and in situ soil moisture observations are inherently different with respect to each other. In situ soil moisture measurements contain significant uncertainties related to accuracy, precision, and spatial support (Susha Lekshmi et al., 2014). These uncertainties limit validation possibilities on local scales. Upscaling in situ measurements to regional averages reduce sampling errors (Cosh et al., 2006; Crow et al., 2012; Zhao and Yang, 2018). Therefore, we evaluate the results on both regional and local spatial scales. A typical regional scale is the management area of a regional water authority, which is approximately the size of the study area. We define field scale as a typical local scale, which is resembled by individual soil moisture monitoring stations. First, the regional scale applicability of the SMAP L3 Enhanced product for data assimilation is assessed by evaluating the performance indicators for both the in situ data and the model estimates. The in situ data and model estimates are spatially averaged. We refer to these results as SMAP-EnKF-AVG. The following twelve stations have a complete data series for the year 2016 and are used for the averaging: 1, 2, 4, 7, 9, 12, 13, 15, 17, 18, 19, 20. The locations are shown in Figure 3.2. Then, the local scale applicability of the SMAP L3 Enhanced product is assessed by evaluating the performance indicators for the same stations used for the regional averaging.

As described in section 3.2.2, data assimilation results using the MetaSWAP-model are only comparable for periods with similar root zone depths. Therefore, we split the year 2016 in a summer and winter period. The length of the summer period depends on the parametrized vegetation type. The root zone depth of the grass vegetation type varies between 0.20 *m* in winter and 0.40 *m* in summer. The root zone depth of the maize vegetation type varies between 0.10 *m* in winter and 0.40 *m* in summer. The root zone depth of the forest vegetation type does not vary. To define a summer period for this vegetation type, we split the year in half. Table 3.1 shows the parametrized vegetation type and summer period length. Since the first aggregation box of MetaSWAP represents the root zone up to 40 cm depth, we use the in situ measurements at 10 cm depth for the winter period and the in situ measurements at 20 cm depth for the summer period. Because the model result is an aggregate of the root zone soil moisture profile, we consider the measurements at these depths representative for the winter and summer periods. Since the most abundant vegetation type in the list of selected stations is grass, we assume that the summer period of grass is representative for the regional average results.

Table 3.1: Vegetation type and length of summer period for each station as parametrized in the MetaSWAP model.

Station	Vegetation type	Summer period
1	Grass	April 1 – November 1
2	Grass	April 1 – November 1
4	Grass	April 1 – November 1
7	Maize	June 1 – October 12
9	Grass	April 1 – November 1
12	Grass	April 1 – November 1
13	Grass	April 1 – November 1
15	Grass	April 1 – November 1
17	Maize	June 1 – October 12
18	Grass	April 1 – November 1
19	Grass	April 1 – November 1
20	Forest	April 1 – October 1

3.3 Results

3.3.1 Twin experiment

First, we show the synthetic twin experiment results. Figure 3.4 shows the performance indicators for the TWIN-OL and TWIN-EnKF runs. As described in section 3.2.6, the TWIN-OL run represents a model run with randomly added errors. The TWIN-EnKF run is the result of assimilating synthetic observations of perfect accuracy to update the soil moisture model state estimates.

In general, the results indicate that the MetaSWAP-OpenDA implementation is able to correct for synthetically added errors for which the error structure is known. In terms of RMSE and model bias, the accuracy of model estimates improves in the TWIN-EnKF run in comparison with the TWIN-OL run. The RMSE of the TWIN-OL run ranges from 0.0013 to 0.010 $m^3\ m^{-3}$, while the RMSE of the TWIN-EnKF run ranges from 0 to 0.0032 $m^3\ m^{-3}$. The bias of the TWIN-OL run ranges from 0.0010 to 0.0090 $m^3\ m^{-3}$, while the bias of the TWIN-EnKF run ranges from 0.00010 to 0.0024 $m^3\ m^{-3}$. Furthermore, in terms of correlation coefficient r, the accuracy of model estimates generally increases in the TWIN-EnKF run compared with the TWIN-OL run. The correlation coefficient of the TWIN-OL run ranges from 0.98 to 1 $[-]$, while the correlation coefficient of the TWIN-EnKF run ranges from 0.99 to 1 $[-]$. However, the accuracy of the TWIN-EnKF run is lower for three stations (7, 11, and 16) in terms of correlation coefficient.

Furthermore, we assessed whether the ensemble size of 32 members is sufficient. Fig-

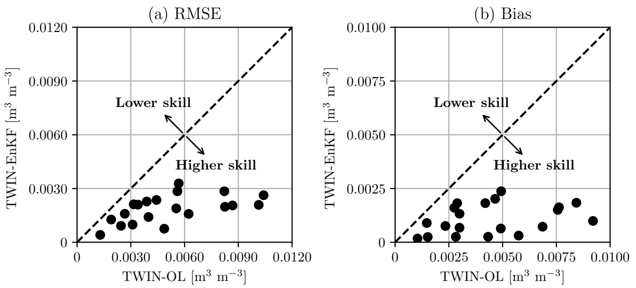

Figure 3.4: (a) RMSE, (b) model bias and (c) correlation coefficient r for TWIN-OL and TWIN-EnKF runs. Arrows show if the skill of the TWIN-EnKF run is higher or lower than the TWIN-OL run.

ure 3.5 shows the change in RMSE of the TWIN-EnKF run when increasing the number of ensemble members. The RMSE of the ensemble mean decreases for larger ensemble sizes. The decrease in RMSE flattens out for an ensemble size larger than 32. Therefore, we assume that an ensemble of 32 members is a good balance between accuracy and computational requirements.

3.3.2 SMAP assimilation: regional comparison

This section presents the findings of assimilating SMAP data into the metamodel MetaSWAP. Figure 3.6 shows the EnKF data assimilation results for the regional soil moisture estimates in the year 2016. The regional estimates are obtained by spatially averaging the soil moisture model estimates of each in situ location. A visual comparison of the SMAP-OL and SMAP-EnKF-AVG runs shows an improvement for both the winter and summer periods of the SMAP-EnKF-AVG run, except in the beginning of May. Furthermore, the accuracy slightly improves in the period between January 1 – April 1.

Table 3.2 shows the RMSE, model bias, and correlation coefficient for the winter and summer periods. In terms of RMSE and model bias, the accuracy improves in the SMAP-EnKF run in comparison with the SMAP-OL run. The decrease in RMSE and model bias is larger in the summer period. In terms of correlation coefficient, the accuracy of model estimates decreases in the SMAP-EnKF run in comparison with the SMAP-OL run. The decrease in correlation coefficient is smaller in the summer period.

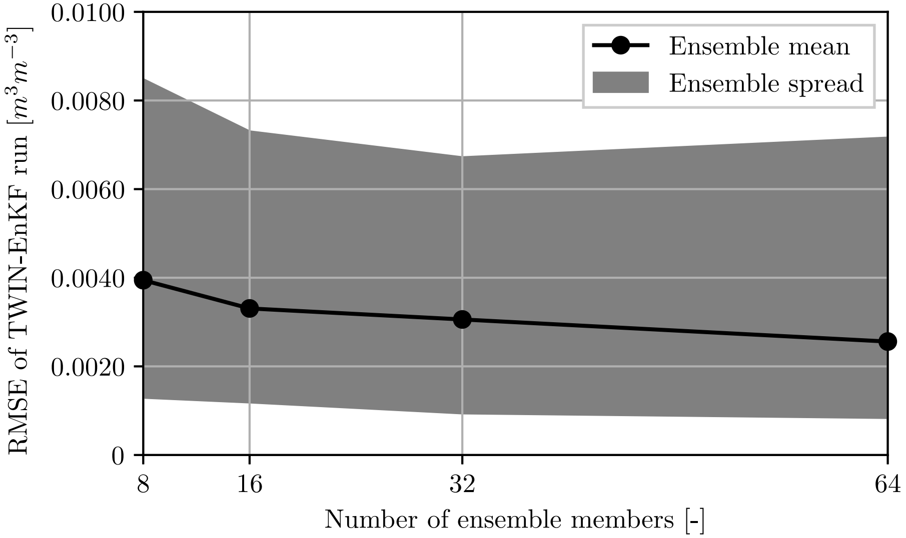

Figure 3.5: The decrease in RMSE of the TWIN-EnKF run when the ensemble size is varied from 8, 16, 32 up to 64 members.

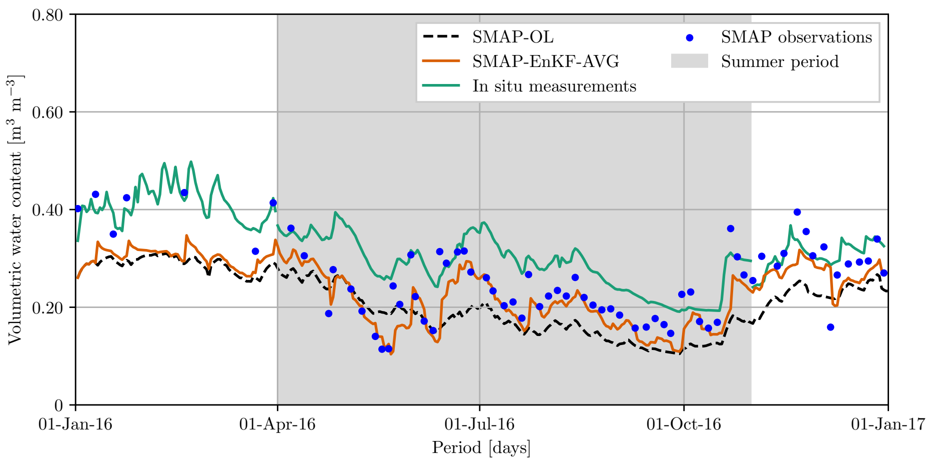

Figure 3.6: Regional soil moisture estimates in the Twente region in the year 2016. The black dashed line is the spatially averaged deterministic SMAP-OL run. The orange line represents the spatially averaged updated root zone soil moisture estimates. We refer to these data as SMAP-EnKF-AVG. The green line represents the spatially averaged in situ soil moisture measurements. The blue dots represent the spatially averaged SMAP L3 Enhanced surface soil moisture observations. The grey area indicates the summer period. In the winter period, the in situ soil moisture measurements at 10 cm depth are used. In the summer period, the in situ soil moisture measurements at 20 cm depth are used.

Table 3.2: RMSE, bias, and correlation coefficient for regional and local SMAP-OL and SMAP-EnKF winter and summer results. The station locations are found in Figure 3.2. Improvements in the SMAP-EnKF run are indicated by underlining.

	Winter						Summer					
	SMAP-OL			SMAP-EnKF			SMAP-OL			SMAP-EnKF		
Station	RMSE $[m^3\ m^{-3}]$	Bias $[m^3\ m^{-3}]$	r [–]	RMSE $[m^3\ m^{-3}]$	Bias $[m^3\ m^{-3}]$	r [–]	RMSE $[m^3\ m^{-3}]$	Bias $[m^3\ m^{-3}]$	r [–]	RMSE $[m^3\ m^{-3}]$	Bias $[m^3\ m^{-3}]$	r [–]
Regional	0.11	0.11	0.94	$\underline{0.094}$	$\underline{0.082}$	0.74	0.11	0.11	0.88	$\underline{0.091}$	$\underline{0.085}$	0.83
1	0.12	-0.053	0.57	0.12	-0.057	0.43	0.13	-0.12	0.74	$\underline{0.12}$	$\underline{-0.10}$	0.51
2	0.21	0.16	-0.82	$\underline{0.16}$	$\underline{0.11}$	$\underline{-0.70}$	0.092	0.081	0.73	$\underline{0.071}$	$\underline{0.052}$	$\underline{0.82}$
4	0.48	0.47	0.57	$\underline{0.46}$	$\underline{0.44}$	0.33	0.58	0.58	0.51	$\underline{0.55}$	$\underline{0.55}$	0.45
7	0.093	0.052	0.74	$\underline{0.089}$	0.054	$\underline{0.79}$	0.12	0.11	0.76	0.12	$\underline{0.11}$	0.70
9	0.040	0.022	0.77	$\underline{0.038}$	$\underline{-0.016}$	0.68	0.12	0.11	0.68	$\underline{0.078}$	$\underline{0.055}$	$\underline{0.74}$
12	0.15	-0.039	0.83	0.15	-0.047	0.76	0.11	-0.098	0.90	$\underline{0.10}$	$\underline{-0.092}$	0.74
13	0.041	0.0046	0.73	0.046	-0.039	0.50	0.055	0.042	0.87	0.066	$\underline{-0.025}$	0.61
15	0.038	0.028	0.77	$\underline{0.028}$	$\underline{-0.0024}$	0.48	0.066	0.051	0.75	$\underline{0.050}$	$\underline{0.015}$	0.71
17	0.081	-0.030	0.18	0.087	-0.041	0.17	0.26	0.25	-0.00068	$\underline{0.18}$	$\underline{0.17}$	$\underline{0.48}$
18	0.12	0.080	0.76	$\underline{0.12}$	$\underline{0.069}$	0.63	0.069	-0.022	0.49	$\underline{0.067}$	-0.030	$\underline{0.60}$
19	0.39	0.30	0.84	$\underline{0.39}$	$\underline{0.27}$	0.77	0.12	0.095	0.89	$\underline{0.11}$	$\underline{0.049}$	0.53
20	0.12	0.12	0.44	$\underline{0.042}$	$\underline{0.041}$	$\underline{0.71}$	0.18	0.17	0.64	$\underline{0.14}$	$\underline{0.14}$	$\underline{0.67}$

3.3.3 SMAP assimilation: local comparison

An overview of the local-scale assimilation results is shown in Table 3.2. For the winter period, in terms of RMSE, the assimilation increases the accuracy of local soil moisture estimates for 8 out of 12 stations. In terms of model bias, the assimilation increases the accuracy for 7 out of 12 stations. In terms of correlation coefficient, the assimilation increases the accuracy for 3 out of 12 stations. For the summer period, in terms of RMSE, the assimilation increases the accuracy of local soil moisture estimates for 10 out of 12 stations. In terms of model bias, the assimilation increases the accuracy for 11 out of 12 stations. In terms of correlation coefficient, the assimilation increases the accuracy for 5 out of 12 stations. Furthermore, the EnKF corrects the low correlation found during the summer period in the SMAP-OL run for station 17. However, the EnKF is not able to correct for the negative correlation found during the winter period in the SMAP-OL run for station 2.

Next, we focus on local results for two stations: station 9 where the updated estimates clearly improve, and station 7 for which the accuracy declines. Figure 3.7 shows the assimilation results for station 9. The accuracy of the model estimates increases in the EnKF run, similar to the patterns found for the regional soil moisture estimates. In terms of RMSE and model bias, the accuracy of model estimates improves in both the winter and summer period. In terms of correlation coefficient, the accuracy of model estimates improves in the summer period and declines in the winter period.

Figure 3.8 shows the assimilation results for station 7. Since the parametrized vegetation type at this station is maize, the length of the summer period is different than for station 9, see Table 3.1. While the accuracy of model estimates slightly improves in terms of RMSE and correlation coefficient, the accuracy in terms of model bias declines in the winter period. Furthermore, the accuracy of model estimates shows no improvement in terms of RMSE and model bias and a small decline in terms of correlation coefficient in the summer period. The EnKF does not significantly affect the model estimates. A possible explanation is that the SMAP L3 Enhanced product does not reflect local root zone conditions for this station. A thick clay layer can be found below the root zone at station 7. In addition, the subsurface of the field contains pipes which drain excess water during wet winter periods.

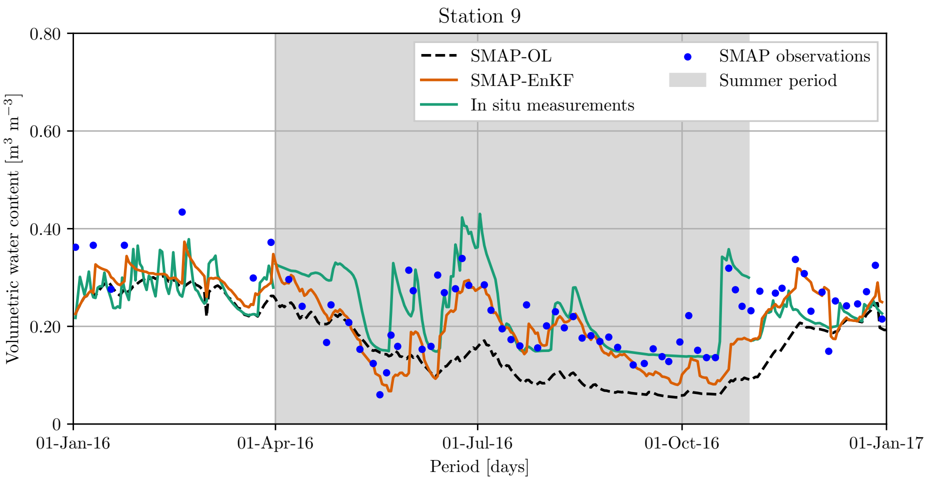

Figure 3.7: Results for station 9 in the year 2016. For a detailed description of the visualized features, see Figure 3.6.

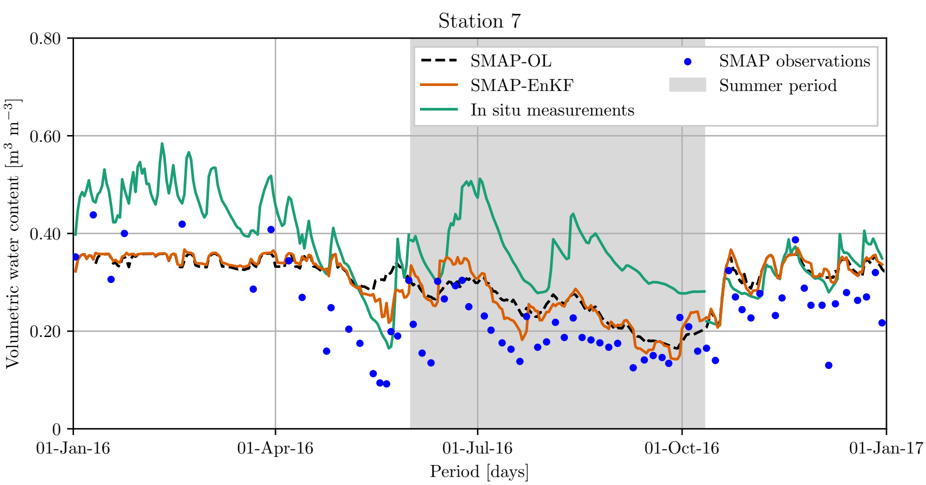

Figure 3.8: Results for station 7 in the year 2016. For a detailed description of the visualized features, see Figure 3.6.

3.4 Discussion

3.4.1 Application of data assimilation for metamodelling: twin experiment

We assessed whether data assimilation can be a tool to integrate soil moisture observations into unsaturated zone metamodels. The metamodelling concept of MetaSWAP depends on the database with pre-calculated soil saturation profiles. Updating this database is a time-consuming process. The twin experiment and SMAP-EnKF runs show that data assimilation is a good alternative to update the metamodel. The twin experiment indicates that applying an EnKF with perfectly accurate synthetic observations increases the accuracy of the soil moisture estimates of MetaSWAP and does not lead to model instabilities or other spurious model behaviour. We conclude that the MetaSWAP-OpenDA implementation is suitable for assimilating soil moisture observations into the metamodel MetaSWAP. Also, we found that an ensemble size of 32 members gives a good representation of model uncertainty. It is important to note that, although Figure 3.4 shows that the accuracy of soil moisture estimates increases in the TWIN-EnKF run, also an inherent model uncertainty exists that cannot be mitigated using data assimilation. The EnKF reduces the RMSE to a lower limit, even when using observations of perfect accuracy. This inherent uncertainty is among others caused by the restart procedure of MetaSWAP after each update step, as is described in section 3.2.2.

3.4.2 Application of data assimilation for metamodelling: SMAP experiment

Table 3.2 shows that the MetaSWAP-OpenDA implementation has value in an experiment with SMAP L3 Enhanced surface soil moisture observations. The accuracy of model estimates improves on both regional and local scales in terms of RMSE and model bias. The improvement is larger for the summer period than for the winter period. In terms of correlation coefficient, the improvement in accuracy is less distinct. In the winter period, only three stations show an improvement in correlation coefficient, in the summer period, almost half of the stations show an improvement in correlation coefficient. The larger variability of the SMAP surface soil moisture observations with respect to the in situ root zone measurements might explain the impact of the assimilation on the correlation coefficient. Also, the availability of SMAP observations influences the effectiveness of the assimilation. For example, less SMAP observations are available in the period January 1 2016 – April 1 2016 in comparison with the rest of 2016. Consequently, the model state is less often updated during the SMAP-EnKF run in the period up to April 1 2016, affecting the performance of the EnKF in the defined winter period.

3.4.3 Regional versus local spatial scales

The SMAP L3 Enhanced product corresponds well with the in situ measurements on a regional scale (Chan et al., 2018). Therefore, the accuracy of regional-scale soil moisture model estimates increase after assimilation of the SMAP L3 Enhanced product in terms of RMSE and model bias. Data assimilation results on local scales largely depend on how well the SMAP L3 Enhanced product represents local field conditions. We want to stress that both the in situ measurements and LHM simulations contain uncertainties, e.g. they might not be representative for local field conditions, as explained in section 3.2.6. New remote sensing products from satellites such as Sentinel-1 are expected to make the leap from regional to local field scales (Balsamo et al., 2018). For example, Bauer-Marschallinger et al. (2019) developed a high-resolution surface soil moisture product based on Sentinel-1 satellite data and a change-detection algorithm. The spatial resolution of this product is 1 km by 1 km. We expect that such high-resolution surface soil moisture products will lead to new possibilities for soil moisture data assimilation in operational water resources management.

Furthermore, the model bias and correlation coefficient show that while the EnKF is able to correct for systematic model errors, the variability of the SMAP L3 Enhanced surface soil moisture product does not always reflect dynamics in deeper layers. Carranza et al. (2018) show a strong vertical variability between soil moisture at 5 and 40 cm depth in the Twente region. The vertical variability forms a challenge for data assimilation applications, since most (if not all) remotely sensed soil moisture data concerns surface soil moisture due to sensor constraints. However, the SMAP-EnKF run shows that a root zone soil moisture model can be updated by assimilating SMAP surface soil moisture observations. The results in Table 3.2 show that assimilating the 9 km resolution surface SMAP L3 Enhanced observations increases the accuracy of local soil moisture model estimates for more than half of the stations. Thus, the SMAP surface soil moisture product has significant value in data assimilation approaches. Renzullo et al. (2014), Dumedah et al. (2015), and Blyverket et al. (2019) also show the value of assimilating satellite-based surface soil moisture observations into a hydrological model to update root zone soil moisture estimates. We want to accentuate the impact of the SMAP observation on December 6 2016. This observation significantly impacts the assimilation run, as visible in Figure 3.6 and Figure 3.7. The in situ measurements do not indicate a steep reduction in soil moisture on that day, so the SMAP observation may be erroneous. Temperatures dropped below 0 °C on December 6 2016, which probably significantly affected the SMAP reading. Similarly, the SMAP L3 Enhanced product does not reflect field conditions well during May 2016, significantly affecting the assimilation run.

3.4.4 Implications for operational water resources management

The assimilation of high-resolution remotely sensed soil moisture products leads to new possibilities for integrated physically-based hydrological models in operational water resources management. Pezij et al. (2019a) found that hydrological models are currently not considered by Dutch regional operational water managers as important tools for decision-making. Among others, regional operational water managers identified model accuracy as a limiting factor, which limits application. Data assimilation is a tool to increase the accuracy and hence the application of hydrological modelling in operational water management.

Yet, combining data assimilation schemes and integrated physically-based modelling for operational water resources management is currently limited due to, among others, computational requirements (Sun et al., 2016). Even with the application of metamodels for simulating hydrological processes at field scale, high performance computing (HPC) facilities are often required for efficient implementation of data assimilation schemes. Furthermore, the implementation of remote sensing data in operational management requires additional investments in data acquiring, processing and storage facilities. However, we expect that due to the development of new computational methods, these challenges become less of an issue in the future (He et al., 2019). For example, Kurtz et al. (2017) show the potential of combining data assimilation and integrated physically-based hydrological modelling with cloud computing techniques for operational water resources management. Ma et al. (2015) identifies several promising tools, such as cluster-based HPC systems and cloud computing for fast calculations, and parallel file systems for big data storage. However, the implementation of such tools requires investments in computational infrastructure. We expect that in the future research and investments into these promising new tools will increase, which will help to integrate the application of data assimilation schemes in operational water resources management.

3.5 Conclusions

We assessed the applicability of satellite-based regional-scale surface soil moisture observations to increase the accuracy of root zone soil moisture estimates of an unsaturated zone metamodel. This study shows that combining metamodels with data assimilation schemes allows incorporating new information in metamodels. Therefore, integrating satellite-based soil moisture observations and hydrological metamodelling lead to new opportunities for operational water resources management.

A data assimilation scheme was developed for the metamodel MetaSWAP using the open-source data assimilation framework OpenDA. A synthetic experiment, known as a twin experiment, showed the value of integrating metamodelling and an Ensemble Kalman Filter (EnKF) data assimilation scheme. Furthermore, the applicability of the 9 km resolution SMAP L3 Enhanced surface soil moisture product for the MetaSWAP-OpenDA framework was assessed for the year 2016. On a regional scale, the updated root zone soil moisture model estimates show a larger skill in terms of RMSE and model bias. In terms of correlation coefficient, the skill of the updated root zone soil moisture model estimates is slightly lower than in the open loop run. The decline is partly explained by the larger variability of the assimilated surface soil moisture observations with respect to the in situ root zone soil moisture measurements. On a local scale, similar results were found. However, the applicability of the SMAP L3 Enhanced product on local scales depends on how well the SMAP product represents local field conditions. In addition, we show that the assimilation of surface soil moisture observations leads to increased accuracy of root zone soil moisture model estimates. The improvement of the soil moisture model estimates is larger in the summer period than in the winter period of 2016. The limited availability of SMAP L3 Enhanced soil moisture observations in the first months of 2016 might explain this difference. The limited availability is caused by, among others, freezing of the soil in winter periods.

As a final remark, the increasing availability of high-resolution surface soil moisture products will lead to new opportunities for data assimilation schemes in operational water resources management. Nevertheless, significant developments and investments in terms of computation capacities are required for operational application of remote sensing data in data assimilation schemes. However, recent developments in HPC and cloud computing are expected to contribute to the integration of data assimilation in operational water resources management.

Acknowledgments

This work is part of the OWAS1S research programme (Optimizing Water Availability with Sentinel-1 Satellites) with project number 13871, which is partly financed by the Netherlands Organisation for Scientific Research (NWO). We want to thank all OWAS1S programme partners for their contribution. The authors are grateful for the Water Resources Department of the ITC faculty of the University of Twente, the Netherlands, for sharing the in situ soil moisture data from their monitoring network. Furthermore, we want to thank Ruud Hurkmans and Erik Pelgrim for their help on the OpenDA implementation. Last, this work was carried out on the Dutch national e-infrastructure with the support of SURF Cooperative.

3.6 Appendix A

To improve readability, the acronyms are alphabetically summarized in the following list:

AHN: Actueel Hoogtebestand Nederland (Elevation Map The Netherlands)

AMSR-2: Advanced Microwave Scanning Radiometer 2

AMSR-E: Advanced Microwave Scanning Radiometer for EOS

ASCAT: Advanced Scatterometer

BOFEK2012: Bodemfysische Eenhedenkaart (Soil Physical Units Map)

DA: data assimilation

EnKF: Ensemble Kalman Filter

HPC: High-Performance Computing

H-SAF: Satellite Application Facility on Support to Operational Hydrology and Water Management

KNMI: Koninklijk Nederlands Meteorologisch Instituut (Royal Dutch Meteorological Institute)

LGN: Landelijk Grondgebruik Nederland (National Land Use the Netherlands)

LHM: Landelijk Hydrologisch Model (National Hydrological Model)

NHI: Netherlands Hydrological Instrument

OL: Open Loop

REGIS: Regionaal Geohydrologisch Informatie Systeem (Regional Geohydrological Information System)

RMSE: Root Mean Square Error

uRMSE: Unbiased Root Mean Square Error

SCA-V: Single Channel Algorithm at V-polarization

SMAP: Soil Moisture Active Passive

SMOS: Soil Moisture and Ocean Salinity

SVAT: Soil-Vegetation-Atmopshere-Transfer

SWAP: Soil-Water-Atmosphere-Plant

3.7 Appendix B

Due to the size of the model state error covariance matrix P in hydrological model predictions, it is generally not feasible to explicitly calculate P. An alternative approach is to estimate P using a sample of evolved model states, leading to a lower rank estimation of P. This ensemble of model runs is created by perturbing model forcing, parameters and/or states. The model perturbations (η) have to be defined in such a way that the model ensemble represents total model uncertainty. This method, introduced by Evensen (1994), is generally known as an Ensemble Kalman Filter (EnKF). We apply a stochastic (or perturbed observations) EnKF (Burgers et al., 1998; Houtekamer and Mitchell, 1998).

Applying an EnKF consists of a forecast (f) and analysis step (a). The forecast and analysis model state ensembles are represented as:

$$x^{\mathrm{f}} = \left[x_1^{\mathrm{f}}, x_2^{\mathrm{f}}, \ldots x_N^{\mathrm{f}}\right], \tag{3.4}$$

$$x^{\mathrm{a}} = \left[x_1^{\mathrm{a}}, x_2^{\mathrm{a}}, \ldots x_N^{\mathrm{a}}\right], \tag{3.5}$$

where x^{f} is the forecasted model state, x^{a} is the analysis model state, and N is the ensemble size. The subscript indicates the ensemble member. Model states of each ensemble member are propagated forward in time:

$$x_j^{\mathrm{f}} = \mathcal{M}\left(x_j^{\mathrm{a}}\right) + \eta_j, \tag{3.6}$$

where $\mathcal{M}$ is a model operator and η_j is the added model noise for ensemble member j. Note that for the first forecast step, an initial model state estimate is used instead of the previous analysis model state. The forecast mean state $\overline{x^{\mathrm{f}}}$ and model state forecast error covariance matrix P^{f} are:

$$\overline{x^{\mathrm{f}}} = \frac{1}{N-1}\sum_{j=1}^{N} x_j^{\mathrm{f}}, \tag{3.7}$$

$$P^{\mathrm{f}} = \frac{1}{N-1}\sum_{j=1}^{N}\left(x_j^{\mathrm{f}} - \overline{x^{\mathrm{f}}}\right)\left(x_j^{\mathrm{f}} - \overline{x^{\mathrm{f}}}\right)^T, \tag{3.8}$$

where T denotes the transpose of a matrix or vector. The mean $\overline{x^{\mathrm{f}}}$ and covariance P^{f} are used to calculate the Kalman gain K:

$$K = P^{\mathrm{f}}H^T\left(HP^{\mathrm{f}}H^T + R\right)^{-1}, \tag{3.9}$$

where H is a transformation matrix. This matrix is used to transform the observations to the model state space. R is a covariance matrix based on perturbed observations and is defined as:

$$R = \frac{1}{N-1}\sum_{j=1}^{N}\left(d_j - \overline{d}\right)\left(d_j - \overline{d}\right)^T, \tag{3.10}$$

where d_j are perturbed observations (with the addition of noise), which are defined as:

$$d_j = y + \epsilon_j, \tag{3.11}$$

where y are observations and ϵ_i are perturbations sampled from a normal distribution

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$\mathcal{N}$ with zero mean and variance R:

$$\epsilon_i \sim \mathcal{N}(0, R). \tag{3.12}$$

Next, the ensemble mean and error covariance matrix ($\overline{x^{\mathrm{a}}}$ and P^{a}) are updated:

$$x_j^{\mathrm{a}} = x_j^{\mathrm{f}} + K\left(d_j - Hx_j^{\mathrm{f}}\right), \tag{3.13}$$

$$\overline{x^{\mathrm{a}}} = \frac{1}{N-1}\sum_{j=1}^{N} x_j^{\mathrm{a}}, \tag{3.14}$$

$$P^{\mathrm{a}} = \frac{1}{N-1}\sum_{j=1}^{N}\left(x_j^{\mathrm{a}} - \overline{x^{\mathrm{a}}}\right)\left(x_j^{\mathrm{a}} - \overline{x^{\mathrm{a}}}\right)^T. \tag{3.15}$$

CHAPTER 4

Applying transfer function-noise modelling to characterize soil moisture dynamics

This chapter is submitted as:

Pezij, M., Augustijn, D.C.M., Hendriks, D.M.D., Hulscher, S.J.M.H. (submitted) Applying transfer function-noise modelling to characterize soil moisture dynamics: a data-driven approach using remote sensing data.

Abstract

The increasing availability of remotely sensed soil moisture data offers new opportunities for data-driven modelling approaches as alternatives for process-based modelling. This study presents the applicability of transfer function-noise (TFN) modelling for predicting unsaturated zone conditions. The TFN models in this study are trained using SMAP L3 Enhanced surface soil moisture data. We found that soil moisture conditions are accurately represented by TFN models when exponential distributions are used to define impulse-response functions. Impulse-response functions describe the response of soil moisture to input stresses. A sensitivity analysis showed the importance of the selected training period, which should at least cover the full 2016 summer period, including the growing season and the onset of autumn to correctly estimate the dry summer period of 2018. The accuracy of the TFN models can be considerably increased by including the dry summer period of 2018 in the training set. Furthermore, the fitted parameters of the impulse-response functions provide valuable information in describing spatially distributed unsaturated zone characteristics such as the total response of soil moisture to a unit stress of precipitation or evapotranspiration. These characteristics can help water managers in making robust decisions. Finally, we encourage exploring the possibilities of TFN soil moisture modelling for water management, as the prediction of soil moisture conditions is a promising application for operational settings.

4.1 Introduction

Soil moisture is a key component of the hydrological cycle, linking surface and subsurface hydrological processes (Entekhabi and Rodriguez-Iturbe, 1994; Vereecken et al., 2016). Among others, soil moisture governs the partitioning of precipitation into infiltration and runoff, affecting streamflow and groundwater recharge (Brocca et al., 2010, 2017). Up-to-date information on soil moisture helps effective decision-making in operational water management, e.g. for drought assessments (Grillakis, 2019; Mishra et al., 2017; Moravec et al., 2019; Sehgal and Sridhar, 2019), flood predictions (Brocca et al., 2017; Tramblay et al., 2010) and irrigation management (Brocca et al., 2018; Rai et al., 2018). The soil moisture drought caused by the 2018 European heat wave significantly impacted water management and agricultural practices (Vogel et al., 2019), which shows the importance of retrieving up-to-date soil moisture information.

Generally, three methods exist for estimating soil moisture on various spatiotemporal scales: in situ (Dobriyal et al., 2012; Susha Lekshmi et al., 2014), remote sensing (Fang and

Lakshmi, 2014; Petropoulos et al., 2015; Zhuo and Han, 2016) and hydrological modelling (Vischel et al., 2008; Zhuo and Han, 2016). In situ soil moisture sensors provide accurate information on local scales, since soil-specific calibration procedures can be performed. However, in situ sensors typically have limited spatial coverage (Susha Lekshmi et al., 2014). Remote sensing and hydrological modelling are alternative sources for providing spatially distributed soil moisture information on larger scales. Remotely sensed soil moisture information is often retrieved using activate and passive microwave sensors (Petropoulos et al., 2015). The temporal coverage of remote sensing is limited in comparison with in situ methods, as satellite imagery is only available during satellite overpasses. In addition, only surface soil moisture can be retrieved by remote sensing due to sensor capabilities (Zhuo and Han, 2016). Furthermore, vegetation dynamics and surface roughness significantly affect remote sensing retrievals (Petropoulos et al., 2015; Benninga et al., 2019).

Hydrological modelling provides a means to estimate soil moisture at various spatiotemporal scales (Vereecken et al., 2016; Brocca et al., 2017). The complexity of unsaturated zone models ranges from simple conceptual lumped models to complex integrated physically-based distributed models. Water managers often regard model accuracy as a limiting factor for the application of hydrological modelling for decision-making in operational water management, e.g. in the Netherlands (Pezij et al., 2019a). The accuracy of hydrological models is partly based on which dataset is used for calibration. Data assimilation can be applied to update model simulations with available observations, although such schemes often require significant computational power (Liu et al., 2012; Weerts et al., 2014; Pezij et al., 2019b). Furthermore, process-based unsaturated zone models are often based on the Richards equation, which is highly non-linear and poses challenges for numerical solutions (Šimůnek et al., 2003; Vereecken et al., 2016). Furthermore, Richards-based models (e.g. SWAP or Hydrus) are generally developed for local applications (Van Dam et al., 2008; Šimůnek and van Genuchten, 2008). Significant computational power is required to scale such models to regional applications (Van Walsum and Groenendijk, 2008). Therefore, the application of Richards-type soil water flow models is not trivial in operational water management on catchment scales.

Data-driven modelling methods are suitable alternatives for process-based modelling (Todini, 2007; Solomatine and Ostfeld, 2008), especially when large amounts of data are available, such as in the Netherlands. Among others, machine learning methods for the prediction of soil moisture conditions are promising (Kolassa et al., 2017; Cai et al., 2019). In this study, we show the applicability of transfer function-noise modelling for describing soil moisture dynamics in the Netherlands.

Transfer function-noise (TFN) modelling is a data-driven method to model an observed time series by applying a linear transformation of deterministic input series known as stress series (Von Asmuth et al., 2002). The stress series are transformed using impulse-response (IR) functions. The IR functions contain information on the response of a water system to input stresses such as precipitation. A TFN model is a fast and easy-to-construct alternative for complex process-based models. TFN modelling does not need prior assumptions on system characteristics, which is an interesting property since no model structure is expected to work best everywhere (Peterson and Western, 2014). Furthermore, due to their stochastic nature, TFN models can model system dynamics which are not well explained by physical laws (Von Asmuth et al., 2002).

The applicability of TFN modelling for groundwater studies has been shown extensively (Yi and Lee, 2004; Bakker et al., 2007; Manzione et al., 2010; Fabbri et al., 2011; Obergfell et al., 2013; Sutanudjaja et al., 2013; Peterson and Western, 2014; Zaadnoordijk et al., 2018; Bakker and Schaars, 2019). Among others, these studies show that TFN modelling can be used to describe groundwater dynamics. In addition, the IR functions contain valuable information on groundwater system characteristics, such as response times. A commonly applied TFN modelling tool for groundwater modelling in the Netherlands is Menyanthes (Von Asmuth et al., 2012).

The non-linearity of unsaturated zone dynamics can be accounted for by adding a process-based soil moisture model on top of the TFN modelling approach (Peterson and Western, 2014). Ramirez-Beltran et al. (2008) showed the applicability of transfer functions for soil moisture modelling using in situ soil moisture measurements as validation data. In particular, we are interested in the application of TFN modelling as an innovative data-driven method for explicitly calculating soil moisture dynamics, which has not been studied before. The availability of new high-resolution remotely sensed soil moisture data offers new opportunities for data-driven modelling methods such as TFN modelling (Petropoulos et al., 2015). We address the following research question in this study: to what extent can transfer function-noise modelling describe and predict soil moisture dynamics using remotely sensed soil moisture information?

This paper is organised as follows: Section 4.2 describes the research methodology. Section 4.3 presents the results, which are discussed in Section 4.4. Finally, conclusions are drawn in Section 4.5.

4.2 Methodology

4.2.1 Transfer function-noise modelling

The approach applied in this study originates from TFN Autoregressive Moving Average (ARMA) modelling (Box and Jenkins, 1970). TFN models are often applied in hydrological applications, since they are fast and yield accurate predictions (Von Asmuth et al., 2008). TFN modelling is comparable to the Unit Hydrograph approach often applied in estimating river discharge rates (Sherman, 1932). A general form of a continuous-time TFN model, formulated for soil moisture dynamics, is (Von Asmuth et al., 2008):

$$h(t) = \sum_{i=1}^{N_{stress}} h_i(t) + d + n_{res}(t), \tag{4.1}$$

where $h(t)$ is the observed soil moisture state at time t $[m^3\ m^{-3}]$, N_{stress} is the number of stress series which influence the soil moisture state $[-]$, $h_i(t)$ is the change in the soil moisture state due to a stress series i at time t $[m^3\ m^{-3}]$, d is the baseline soil moisture state $[m^3\ m^{-3}]$, and $n_{res}(t)$ is a residual time series $[m^3\ m^{-3}]$.

$h_i(t)$ is determined by solving a convolution integral in continuous time using impulse-response (IR) functions (Von Asmuth et al., 2002). IR functions describe the variation of the soil moisture state due to an individual stress series. The type and shape of the functions depend on the type of stress and water system characteristics. $h_i(t)$ is defined by the following convolution integral:

$$h_i(t) = \int_{-\infty}^{t} R_i(\tau)\Theta_i(t-\tau)d\tau, \tag{4.2}$$

where R_i is the value of a stress series i $[mm]$ at time t and Θ_i is an IR transfer function of the corresponding stress series i. To solve Equation 4.2, Θ_i should be known. However, the IR functions are not known a priori and have to be estimated (Von Asmuth et al., 2012). The IR functions can be estimated using the Predefined Impulse Response Function In Continuous Time (PIRFICT) method (Von Asmuth et al., 2002; Von Asmuth and Bierkens, 2005). The PIRFICT method defines IR functions as analytical expressions. Von Asmuth et al. (2002) show that the PIRFICT method overcomes the following limitations of estimating IR functions in regular TFN ARMA models: (1) PIRFICT allows the use of data with an irregular time interval, and (2) since the distribution of the IR functions has to be defined a priori, the order of the IR functions does not have to be defined in a Box-Jenkins model identification procedure (Box and Jenkins, 1970). The PIRFICT method allows selecting a typical IR function for a specific type of input series (Von Asmuth et al., 2008). We assume that the main drivers of soil moisture dynamics are precipitation (Entekhabi and Rodriguez-Iturbe, 1994; Vereecken et al., 2016) and evapotranspiration (Syed et al., 2004). Therefore, we use time series of precipitation and evapotranspiration as stress series for the TFN model.

An IR function can be expressed as a step response function:

$$s(t) = \int_0^t \Theta(\tau) d\tau. \tag{4.3}$$

A step response function describes the long-term response of soil moisture due to a continuous unit stress. The soil moisture response due to a unit stress is defined as the block response. The block response can be derived from the step response function:

$$b(t) = s(t) - s(t-1) \tag{4.4}$$

Von Asmuth et al. (2012) state that, independently of system properties, statistical distributions such as the scaled gamma distribution fit the behaviour of many hydrogeological systems. The scaled gamma step response function is a commonly applied IR function for precipitation and evapotranspiration stress series in groundwater TFN modelling (Von Asmuth et al., 2012). The scaled gamma IR function is defined as:

$$\Theta(t) = A \frac{t^{n-1} exp(-t/a_{gam})}{{a_{gam}}^{n} \Gamma(n)} \tag{4.5}$$

where A corresponds to the unit step response of the state variable to the input stress $[m^3\ m^{-3}]$, a_{gam} is a shape parameter $[day]$, n is a shape parameter $[-]$, and $\Gamma(n)$ is the gamma function of the form $(n-1)!$ $[-]$. Typical forms of the gamma block response function are visualized in Figure 4.1.

Next to the gamma distribution, we studied whether an exponential distribution is a better representation of the unit response of soil moisture to precipitation and evapotranspiration, as we expect that soil moisture shows a fast response to precipitation and

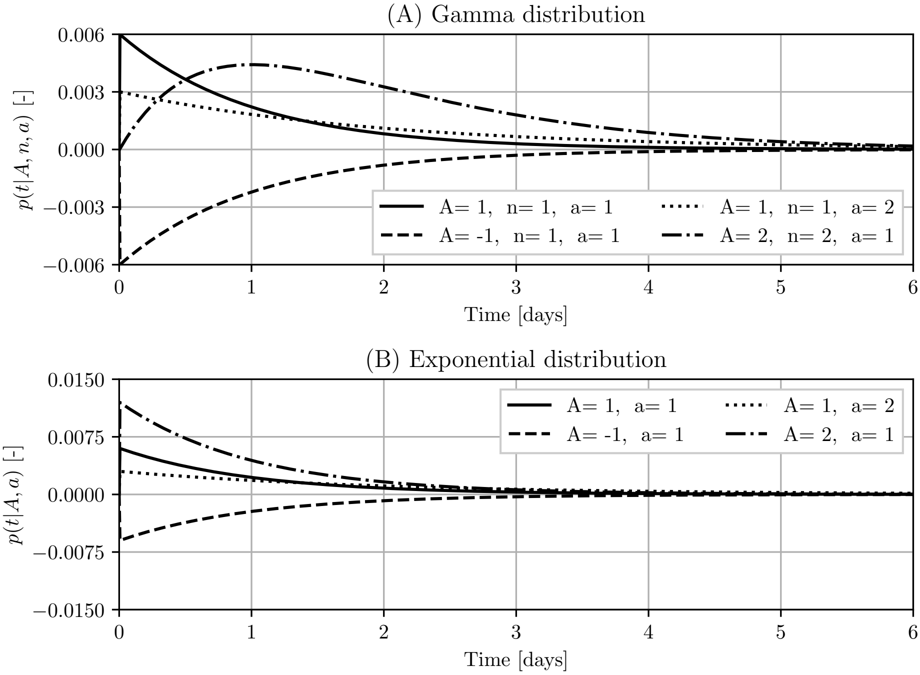

Figure 4.1: Various forms of the (A) gamma and (B) exponential block response functions for different parameter values.

evapotranspiration. The exponential IR function is defined as:

$$\Theta(t) = \frac{A}{a} exp(-t/a) \tag{4.6}$$

where A corresponds to the unit step response of the state variable to the stress $[m^3\ m^{-3}]$ and a is a shape parameter $[day]$. Figure 4.1 also shows typical forms of the exponential block response function.

The parameters of the IR functions are unique for every location which is analysed (Bakker et al., 2008). An initial estimate of the IR function parameters is used to evaluate the TFN model equations. Furthermore, the residual time series $n_{res}(t)$, defined in equation 4.1, is modelled using a noise model, which is formulated as:

$$n_{res}(t_j) = v(t_j) + exp(-\frac{\Delta t_j}{\alpha}) n_{res}(t_{j-1}) \tag{4.7}$$

where $\upsilon(t)$ is white noise resulting from a random process for time step j [$m^3\ m^{-3}$], α is a decay parameter [day], and Δt is the time step [day] (Von Asmuth and Bierkens, 2005; Collenteur et al., 2019a). The subscript j indicates the day. The noise model allows the application of a least squares objective function (Peterson and Western, 2014). The goal of training a TFN model is to find optimal parameter sets for the IR functions used in equations 4.1 and 4.2 by minimizing the objective function. More information on the parameter estimation procedure and the noise model can be found in Von Asmuth and Bierkens (2005).

4.2.2 Study area and data

We assessed the extent to which TFN modelling is applicable for soil moisture predictions in the Twente region in the eastern part of the Netherlands, see Figure 4.2. The study area is situated in a temperate marine climate zone (Hendriks et al., 2014), has an elevation ranging between 3 to 85 m.a.s.l. and has a size of approximately 40 km by 50 km. The main soil types are sand and loamy sand (Wösten et al., 2013). The primary land use is agriculture. Annual precipitation varies between 800 and 850 mm.

We use two types of input stress series: precipitation and Makkink reference crop evapotranspiration. Makkink reference crop evapotranspiration (in the following evapotranspiration) describes the potential evapotranspiration from a reference surface covered with grass (Makkink, 1957). Open source precipitation and evapotranspiration data from the Royal Netherlands Meteorological Institute (KNMI) are used (KNMI, 2018a,b). The precipitation data are based on radar data which are corrected using KNMI station data by applying ordinary kriging. The precipitation data have a spatial resolution of 1 km by 1 km. The evapotranspiration data are based on extrapolating KNMI station data using Thin Plate Spline interpolation. The station data are calculated by KNMI using incoming shortwave radiation and mean daily temperature measurements at the KNMI stations. The evapotranspiration data have a spatial resolution of 10 km by 10 km.

We use the SMAP (Soil Moisture Active Passive) L3 Enhanced radiometer-only daily gridded soil moisture product to train the TFN models (Entekhabi et al., 2010; Chan et al., 2018; O'Neill et al., 2018). The surface soil moisture estimates are obtained by processing interpolated brightness temperature observations from the SMAP satellite (Das et al., 2018). In general, SMAP soil moisture products perform well in the Twente region (Colliander et al., 2017). Chan et al. (2018) found an unbiased root mean square error of 0.056 $m^3\ m^{-3}$ for the Twente region when assessing the SMAP L3 product using in situ soil moisture measurements. The SMAP observations are available for the study area

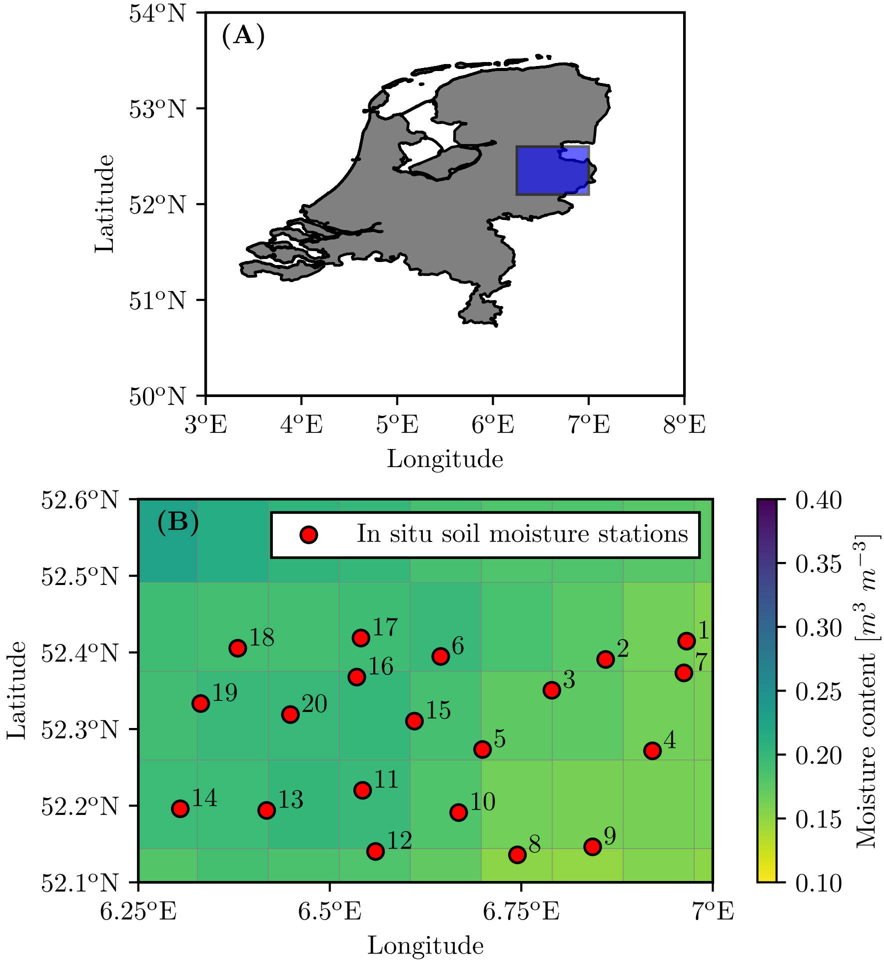

Figure 4.2: (A) Location of the Twente study area in the Netherlands, indicated by the blue rectangular shape. (B) Overview of the study area including the station locations of the in situ soil moisture monitoring network and the footprint of the SMAP L3 Enhanced surface soil moisture data for September 9 2017.

approximately every 2–3 days and have a spatial resolution of 9 *km* by 9 *km*. The footprint of the SMAP L3 Enhanced product in the Twente region is visualized in Figure 4.2. We have analysed the SMAP data for the period January 1 2016 – January 1 2019.

Additionally, we use in situ soil moisture measurements from a monitoring network to assess whether the TFN models can describe soil moisture field conditions. The monitoring network, operating since 2009, is maintained by the ITC faculty of the University of Twente (Dente et al., 2012; Van der Velde, 2018; Van der Velde et al., 2019). Both volumetric moisture content and soil temperature are measured at 20 locations in the Twente region. The stations cover agricultural fields, except station 20, which is installed in a forest area. The station locations are shown in Figure 4.2. The monitoring network consists of Decagon 5TM probes at 5, 10, 20, 40, and 80 cm soil depth and provide a reading every 15 minutes. We use daily averaged measurements at 5 cm soil depth, since remotely sensed soil moisture data are limited to surface soil moisture (Petropoulos et al., 2015; Benninga et al., 2019). Figure 4.2 provides an overview of the SMAP L3 Enhanced footprint relative to the in situ locations in the study area. Seventeen pixels provide information for the 20 stations.

4.2.3 TFN modelling library: Pastas

To set up the TFN models, we use the open source library Pastas (Collenteur et al., 2019b), which is a Python 3 implementation of the TFN modelling approach described in section 4.2.1. A description of Pastas can be found in Collenteur et al. (2019a). In order to solve equation 4.1, we use a least squares optimization approach to fit the parameters of the IR functions in Pastas (equations 4.5 and 4.6). More information on the Pastas library can be found at `https://pastas.readthedocs.io`.

4.2.4 General workflow

Figure 4.3 shows the general research workflow. The workflow focuses on three main parts, indicated by the yellow boxes in the figure. First, the TFN models are set up and trained using SMAP data (*SMAP training*). Next, these models are validated using SMAP data for a different period (*SMAP validation*). Last, we assess the applicability of the TFN models for estimating soil moisture on field scales using in situ measurements (*Field validation*). We will elaborate on each research step. The numbers in the following sections refer to the steps shown in Figure 4.3.

SMAP training

First, (1) the input datasets, which are described in section 4.2.2, are selected. The datasets are split in a (2) training set and a (3) validation set. The training set is used to train the TFN models by deriving the parameter sets for the IR functions. The validation set is used to assess the trained TFN model results. We want to use a training period which covers at least the response time of the hydrological system that we observe. We used the shape of the IR distributions to estimate the response time, see Section 4.3.3.

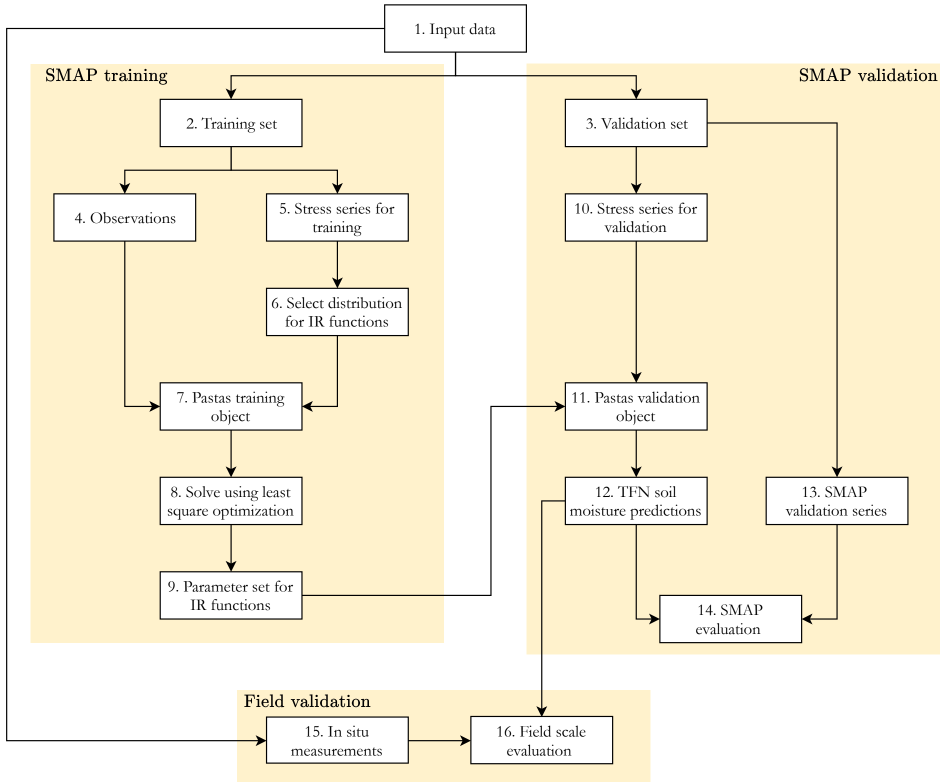

Figure 4.3: Flowchart visualizing the research steps to set up and validate a TFN model with SMAP observations and in situ measurements. The individual steps are described in Section 4.2.4.

Especially, we are interested in the predictive capabilities of the TFN model for the dry summer period of 2018. Therefore, the training set covers the period January 1 2016 – January 1 2018, while the validation set covers the period January 1 2018 – January 1 2019. Since more SMAP observations are becoming available, the training period can be continuously extended in an operational setting.

We assessed the influence of the training period length by performing a sensitivity analysis in which both the length and period of training set are varied. The training periods used for the sensitivity analysis are a summer period (April – October 2016), a winter period (October 2016 – April 2017), the full year 2016 and the full year 2017. In addition, we assessed the TFN model capabilities by switching the training and validation period: January 1 2017 – January 1 2019 for the training set and January 1 2016 – January 1 2017 for the validation set. Section 4.4.1 elaborates on the results of the sensitivity analysis

Table 4.1: Combinations of statistical distributions assessed for the IR functions.

Precipitation	Evapotranspiration	Code
Gamma	Gamma	**GG**
Exponential	Exponential	**EE**
Gamma	Exponential	**GE**
Exponential	Gamma	**EG**

and the implications for TFN modelling.

The SMAP soil moisture observations of the training set are used as the (4) observational training dataset for the TFN model. Then, (5) the stress series are defined for the training period. Subsequently, (6) a statistical distribution is defined for each stress series. Both the observations and the stress series are added to a (7) Pastas model object. Next, Pastas applies (8) a least squares optimization approach to find (9) optimal parameter sets for the precipitation and evapotranspiration IR functions for each in situ location by solving equation 4.1. These sets are assumed to best fit the SMAP soil moisture observations for the training period. The sets can subsequently be used to estimate soil moisture dynamics in the validation period.

We assessed the applicability of two distribution functions to define the IR function of each stress series: a gamma and an exponential distribution. Table 4.1 lists the combinations. The explained variance percentage (EVP) is calculated to assess the applicability of each combination. The EVP is defined as:

$$EVP = 100\frac{\sigma_h^2 - \sigma_n^2}{\sigma_h^2}, \tag{4.8}$$

where σ_h^2 is the variance of the SMAP soil moisture observations $[(m^3\ m^{-3})^2]$ and σ_n^2 is the variance of the TFN model residuals as defined in equation 4.1 $[(m^3\ m^{-3})^2]$ (Von Asmuth et al., 2002). An EVP of 100% indicates a perfect simulation of the observations, since no residuals exist in that case. As a rule of thumb, one generally accepts the results of a TFN model if the EVP $\geq$ 70%.

Additionally, the noise series should not be autocorrelated. Autocorrelation would indicate that the white noise assumption does not hold (Von Asmuth et al., 2002). We use the Ljung-Box test to determine whether the noise series shows significant autocorrelation (Ljung and Box, 1978).

SMAP validation

Next, we use SMAP observations from the year 2018 to validate the TFN models. We define (10) the precipitation and evapotranspiration stress series for the period January 1 2018 – January 1 2019. These series are used to (11) set up a Pastas model for the validation period. The (9) optimized parameter sets from the training set are applied to define the IR functions. Again, Pastas solves equation 4.1 using the defined IR functions, the optimized parameter sets, and the stress series, resulting in (12) predictions of soil moisture for the validation period. We use (13) the SMAP validation set to (14) assess the TFN model results using the unbiased Root Mean Square Error (uRMSE), bias, and Pearson correlation coefficient. Appendix A provides a definition of these error metrics.

Field validation

Furthermore, we are interested in the applicability of the TFN models on field scales compared to the regional scales represented by the SMAP observations. Therefore, we use (15) in situ soil moisture measurements from the soil moisture monitoring network to (16) evaluate the TFN model results on field scales using the error metrics. The evaluation is performed for all in situ location for which measurement data is available for the validation period. The following eleven stations provide data for the 2018 validation period: 2, 4, 7, 9, 10, 11, 13, 14, 15, 16, and 17.

4.3 Results

4.3.1 Selection of distribution functions

First, we evaluated which combination of statistical distributions leads to the best fit of the TFN models in terms of EVP. Figure 4.4 shows the spatially averaged EVP for the four distribution combinations as defined in Table 4.1. The GG and GE combinations lead to TFN models which cannot sufficiently explain soil moisture dynamics. Both the GG and GE combinations score spatially averaged EVP values lower than 50%. The Exponential-Exponential (EE) and Exponential-Gamma (EG) combinations show the best model behaviour. The EG combination leads to a rejection of the TFN model for one location, i.e. station 16 (67%). The EVP of the EE combination is consistently larger than 70% for all stations, exceeding the model acceptance criterion. Since the EE combination consistently shows good accuracy, we use the exponential distribution for both the precipitation and evapotranspiration IR functions in the remainder of the study.

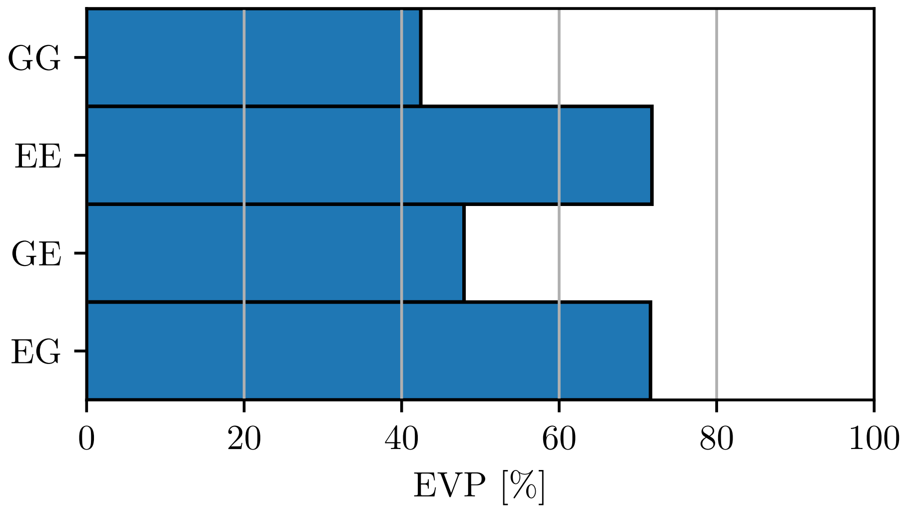

Figure 4.4: Spatially averaged EVP per combination of distributions for precipitation and evapotranspiration stress series.

The TFN models will be rejected when a gamma distribution is used for the precipitation stress series. An exponential distribution is a better choice for the precipitation stress series. The difference is less distinct for the evapotranspiration stress series. Either a gamma or exponential distribution leads to similar results in terms of EVP. So, although Von Asmuth et al. (2002) show that the gamma distribution is suitable to model the response of groundwater head to recharge using precipitation stress series, the gamma distribution is not the best choice for precipitation stress series when modelling surface soil moisture dynamics.

4.3.2 Assessment of soil moisture modelling

We will show the TFN model results for the first in situ location for which field validation data are available, which is location 2. Figure 4.5 shows the TFN model results, SMAP observations, and in situ measurements for location 2 during the period January 1 2016 – January 1 2019. The in situ measurements are only shown for the validation period, which is the year 2018. In both the training and validation period, the TFN model can correctly simulate the summer-winter cycle of drying and wetting. Large deviations between the SMAP observations and the TFN model results can be observed in winter periods such as December 2016 and February 2018. The soil can freeze in winter periods, which significantly affects SMAP satellite as well as in situ sensor readings (Van der Velde et al., 2019). As temperature is not an input, the TFN model is not affected by this limitation. On the other hand, the TFN model underestimates soil moisture during July-August 2018. Last, the SMAP observations overestimate soil moisture in the transition from summer to fall in 2018. Van der Velde et al. (2019) evaluated SMAP surface soil moisture data in the Twente region and stated that "in the summer/fall of 2018, dry spells were ended by a sequence of substantial rain events that exposed the disparity in sampling depth between SMAP and the in situ sensors". Shellito et al. (2016) and Benninga et al. (2018) found similar results.

We quantify the accuracy of the TFN models by calculating the uRMSE, bias and correlation coefficient error metrics with respect to the SMAP observations for each in situ location in the 2018 validation period. The dots in Figure 4.6 (*SMAP validation 2018*) visualize the error metrics of the TFN models results with respect to the SMAP observations for the year 2018. The uRMSE varies between 0.059–0.070 m^3 m^{-3} for all locations.

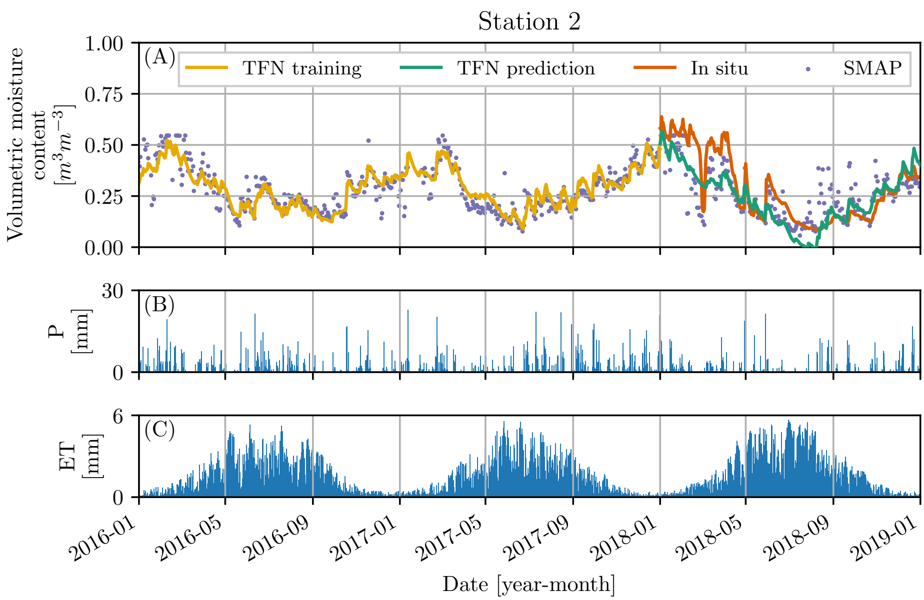

Figure 4.5: (A) TFN model results for location 2. The yellow line indicates the TFN model results in the training period. The green line indicates the TFN model results in the validation period. The purple dots represent the SMAP observations, while the brown line represents the in situ soil moisture measurements. (B) Corresponding precipitation stress series. (C) Corresponding evapotranspiration stress series.

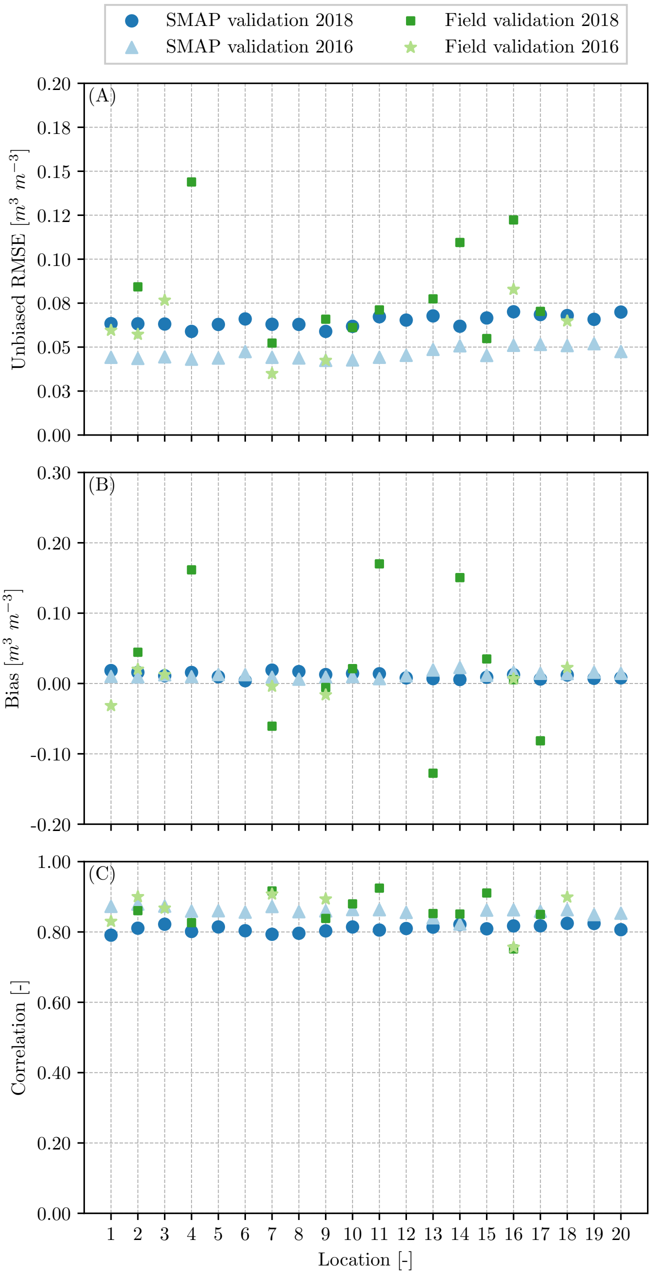

Figure 4.6: Evaluation of the TFN model accuracy in terms of (A) unbiased root mean square error, (B) bias, and (C) Pearson correlation coefficient for the 2018 validation and 2016 sensitivity analysis periods. We evaluated the TFN models against the SMAP data (SMAP validation) and the TFN models versus in situ data (Field validation).

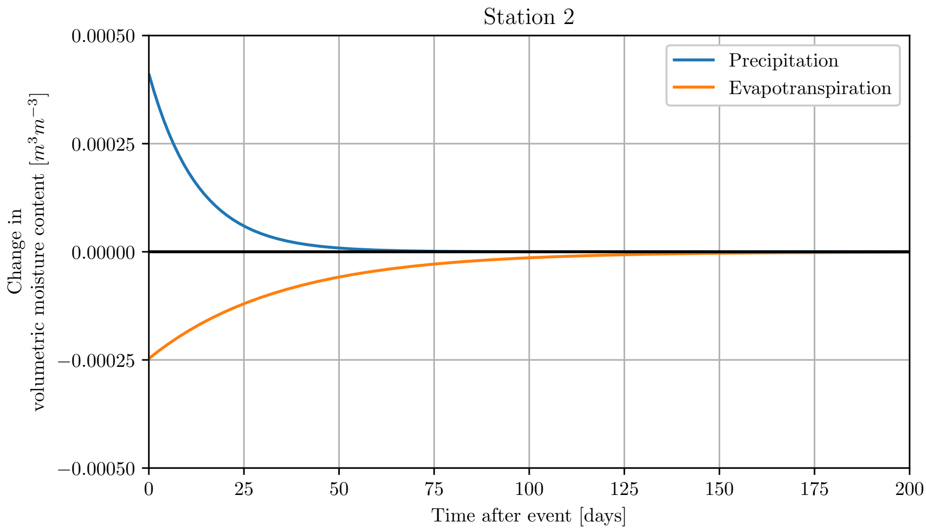

Figure 4.7: Trained block response functions for precipitation and evapotranspiration at location 2 based on the 2016-2017 training set.

The bias varies between 0.0040–0.019 $m^3\ m^{-3}$ for all locations. The correlation coefficient varies between 0.79–0.82 $[-]$ for all locations. Recognizing that the TFN models do not consider the over- and underestimation of SMAP in frozen and dry conditions, the TFN models perform well in predicting SMAP surface soil moisture. An implication is that the trained TFN model can be used to estimate surface soil moisture and extend SMAP data if precipitation and evapotranspiration data are available. Furthermore, one could use the TFN models to construct historical surface soil moisture time series, since the KNMI meteorological datasets cover a long period.

In addition, Figure 4.6 shows the RMSE of the TFN model results with respect to the in situ measurements for eleven locations in the 2018 validation period (*Field validation 2018*). The spread in RMSE is more substantial than for the SMAP 2018 validation. Although a fundamental difference exists in spatial scales represented by the SMAP satellite footprint and the in situ measurements, the TFN models accurately predict field scale soil moisture for seven out of eleven locations in terms of uRMSE, for four out of eleven locations in terms of bias, and for all locations in terms of correlation coefficient.

4.3.3 Trained IR functions

The IR functions contain valuable information on the soil moisture response to the stress series. As described in section 4.2.1, the block response function describes the response of soil moisture to a unit stress of one day. Figure 4.7 shows the trained block response functions of the precipitation and evapotranspiration stresses for location 2. As expected, the precipitation stress series has a positive impact on the soil moisture state, while the evapotranspiration stress series decreases the soil moisture state. Also, the time scale of the precipitation stress series is smaller than the time scale of the evapotranspiration stress series. Furthermore, the initial response of soil moisture at day one is much larger for the precipitation stress series than for the evapotranspiration stress series. Similar observations hold for all individual locations. These findings are physically reasonable, since precipitation causes immediate spikes in soil moisture, while drydown due to evapotranspiration takes place on longer time scales.

In addition, Figure 4.7 shows that the length of the precipitation IR function for location 2 is approximately 75 days, while the evapotranspiration IR function has a length of approximately 150 days. The length of the IR functions can be interpreted as the system response to that specific stress series. The training period of two year covers this length multiple times. Therefore, we can conclude that the training period is of sufficient length to estimate soil moisture dynamics in the Twente region.

4.4 Discussion

4.4.1 Verification of TFN modelling approach

The results show that TFN modelling using the PIRFICT method can be applied to predict surface soil moisture conditions in the Twente region using SMAP surface soil moisture remote sensing data as training set. As part of the TFN model verification, we assess whether the noise series show autocorrelation using the Ljung-Box statistical test (Ljung and Box, 1978). The autocorrelation is assessed considering a significance level of 0.05 [−]. The Ljung-Box test shows that no significant autocorrelation is observed for all stations. Therefore, the white noise assumption holds for all stations.

In addition, because of the data-based nature of TFN models, there is a risk in extrapolating results to situations for which no references are available in the training set (Von Asmuth et al., 2012). For example, the TFN model of location 2 does not capture the extremely dry summer period of 2018 well, as seen in Figure 4.5. According to the

TFN model, the volumetric moisture content drops to almost 0 m^3 m^{-3} in that period. However, both the SMAP observations and the in situ measurements show that soil moisture seems to have a physical lower limit of approximately 0.1 m^3 m^{-3}. The TFN models do not identify the lower limit. This limitation might be explained by evapotranspiration reduction, which is a mechanism which reduces actual evapotranspiration when only low amounts of moisture are available. Thus, evapotranspiration reduction occurs in dry periods. Since the training period does not include long dry periods, the TFN models do not consider evapotranspiration reduction. The influence of the training period will be assessed in the next section.

4.4.2 Sensitivity of training period

We performed a sensitivity analysis on both the training set period and length based on the RMSE error metric. Figure 4.8 shows the results of the sensitivity analysis. Soil moisture dynamics at some stations cannot be properly explained using the 2016–2017 winter period as training period. The difference between the summer of 2016, the year 2016, 2017, and 2016-2017 training periods is not significant. The 2016–2017 winter period shows the largest RMSE values. The 2016 summer training set shows the smallest RMSE values. Figure 4.5 showed that the 2016-2017 training set leads to a large underestimation of the 2018 dry summer period. The same finding holds for the 2016 and 2017 training sets. Using the 2016 summer training set, the TFN models can simulate the dry period of 2018 correctly. We refer to Figure 4.10 in Appendix B which shows the TFN model results for location 2 when only the 2016 summer period is used as training set. Thus, the TFN models can represent the drought period of 2018 when a representative training period is selected.

The dry period in the summer of 2018 is an extreme event. Probably, the sensitivity analysis results are case-specific and thus not generalizable. To test the applicability of the TFN models in more regular situations, we switched the training and validation set periods. The TFN models are trained for the period January 1 2017 – January 1 2019 and validated for the year 2016. The triangles in Figure 4.6 (*SMAP validation 2016*) show the uRMSE, bias, and correlation coefficient of the TFN models with respect to the SMAP observations when the year 2016 is used as validation set. The 2016 results have consistently higher accuracies than the SMAP 2018 validation results. The uRMSE varies between 0.042 and 0.052 m^3 m^{-3} for the locations. The bias varies between 0.0061 and 0.023 m^3 m^{-3} for the locations. The correlation coefficient varies between 0.82 and 0.88 $[-]$ for the locations.

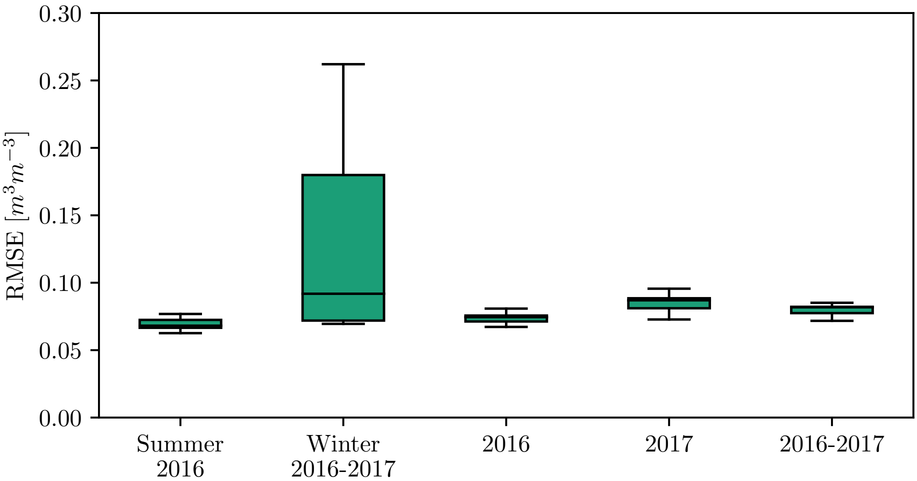

Figure 4.8: The results of the sensitivity analysis illustrating the effect of the training period length. The box plots show the distribution of the RMSE of the TFN model with respect to the in situ measurements in the 2018 validation period for different training periods.

Furthermore, the star shapes in Figure 4.6 (*Field validation 2016*) show the error metrics of the TFN models with respect to the in situ measurements when the year 2016 is used as validation set. No apparent change in accuracy is found for the 2016 validation results on field scales, which are represented by the in situ measurements. These results indicate that a training period including the extreme dry summer of 2018 will lead to more accurate TFN models for drought predictions, especially on spatial scales similar to the SMAP satellite footprint.

Table 4.2 shows the performance of the soil moisture TFN modelling approach in comparison with the SMAP validation studies of Colliander et al. (2017) and Chan et al. (2018), as well as the data-driven soil moisture modelling approach of Kolassa et al. (2017), who also used SMAP observations as training data. As these studies applied spatially averaged results for the Twente study area, the TFN model results are also spatially averaged. Especially the TFN model validated for the year 2016 performs well as shown by the uRMSE, bias, RMSE, and correlation coefficient error metrics. The comparison with the data-driven approach by Kolassa et al. (2017) shows that SMAP TFN modelling for the year 2016 has a similar accuracy.

Table 4.2: Spatially averaged error metrics (uRMSE, bias, RMSE, and r) for TFN model results versus in situ measurements and a comparison with literature. NA indicates error metric is not available. NumStat is the number of field stations included in the analysis.

Source	Period	uRMSE $[m^3\ m^{-3}]$	Bias $[m^3\ m^{-3}]$	RMSE $[m^3\ m^{-3}]$	r [-]	NumStat [-]
TFN versus in situ	Jan 2018 - Jan 2019	0.083	0.028	0.12	0.86	11
TFN versus in situ	Jan 2016 - Jan 2017	0.060	0.0014	0.063	0.86	7
Colliander et al. (2017)	Apr 2015 - Mar 2016	0.044	0.014	0.046	0.92	5
Chan et al. (2018)	Apr 2015 - Oct 2016	0.056	-0.0010	0.052	0.90	5
Kolassa et al. (2017)	Apr 2016 - Mar 2017	0.057	NA	NA	0.70	9

4.4.3 Water system characteristics

Generally, IR functions can provide information on characteristics of the system which is observed. Among others, these functions describe the unit step response and response time of groundwater dynamics when a groundwater system is observed (Bakker et al., 2008; Zaadnoordijk et al., 2018). The exponential distribution applied in this work consists of two parameters: A and a, see equation 4.6. The parameter A relates to the total change in soil moisture volume due to a unit stress. A large A indicates a large total change in volume. The shape parameter a is related to the time scale on which a unit stress affects soil moisture. A large a indicates a fast response.

Figure 4.9 shows the trained parameters for the precipitation and evapotranspiration IR functions for all locations based on the 2016–2017 training set. The colours indicate the station numbering as shown in Figure 4.2. Approximately, the lower numbers are situ-

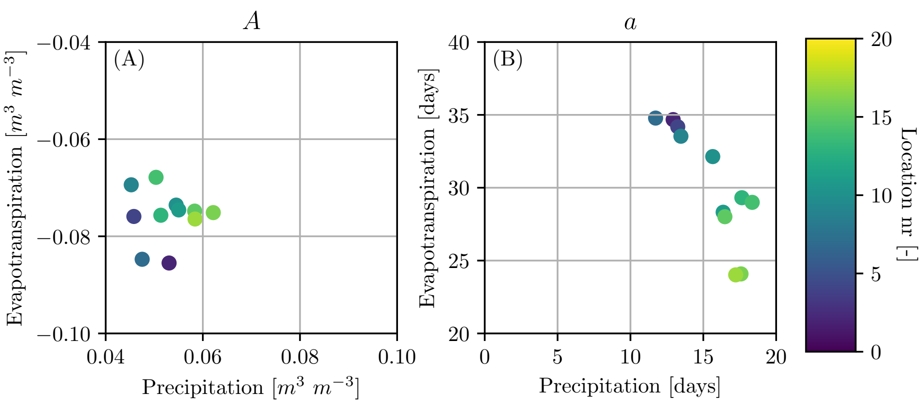

Figure 4.9: Distribution of (A) parameter A and (B) parameter a of the precipitation and evapotranspiration IR functions. The colourbar represents the 11 stations as shown in Figure 4.2.

ated in the eastern part, while the higher numbers are situated in the western part of the study area. No clear pattern can be found for parameter A, which represents the total soil moisture change. The total change is probably related to soil physical characteristics and vegetation dynamics. These features are quite similar for the locations in the study area, with mainly sandy soils and grass vegetation, which is possibly why we do not observe distinct differences. A valuable addition can be to study whether different IR functions and corresponding parameters are found in areas with other soil characteristics, such as peaty or clayey areas, or areas with different vegetation types.

On the other hand, a trend is seen in the spatial distribution of parameter a, which describes the time scales of the IR functions. In general, if a large soil moisture response time to precipitation is found at a specific location, the corresponding soil moisture response time to evapotranspiration is relatively small and vice versa. The length scale of the precipitation IR function is larger for locations in the western part of the study area. A possible explanation is the local variation in precipitation patterns. Also, the subsurface in the western part of the study area contains thick sand layers. Precipitation infiltrates relatively easy in sandy layers, which causes a slow response of shallow moisture. Moraines of clay are found in the eastern part of the study area. Clay layers have low infiltration rates, which results in a fast increase of soil moisture content. However, more research is needed to generalize these findings.

Also, one should be careful in relating these parameters to physical processes as the selection of an IR function is an assumption (Von Asmuth et al., 2012). For example, Figure 4.7 shows that the time scale of the precipitation IR function is approximately 75 days. To our knowledge, this time scale cannot be directly connected to physical phenomena. More research on the IR function parameters is needed to increase the understanding of their physical meaning.

4.5 Conclusions

We studied the applicability of transfer function-noise modelling (TFN) for describing and predicting soil moisture dynamics. TFN modelling is a fast alternative for process-based models, taking only seconds to simulate a full year of daily soil moisture conditions. TFN modelling is based on the assumption that soil moisture dynamics can be explained by linearly transforming precipitation and evapotranspiration stress series using impulse-response (IR) functions. The SMAP L3 Enhanced surface soil moisture product is used to train the TFN models. We found that exponential distributions describe the

IR functions of both the precipitation and evapotranspiration stress series better than gamma distributions.

TFN models describe soil moisture conditions well when comparing the TFN model results with the SMAP observations. In addition, the TFN model results were compared with in situ soil moisture measurements to assess the field scale applicability of TFN modelling. The accuracy of the TFN models mainly depends on the representation of the SMAP satellite product for that specific spatial scale.

A practical application for operational water management is that the TFN modelling approach can be used to estimate soil moisture dynamics using predictions of precipitation and evapotranspiration. The application is promising if sufficient training data are available, although one should be careful when interpreting results in extreme situations, since the TFN models do not consider the physical lower and upper limits of soil moisture. However, a sensitivity analysis showed that a suitable training period can significantly increase the TFN model capabilities in both regular and extreme situations. In addition, the IR function parameters potentially provide valuable information on water system characteristics, such as response times of soil moisture to precipitation and evapotranspiration. However, more research on the physical meaning of the parameters is needed to understand their applicability. Concluding, we consider the applicability of TFN modelling for explaining soil moisture dynamics promising and propose to explore the possibilities of TFN modelling for operationally predicting soil moisture.

Acknowledgements

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4.6 Appendix A

The Root Mean Square Error (RMSE) is defined as:

$$RMSE = \sqrt{\frac{\sum_{j=1}^{N}\left(\theta_j^{obs} - \theta_j^{pred}\right)^2}{N}}, \tag{4.9}$$

in which θ_j^{obs} are the SMAP soil moisture measurements for each day j [$m^3\ m^{-3}$], θ_j^{pred} are the TFN model results for each day j [$m^3\ m^{-3}$], and N is the number of observations [–].

The unbiased Root Mean Square Error (uRMSE) is defined as:

$$uRMSE = \sqrt{\frac{\sum_{j=1}^{N}\left(\left(\theta_j^{obs} - \overline{\theta^{obs}}\right) - \left(\theta_j^{pred} - \overline{\theta^{pred}}\right)\right)^2}{N}}, \tag{4.10}$$

in which $\overline{\theta^{obs}}$ is the arithmetic mean of the SMAP soil moisture measurements [$m^3\ m^{-3}$] and $\overline{\theta^{pred}}$ is arithmetic mean of the TFN model results [$m^3\ m^{-3}$].

The bias is defined as:

$$Bias = \overline{\theta^{obs}} - \overline{\theta^{pred}}. \tag{4.11}$$

The Pearson correlation coefficient r is defined as:

$$r = \frac{\sum_{j=1}^{N}\left(\left(\theta_j^{obs} - \overline{\theta^{obs}}\right)\left(\theta_j^{pred} - \overline{\theta^{pred}}\right)\right)}{\sqrt{\sum_{j=1}^{N}\left(\theta_j^{obs} - \overline{\theta^{obs}}\right)^2}\sqrt{\sum_{j=1}^{N}\left(\theta_j^{pred} - \overline{\theta^{pred}}\right)^2}}. \tag{4.12}$$

4.7 Appendix B

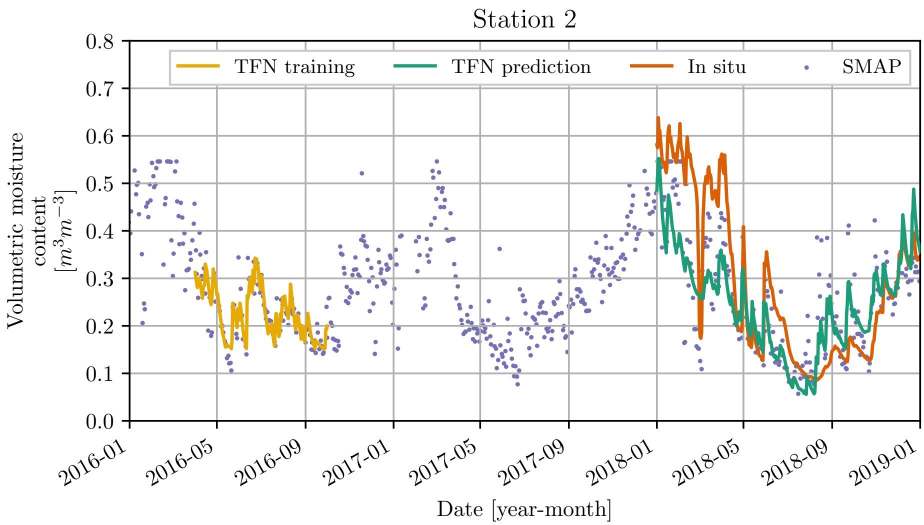

Figure 4.10: TFN model results for location 2 when the summer 2016 period is used as training period.

CHAPTER 5

Discussion

This chapter contains a discussion on the thesis results. First, we elaborate on the scientific implications. Next, we show several applications for water management. Last, we focus on the applicability of the results for other practical and scientific areas.

5.1 Scientific implications

5.1.1 Spatiotemporal variability of soil moisture

Section 1.4 discussed the spatiotemporal overlap and mismatch between the three main methods of estimating soil moisture (in situ, remote sensing, and hydrological modelling). Each method leads to soil moisture estimates which have to be interpreted on a different spatiotemporal scale. The three methods can complement each other, although critical evaluations are needed when applying integral approaches.

Data from the three soil moisture estimation methods were combined in this research to retrieve more accurate soil moisture estimates. Chapter 3 showed how regional scale remote sensing estimates can be used to update regional scale hydrological modelling estimates by applying a perturbed observations EnKF data assimilation scheme, as seen in Figure 3.6. On a local scale, the impact of the data assimilation scheme largely depends on the representativeness of the remote sensing estimates concerning the spatial scale. Chapter 4 showed that remote sensing estimates have value on field and local scales, as the TFN models represent the in situ estimates as visualized in Figures 4.5 and 4.10. In addition, the data assimilation approach enables to translate surface soil moisture information to root zone soil moisture information, extending purely statistical methods (e.g. Albergel et al., 2008; Carranza et al., 2018). Furthermore, the approach integrated the remote sensing data, which are available every 2–3 days for the Twente study area, to daily information using the hydrological model. Also, the TFN models have value in retrieving information on days for which no remote sensing imagery is available. A more detailed discussion of the possibilities of TFN modelling is given in Section 5.1.3. We expect that new sources of high-resolution remotely sensed soil moisture information, for example from Sentinel-1 satellite retrievals (Bauer-Marschallinger et al., 2019; Benninga et al., 2019) or combining SMAP and Sentinel-1 retrievals (Das et al., 2019), will help to increase the effectiveness of these methods for relating soil moisture estimates on both regional and field scales.

Substantial biases exist between in situ, remote sensing, and model estimates (both process-based and TFN). The differences in both the horizontal and vertical spatial scales between in situ, remote sensing and hydrological modelling estimates lead to large uncertainties in hydrological research, validation procedures and practical applications. For example, the model results of Chapters 3 and 4 are validated using in situ soil moisture estimates, which are valid on point scales. Although not investigated in this research, several other approaches have been proposed to relate the various soil moisture estimation methods. Ford and Quiring (2019) employed various soil moisture comparison and verification methods to develop a comprehensive soil moisture validation framework and assess the fidelity of the three estimation methods. Crow and Wood (2003) applied a model-based approach to upscale in situ estimates to be representative on a satellite footprint scale. Van der Velde et al. (2019) showed the applicability of a similar approach for the validation of a SMAP soil moisture product using the in situ soil moisture estimates of the Twente network. Another approach is triple collocation analysis (Scipal et al., 2010; Gruber et al., 2016). Triple collocation analysis can be applied to estimate the error structure of three soil moisture datasets (e.g. in situ, remote sensing, and hydrological modelling) and serves as a valuable addition to harmonize the different spatiotemporal scales of the soil moisture estimation methods. Nonetheless, new methods for in situ soil moisture estimation on field scales will have to be developed and studied to overcome the difference in spatiotemporal scales. Future research should continue to focus on developing methods to relate soil moisture estimates on various spatiotemporal scales.

One can argue whether the soil moisture modelling assumptions and concepts applied for point or field studies are still valid when moving towards regional, national, and global studies. For example, the complexity of physical processes which have to be taken into account differs when moving from field to larger spatial scales. Special attention is needed during the development of soil moisture modelling tools to identify the relevant spatiotemporal scales. Decades of research on process-based unsaturated zone modelling led to complex hydrological models which heavily depend on rather coarse soil physical and vegetation parametrizations (Vereecken et al., 2016). Chapter 3 and 4 show that data-driven methods have the potential to integrate soil moisture information on several spatiotemporal scales. A powerful aspect of many data-driven methods is that, in general, they often do not need a priori assumptions on system characteristics, which is an interesting property when studying subsurface processes. Already, data-driven methods are an important research field in soil and hydrological sciences (Remesan and Mathew, 2015). We expect that the application of these methods will keep growing, especially with a focus on the integration with process-based modelling.

5.1.2 Impact of soil moisture data assimilation on other hydrological variables

The process-based hydrological modelling framework NHI applied in Chapter 3 consists of several coupled components related to unsaturated zone (MetaSWAP), saturated zone (MODFLOW) and surface water dynamics (Mozart and DM). The simulations of each component affect other components, see Figure 3.1. For example, Crow and Ryu (2009), Alavi et al. (2010), Brocca et al. (2010), Koster et al. (2018), and Naz et al. (2019) showed that the assimilation of soil moisture data not only increases the accuracy of soil moisture simulations, but also affects evapotranspiration, phreatic groundwater levels, and runoff simulations. The next sections will describe the effect of assimilating SMAP surface soil moisture observations on other simulated hydrological variables within the LHM model, such as evapotranspiration and groundwater levels.

Evapotranspiration

Zhang et al. (2016) showed that assimilating soil moisture observations in an integrated hydrological model improves the accuracy of evapotranspiration model estimates. Evapotranspiration data can help in monitoring the growth and water demand of vegetation, which is valuable for agricultural activities. The unsaturated zone metamodel MetaSWAP within LHM calculates actual evapotranspiration (ET_{act}) using Makkink reference crop evapotranspiration input data (ET_{ref}). ET_{act} depends on root extraction rates, which in turn depend on the availability of soil moisture. The Feddes reduction curve introduced by Feddes et al. (1978) describes the relation between soil moisture availability and root extraction rates.

Figure 5.1 shows two ET_{act} simulations of the unsaturated zone model MetaSWAP for station 1 of the Twente in situ soil moisture monitoring network (Dente et al., 2012), based on the simulations described in Chapter 3. Figure 3.2 displays the location of this station within the Twente study area. Overall, the assimilation of soil moisture estimates does affect the actual evapotranspiration simulations. Small differences can be observed between the open loop and the data assimilation run, as can be seen in the lower panel. The lower panel shows that the change in ET_{act} is not strictly positive or negative, indicating that the model is not correcting for biases in the evapotranspiration simulations. Remarkable is the large increase of ET_{act} in the EnKF run around the end of November. A model artefact causes this peak. The model cannot solve the water balance terms during that time step and artificially adds water via a model variable known as *virtual water creation*. Subsequently, the remaining water volume is removed from the

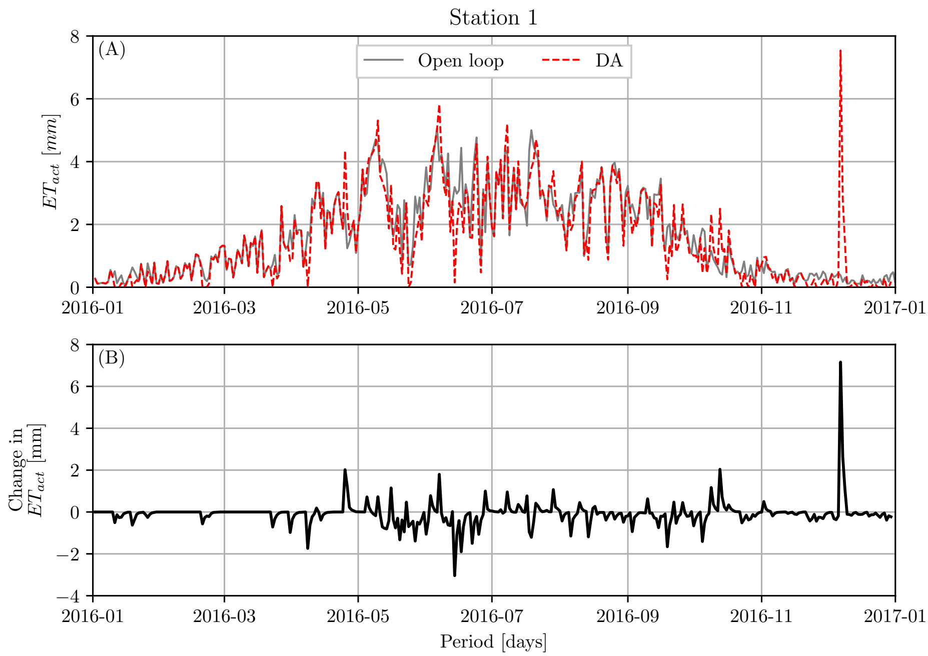

Figure 5.1: (A) Actual evapotranspiration (ET_{act}) model estimates of a LHM open loop run and an EnKF data assimilation run updated with soil moisture observations. (B) Difference in ET_{act} estimates between an open loop and an EnKF run.

model using the ET_{act} model output variable, causing the spike in ET_{act}. We want to stress that the validation of ET_{act} data is challenging, since hardly any measurement data on ET_{act} is available. However, we expect that recent and future breakthroughs in the development of actual evapotranspiration data products will bridge this gap (e.g. Martens et al., 2018; McCabe et al., 2019; Xu et al., 2019).

Groundwater

Carranza et al. (2018) showed that surface soil moisture shows high correlations with soil moisture at greater depths during wet conditions in the Twente study area. They refer to the correlated period as coupled conditions, while periods with low correlation are referred to as decoupled conditions. In general, phreatic groundwater levels in the Twente area are characterized as shallow, and the unsaturated zone is relatively thin. The depth to the phreatic groundwater level varies between 0 and 12 m (Van Thienen-Visser et al., 2014), implying that the assimilation of surface soil moisture estimates in an integrated hydrological model affects phreatic groundwater head simulations.

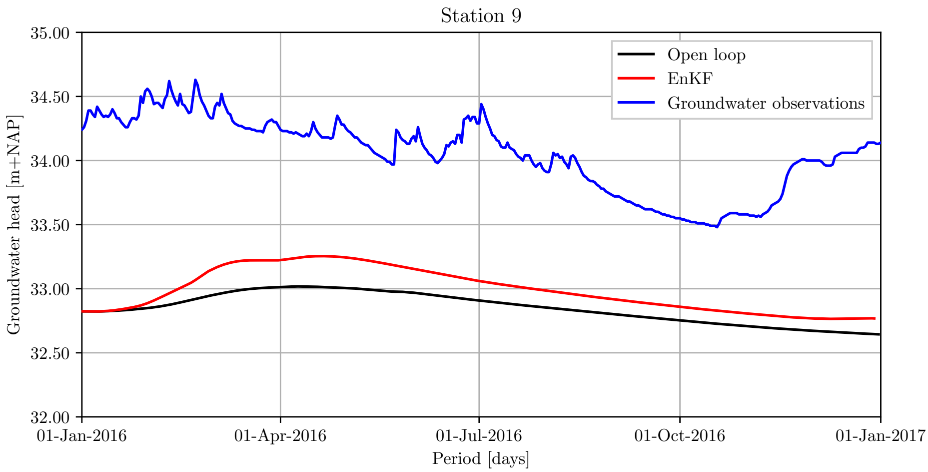

Figure 5.2: Impact of MetaSWAP soil moisture data assimilation on MODFLOW groundwater simulations for location 9 of the Twente soil moisture monitoring network. The unit of the groundwater head is m +NAP, which is the height above the Dutch vertical reference datum.

Indeed, the assimilation of soil moisture observations affects simulated groundwater levels due to the coupling of the MetaSWAP metamodel with the MODFLOW model, as shown in Figure 3.1. Figure 5.2 shows two phreatic groundwater head simulations of the MODFLOW model within LHM for station 9 of the in situ Twente soil moisture monitoring network, based on the simulations described in Chapter 3. Note that Figure 3.2 shows the location of this station within the Twente region. The blue line represents groundwater observations from observation well *B34F1353*. The groundwater observations are obtained from DINOloket, the Dutch online database for subsurface and groundwater data (`https://www.dinoloket.nl`). The black line shows the groundwater head estimates of an open loop model run for a grid cell in which the groundwater well is located. The red line shows the groundwater head estimates when soil moisture observations are assimilated into the unsaturated zone model MetaSWAP using the EnKF data assimilation scheme. Initially, the open loop run shows a large bias with respect to the groundwater head observations. The EnKF run starts to deviate from the open loop run in February 2016. In general, the accuracy of the EnKF run is higher than the accuracy of the open loop run in terms of bias. Still, a large bias exists between the EnKF run and the groundwater head observations.

These results should be interpreted with caution, as one could not expect that increasing the accuracy of unsaturated zone fluxes would significantly remove biases in groundwater head simulations in short term simulations. Although related, groundwater dynamics should be studied on much longer time scales than soil moisture dynamics. Therefore, it would make sense to update both the soil moisture state as well as groundwater heads in a data assimilation procedure to update phreatic groundwater levels. For example, Zhang et al. (2016) found that univariate assimilation of either soil moisture or groundwater head states improves the accuracy of the variable being assimilated, but does not improve the accuracy of other variables. However, they show that the simultaneous assimilation of soil moisture and groundwater head into a hydrological model improves the accuracy of both the soil moisture and groundwater head simulations. Similar findings were found by Camporese et al. (2009b). Moreover, He et al. (2019) show that assimilating both surface water and groundwater head observations in a process-based hydrological model increases the accuracy of both surface water and groundwater head simulations. Although the application of multivariate data assimilation is promising, more research is required before implementation in operational applications. For example, multivariate data assimilation can lead to trade-offs. Botto et al. (2018) shows that assimilating three related variables (pressure head, soil moisture, and subsurface outflow) in the CATHY hydrological model using an EnKF scheme leads to a decrease in accuracy of other hydrological variables which were otherwise simulated well.

Outlook

We expect that, due to the increasing availability of hydrological observations, the applicability of data assimilation schemes for operational water resources management will increase. Lessons might be learned from the meteorological sciences, as operational weather forecasting centres already have considerable experience with integrating data assimilation schemes into operational modelling and forecasting systems. Conversely, weather centres can learn from the lessons learned in terrestrial data assimilation, as subsurface processes concerning soil moisture significantly affect meteorological processes (Drusch et al., 2009; De Rosnay et al., 2013).

Although national water authorities might have sufficient in-house knowledge on data assimilation schemes, regional water authorities generally lack such knowledge. In addition, water authorities may not have access to high-capacity computing facilities which are often needed for data assimilation schemes due to budget constraints. The emergence of parallel computing abilities (Rajabi et al., 2018) and new cloud computing techniques offer solutions for real-time applications (Bürger et al., 2012; Kurtz et al., 2017; Yang et al., 2017). Also, the Model as a Service (MaaS) concept is promising (Chen et al., 2018). MaaS consists of a set of services which users such as water managers can use to quickly run pre-built hydrological models which are run on cloud computing services. The MaaS concept allows users to control model input and concepts and use their data for data assimilation without having to implement data assimilation schemes themselves. An example is the eWaterCycle project (`https://www.ewatercycle.org`), which is an initiative to work collaboratively with existing hydrological models in one framework. MaaS shows overlap with participatory modelling approaches, which are discussed in Section 5.2.3.

Last, the previous sections elaborated on the effect of soil moisture data assimilation on updating of model state variables. Although not studied in this work, data assimilation can also be used in parameter calibration studies. Several studies showed the value of assimilating remotely sensed soil moisture information for calibrating parameters of hydrological models (Wanders et al., 2014a; Shin et al., 2016; Baldwin et al., 2019). An interesting application is updating of subsurface model parameters, as we found that updating of a soil moisture state variable does not directly lead to increased accuracy of groundwater simulations. Updating subsurface model parameters, such as hydraulic conductivity, can lead to increased accuracy of groundwater modelling simulations as shown by, for example, Hendricks Franssen et al. (2011).

5.1.3 Exploring the possibilities of TFN modelling

Since TFN modelling is a data-driven method, the applicability depends on the availability of reliable training datasets. However, the sensitivity analysis performed in Chapter 4 shows that soil moisture TFN models already perform quite well using training set with a length of half a year to one year. This finding is an interesting property of TFN modelling as hardly any long-term soil moisture datasets are available, besides the ESA CCI soil moisture climate records (Gruber et al., 2019). In the following sections, we discuss four possible TFN modelling applications which are interesting to study in the future.

Predicting soil moisture

The fitted IR functions of the TFN models can provide predictions of surface soil moisture using predictions of precipitation and evapotranspiration. The Dutch meteorological institute KNMI provides forecasts of these input variables. One could use ensemble forecasting methods to include uncertainty aspects in the predictions. The TFN models are especially suited for ensemble predictions due to the efficiency and fast calculation times. Additionally, projections of climate variability on historical time series of precipitation and evapotranspiration can be used to assess the effect of climate change on soil moisture dynamics by means of scenario analyses. On the other hand, the limitations of TFN models should be taken into account. Changes in hydrology, land use, and soil type are not considered due to the data-driven nature of the TFN approach.

Relate IR function parameters to physical phenomena

Chapter 4 elaborates on the spatial variation of the trained IR function parameters. The variations could not be directly attributed to physical processes and spatial characteristics. However, Bakker et al. (2007) and Bakker et al. (2008) show that the parameters of IR functions in TFN groundwater modelling can be related to physical processes such as the change in groundwater head. However, we were not able to relate the IR function parameters, visualized in Figure 4.9, to physical processes concerning unsaturated zone dynamics. Therefore, more research into the relationship between the parameters of IR functions and physical processes is needed.

Fill data gaps

The occurrence of data gaps is inherent in satellite remote sensing studies. These gaps exist for various reasons: Firstly, data are only available during satellite overpasses. Also, satellite sensors are prone to malfunctioning. For example, the radiometer sensor of the SMAP satellite temporarily stopped providing data during the summer of 2019. Lastly, soil moisture retrievals by satellites are limitedly possible in periods where temperatures drop below the freezing point, as low temperatures affect the di-electric properties of soil water. The trained TFN models described in Chapter 4 are a means to fill the data gaps. Figures 4.5 and 4.10 show that the TFN models accurately predict soil moisture with respect to the in situ data on days where the SMAP satellite data are not available. Thus, the TFN models allow estimating soil moisture conditions during these gaps.

In addition, the TFN models can help in constructing historical long-term soil moisture datasets. One would need long term input data series of precipitation and evapotranspiration for the development of such datasets. Long-term historical time series of precipitation and evapotranspiration are available in the Netherlands via the meteorological institute KNMI. These time series can be used in combination with the trained IR functions to construct historical soil moisture time series. The validity of such soil moisture time series can be assessed using, for example, long-term ESA CCI soil moisture data (Gruber et al., 2019).

Satellite validation studies

In situ soil moisture data are often used in remote sensing validation studies (Crow et al., 2012; Dente et al., 2012; Wagner et al., 2013; Colliander et al., 2017; Van der Velde et al., 2019). However, Figure 1.8 on page 40 shows that substantial differences in spatial scale exist between in situ and remote sensing soil moisture estimates. The IR functions derived in TFN modelling (Section 4.3.3) are interesting tools to identify which in situ data can be used in the validation procedure, as the IR functions describe the system reaction to input stresses. In such a study, both the IR functions for in situ and remote sensing data should be derived. If the IR functions show similar system behaviour, the in situ data are representative for the remote sensing footprints.

5.2 Applications for water management

We elaborate on various applications of the dissertation findings for water management in the following sections.

5.2.1 Integrating evidence-based and experiential information

Chapter 2 concluded by stressing the need for the development of structured methodologies to increase the integration of evidence-based information in operational water management. The structured methodologies are especially useful in mitigating the use of the opinion-based and limited guidance bypasses as defined in Figure 2.1. For example, Schuwirth et al. (2018) combine a multi-criteria decision support framework for water quality assessments with modelling methods to predict the effectiveness of water management alternatives, using scenario planning to include uncertainties concerning climate variability and socio-economic developments. This example shows the utility of structured methodologies for water management applications.

Decision support systems (DSSs) are tools specifically developed to integrate evidence-based information in operational water resources management (Zhang et al., 2013). Although several DSSs (*Dutch: BOS, or beslissingsondersteunend systeem*) have been developed in recent years, few examples of implementation in operational water management are known (De Kok et al., 2008). For example, Junier and Mostert (2014) evaluated the development and application of a DSS for the implementation of the Water Framework Directive in the Netherlands. They found that the DSS was not used as much as it was intended. Similar results were found in Chapter 2. For example, Figure 2.3 on page 55 shows that hydrological models in a DSS setting are not regarded as important in comparison with other information sources. The interviewed experts indicated that the trust in a DSS firmly declines if an individual decision of the DSS leads to suboptimal water system conditions, independently of the accuracy of the DSS in other situations. In such (often calamity) situations, the experts rather depend on their experiential understanding of the water system. These findings are supported by Fabian et al. (2019), who found that in nature conservation management, experiential information is considered more important than evidence-based information. We should indeed acknowledge that hydrological modelling approaches in DSSs are representations of the real world, so uncertainties exist in the operational application of DSSs. However, water managers probably overestimate their ability to estimate the effects of local measures on catchment and management area scales (Cosgrove and Loucks, 2015; Loucks and Van Beek, 2017). Therefore, structured methodologies can help to find a balance in applying both evidence-based and experiential information for decision-making in operational water management. The framework shown in Figure 2.1 on page 49 provides a guide to develop structured methodologies.

It would be helpful to develop a methodology for building trust in DSSs to increase their applicability. De Kok et al. (2008) state that DSSs can serve several functions: being library systems, learning tools, discussion instruments and operational decision-making tools. An interesting aspect would be to use these different functions to increase the trust in DSSs. Initially, a DSS can be used as a reference work and as a learning tool. Once water managers are familiar with DSSs, they can move towards operational applications. Furthermore, the development and integration of hydrological models in DSSs should be based on the needs of the users, for which participatory modelling approaches should be used. De Kok et al. (2008) describe this process as *appropriate modelling*. Section 5.2.3 elaborates on the value of participatory modelling in the context of this research.

5.2.2 Translating data into information

It is not sufficient to only focus on how we can integrate hydrological modelling into operational water management. Also, we have to focus on general methods for effectively translating and presenting information. One way of translating data into rational information for decision-making is the use of indicators. Indicators are qualitative or quantitative parameters which offer spatiotemporal information. Several studies propose the use of indicators to translate data into applicable and valuable information (Juwana et al., 2012; Maiello et al., 2015; De Girolamo et al., 2017).

Table 5.1: Drought categorization of the SWDI indicator as defined by Martinez-Fernandez et al. (2015).

SWDI	Drought categorization
>0	No drought ($\theta > \theta_{fc}$)
0 to -2	Mild
-2 to -5	Moderate
-5 to -8	Serious
-8 to -10	Severe
<-10	Extreme ($\theta < \theta_{wp}$)

Examples of soil moisture indicators which are useful for drought monitoring are the Soil Water Deficit Index (SWDI) (Martinez-Fernandez et al., 2015), the Drought Severity Index (DSI) (Cammalleri et al., 2016), the Soil Moisture Agricultural Drought Index (SMADI) (Sanchez et al., 2016), and the Storage Capacity Indicator (SCI) (De Heus, 2019). Examples of soil moisture indicators which are useful for flood monitoring are the Soil Wetness Index (SWI) (Mallick et al., 2009) and various relative soil moisture indices proposed by Massari et al. (2014). Furthermore, wildfire risk soil moisture indicators give valuable information in dry periods (Chaparro et al., 2015; Krueger et al., 2017).

We give an example application of the SWDI drought indicator for the dry summer period of 2018, as Vogel et al. (2019) showed that heat waves will occur more frequently in the future. Martinez-Fernandez et al. (2015) define the SWDI as:

$$SWDI = \frac{\theta - \theta_{fc}}{\theta_{aws}} * 10, \tag{5.1}$$

$$\theta_{aws} = \theta_{fc} - \theta_{wp}, \tag{5.2}$$

where θ_{fc} is the soil moisture content at field capacity [$m^3\ m^{-3}$], θ_{aws} is the available water storage [$m^3\ m^{-3}$], and θ_{wp} is the soil moisture content at wilting point [$m^3\ m^{-3}$]. θ_{aws} indicates the maximum amount of soil water available for vegetation and crops. SWDI quantifies agricultural drought by classifying the water availability for crops in terms of severity. Table 5.1 shows the different SWDI drought categories defined by Martinez-Fernandez et al. (2015). The classification helps water managers to interpret the severity of dry spells.

Figure 5.3 shows an example of the SWDI indicator for two days in the year 2018 for the Twente study area. The root zone soil moisture estimates used for calculating the SWDI

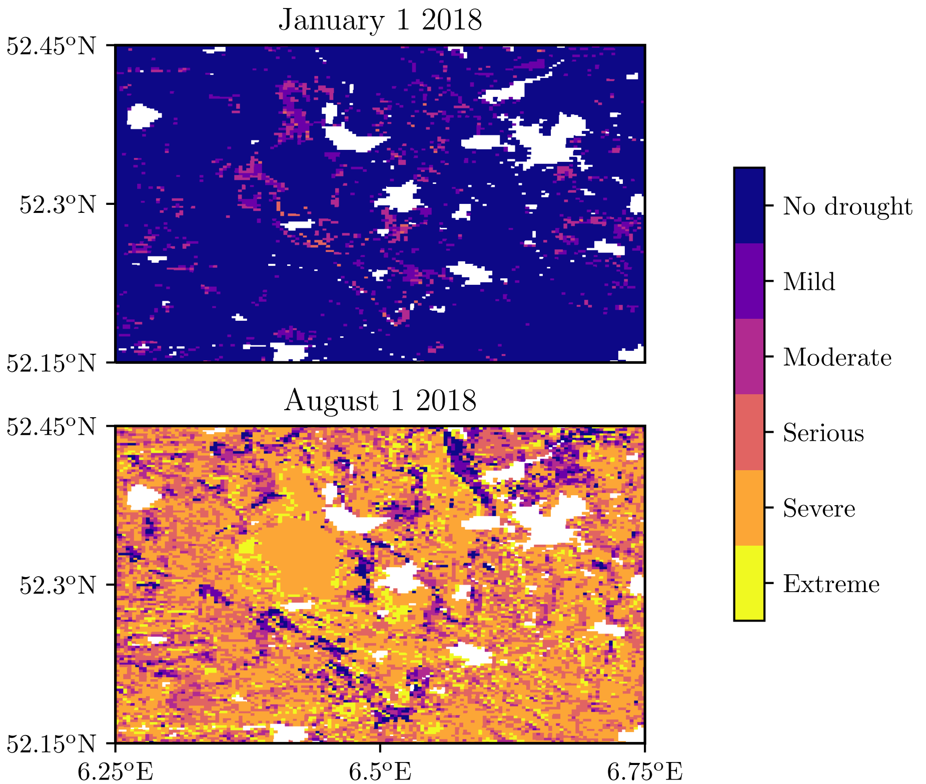

Figure 5.3: SWDI indicator according to the categorization in Table 5.1 for January 1 and August 1 2018 derived from MIPWA model output, which is based on the NHI modelling framework (De Lange et al., 2014). Part of the Twente study area is shown. The white areas indicate built-up areas, which are not considered by MIPWA.

indicator, using equation 5.1, are obtained from a regional hydrological model (MIPWA), which is part of the NHI modelling framework (De Lange et al., 2014). The concepts of MIPWA are similar to the LHM model introduced in Chapter 3. The estimates have a spatial resolution of 25 m by 25 m. Van Gurp (2016) assessed the suitability of MIPWA for soil moisture modelling in the Twente study area. A model description can be found in Chapter 3 and in Van Gurp (2016).

The upper panel of Figure 5.3 shows the SWDI indicator for January 1 2018, which is a wet winter period. The lower panel shows the SWDI indicator for August 1 2018, which is a dry summer period. Analogous to Figure 1.7, the SWDI indicator shows that severe dry conditions existed during the 2018 summer period. The categories show that the severity of the agricultural drought varied over the study area from a moderate to extreme drought. The spatial distribution of the SWDI indicator allows water managers to identify areas which need special attention. In addition, the temporal variation of the SWDI indicator can be used to assess the development of a dry spell and the effectiveness of drought measures.

De Heus (2019) validated the usefulness of the SWDI indicator for drought monitoring in the Twente study area in cooperation with the Dutch regional water authority Vechtstromen. The water managers indicated that the SWDI indicator is useful to support decision-making. In addition, the spatial distribution of SWDI helped the water managers to gain new insights into the spatial variation of drought problems. Finally, the SWDI indicator was considered as easy-to-use.

5.2.3 Participatory modelling

We discussed in Chapter 2 that water resources managers have difficulties interpreting the output of hydrological models. As an example, the water managers indicate that they often do not understand the assumptions behind model conceptualizations, which limits application of hydrological modelling output. Traditionally, hydrological models are developed and run by model developers in response to specific requests from decision-makers, which Cash et al. (2006) and Feldman and Ingram (2009) describe as the loading-dock model of decision support. Model developers prepare models, forecasts or other information for general use without really understanding the end users' needs, which is another example of the science-policy gap, as discussed in Section 1.4.

A proposed method to overcome the science-policy gap regarding hydrological modelling is participatory modelling. Participatory modelling is a process in which water managers are actively involved in model development and simulations (Hanger et al., 2013; Moeseneder et al., 2015). This approach helps water managers to understand the various modelling choices, as well as model developers getting a better understanding of the water managers' needs. In the following, we will give three examples of participatory modelling approaches which were applied in the context of this dissertation. Last, we will reflect on the application of participatory modelling.

Firstly, we applied a participatory modelling approach in Chapter 4. An exploratory study was conducted in cooperation with the Dutch regional water authority Vechtstromen. A student of the University of Twente was positioned at the regional water authority for ten weeks, during which he focused on the development of an initial version of the TFN models described in Chapter 4. The student worked in close cooperation with water managers at the regional water authority. The authors of this work supervised the student. The student and water managers regularly met to discuss the intermediate modelling results. During these meetings, the student presented the recent findings, and the water managers had the opportunity to provide feedback. The final results helped the regional water authority in identifying the possibilities of TFN modelling for application in operational water management (Rorink, 2019). Furthermore, the student had various recommendations which helped to improve the work presented in Chapter 4.

Another example is the validation of a new hydrological subsurface model for the Dutch regional water authority Aa en Maas. This regional water authority shows interest in the application of soil moisture information to increase water management effectiveness. In this context, an in situ soil moisture and temperature monitoring network consisting of 15 locations was developed and installed in cooperation with members of the OWAS1S project team early 2016. The network is situated in the Raam catchment, which is located in the management area of Aa en Maas. The location is shown in Figure 1.5. Benninga et al. (2018) describe the development and characteristics of the Raam monitoring network. All data from the network are freely available and have already resulted in several studies concerning soil moisture applications (Droesen, 2017; Martens et al., 2018; Airlangga and Liu, 2019; Carranza et al., 2019). The development of the network also led to increasing interest in the forecasting of soil moisture and groundwater conditions by the regional water authority, which led to the development of a new subsurface modelling instrument for Aa en Maas. A student of Wageningen University & Research was positioned at the regional water authority and at the research institute Deltares where the modelling instrument is developed. The student used the soil moisture data from the network to validate model output (Droesen, 2017). Next, the student discussed his findings in meetings with water managers from the regional water authority and model developers. Among others, this led to the selection of different model input data concerning soil physical characteristics. Furthermore, the findings of the student contributed to the research methodology applied in Chapter 3.

Last, the MetaSWAP-OpenDA data assimilation framework applied in Chapter 3 was developed using a participatory approach. The coupling of the operational hydrological modelling instrument with the data assimilation framework is a result of a cooperation with a research institute (Deltares), a consultancy firm (HKV), and the authors of this work. During meetings with the software developers of the OpenDA framework, several code requirements were set. Based on these requirements, the software developers developed new software code which was subsequently tested by the user, who in turn gave feedback to the software developers. As a final product, the MetaSWAP-OpenDA framework was added to the official release of the OpenDA software (`http://www.openda.org/`). The source code of the software can be found at `https://github.com/OpenDA-Association/OpenDA`.

The three examples give a good overview of how participatory modelling approaches can help to increase the accuracy and applicability of hydrological models in operational water management. The participatory approach leads to feedback loops between developers and water managers. Furthermore, the frequent meetings with water managers help them become familiar with the processes and different spatiotemporal scales concerning soil moisture. In addition, water managers often consider hydrological models as unreliable for operational water resources management, as was found in Chapter 2. Participatory modelling will help to increase the trust of water managers in hydrological modelling approaches. In our opinion, model developers, policy-makers, and water managers should be encouraged to invest in participatory modelling approaches.

Participatory modelling becomes increasingly included in hydrological model development. For example, the hydrological models based on the NHI modelling framework, such as the LHM model used in Chapter 3 and the MIPWA model discussed in Figure 5.3, have been developed using a participatory approach (De Lange et al., 2014). However, the people from the water authorities and other participating stakeholder organisations who help to develop the models are not always the people who have to apply the models in operational settings. Hence, it is vital that the right people from the water authorities and stakeholder organisations are involved in the modelling process.

5.3 Link to other research areas

Integrating new information in water management

The findings of this study show that integrating new information sources in water management is not just a matter of technical advances. Although the developers of new information may have sufficient knowledge and experience to develop understandable forms of information, external forces largely determine if such information is implemented in water management (Junier and Mostert, 2014). Indeed, several studies stress that the social aspect plays a large role in the integration of new information sources in water management (e.g. Junier and Mostert, 2014; Leskens et al., 2014). Individually, the technical and social aspects have been studied extensively. To develop a consistent framework for integrating new information in water management, we should focus on integrating both the technical and social aspects. Participatory modelling approaches as described in Section 5.2.3 show great potential.

Additionally, serious gaming methods allow water managers to become familiar with new technological advances and simultaneously build trust in new water management methodologies (Den Haan et al., 2019). Furthermore, the storylines developed within the Dutch RiverCare project (`https://kbase.ncr-web.org/rivercare/storylines-overview`) are an interesting development. The storylines can be used to get an easy-to-interpret overview of new methodologies, results, and applications of research output, allowing water managers to relate the new findings to their management challenges (Cortes Arevalo et al., 2018). Such methods are also proposed by Fabian et al. (2019) to increase the application of evidence-based information in nature conservation management.

Soil moisture data assimilation for meteorological research

The land surface part of operational weather forecast modelling instruments is often bounded by the unsaturated zone, as the availability of soil moisture influences evapotranspiration processes. The findings of Chapter 3 may help in increasing the accuracy of meteorological forecasting, as operational assimilation of soil moisture information can improve both regional and local soil moisture model estimates. Since data assimilation schemes are already extensively used in operational numerical weather forecasting, it should be relatively easy to include soil moisture data assimilation in such systems (Drusch et al., 2009; De Rosnay et al., 2013). SWM-EVAP is an example of a project currently focusing on such applications. More information concerning this project can be found at `https://www.knmi.nl/over-het-knmi/nieuws/onderzoek-naar-verdamping-voor-beter-waterbeheer`.

Describing physical systems using TFN modelling

TFN modelling is already used for groundwater modelling applications. The findings on TFN models in this research show potential for application in other research fields. The development of the PIRFICT method (Von Asmuth et al., 2002; Von Asmuth and Bierkens, 2005) lead to easier-to-implement TFN models, as the model identification stage usually needed in TFN modelling (Box and Jenkins, 1970) does not have to be performed. As shown in Chapter 4, TFN models can describe both linear and non-linear systems. In theory, they can be developed for each process or variable which can be described using a set of input time series. The influence of each input time series on the desired process or variable has to be described using a relatively simple statistical distribution function. Furthermore, sufficient training data must be available. As a general rule of thumb, the training data must at least cover the memory of the observed system.

As TFN models are powerful in the sense that they need limited computational requirements, these models have potential in research fields focusing on hydraulic and morphological systems. Model simulations in these fields are generally computationally demanding, so often idealized modelling approaches (e.g. Campmans et al., 2017; Reef et al., 2018; Damveld et al., 2019) and meta-modelling or emulation methods (e.g. Berends et al., 2018; Bomers et al., 2019) are often applied to study system processes. TFN modelling is a promising extension to these methods, e.g. for predictions and uncertainty assessments using ensemble methods.

CHAPTER 6

Conclusions and recommendations

6.1 Conclusions

We answer the research questions, formulated in Section 1.5, in the following section.

Research question 1

To what degree are hydrological models currently applied in operational water management and how can their applicability be increased for operational water management?

Chapter 2 focused on the current application of experiential and evidence-based information in Dutch regional operational water management. A framework was developed to identify which information is used by regional operational water managers, also referred to as decision-makers. We found that water managers use evidence-based information in the form of measurement data, system knowledge, meteorological forecasts, hydrological models, and legislation. However, operational water managers also considerably depend on experiential information, which may lead to opinion-based bypasses. Furthermore, water managers often take limited guidance bypasses (not taking into account all available information), as they are limited due to time and budget constraints. In addition, regional operational water managers often regard evidence-based information in the form of hydrological models as unreliable for decision-making in operational water resources management. To improve the applicability of hydrological models, both scientists and decision-makers should focus on several aspects. Decision-makers should focus on developing structured methodologies for interpreting both evidence-based and experiential information. Researchers have to focus on delivering the appropriate information in an understandable format at the right moment in time. Furthermore, educating decision-makers on hydrological model concepts and assumptions may help to increase the understanding of the relationship between model results, implications for water management, and what water managers observe in the field. The latter aspect will also help water managers to understand the inherent uncertainties related to hydrological modelling. Participatory approaches, serious gaming, and storylines show great potential to build trust in new technological advances in hydrological modelling.

Research question 2

To what extent can the assimilation of a high-resolution remotely sensed surface soil moisture product increase the accuracy of an unsaturated zone hydrological metamodel?

Chapter 3 focused on the utilization of high-resolution remotely sensed soil moisture information for process-based modelling. We found that integrating satellite-based soil moisture observations and hydrological metamodel simulations using a data assimilation scheme leads to new opportunities for operational water resources management. The Bayesian background of data assimilation schemes allows combining the uncertainties of both the remotely sensing data and soil moisture simulations into a new soil moisture estimate of larger accuracy. A perturbed observations Ensemble Kalman Filter (EnKF) was used to assimilate SMAP satellite L3 Enhanced surface soil moisture estimates into the unsaturated zone metamodel MetaSWAP as part of the Netherlands Hydrological Instrument (NHI). First, a synthetic experiment, commonly referred to as a twin experiment, showed the value of applying an EnKF data assimilation scheme for state updating of the MetaSWAP metamodel. Then, a data assimilation run was performed using the SMAP surface soil moisture product for the year 2016. On a regional scale, the updated soil moisture model simulations show a larger skill in terms of root mean square error (RMSE) and model bias. The skill of the updated model simulations slightly decreases in terms of correlation coefficient, which can be explained by the larger variability of the assimilated SMAP observations with respect to the in situ validation data. On a local scale, the skill of updated soil moisture model simulations mainly depends on how well the SMAP surface soil moisture observations represent local field conditions. A particular challenge concerning soil moisture remote sensing is that satellite-retrieved soil moisture is generally limited to the upper part of the soil. The results presented in Chapter 3 show that the assimilation of surface soil moisture observations has value in updating root zone soil moisture model simulations. We expect that recent and upcoming developments in high-performance computing, data storage and data processing facilities will increase the applicability of data assimilation methods for operational water resources management. These developments will help operational water managers to get an up-to-date overview of water system conditions.

Research question 3

To what extent can data-driven modelling, based on high-resolution remote sensing data, be used to provide up-to-date soil moisture information for operational water management?

Chapter 4 focused on a novel data-driven method for soil moisture modelling. We studied the applicability of transfer function-noise (TFN) modelling for explaining soil moisture conditions. We found that exponential distributions can be used to define impulse-response (IR) functions, which describe the response of soil moisture to precipitation and reference evapotranspiration stress series. The TFN models were able to describe soil moisture dynamics using the SMAP L3 Enhanced surface soil moisture product as training data. In terms of RMSE, the TFN models shows similar accuracies with respect to the SMAP data. Also, the TFN models have value on field scales if the SMAP training data is representative for that particular scale. One should note that the availability of training data has a considerable effect on the TFN model results, especially in extreme situations. A sensitivity analysis on the training period length showed that selecting a suitable training period can positively affect the capabilities of the TFN model in extreme situations. Furthermore, the parameters of the IR functions describe water system characteristics, although more research is needed to relate the parameters to physical phenomena. Concluding, TFN models are fast and easy-to-construct alternatives for process-based modelling and can help in retrieving up-to-date information on water system conditions in water management. Several promising applications of TFN soil moisture modelling were identified in Chapter 5, such as ensemble predictions of soil moisture, the reconstruction of historical soil moisture time series, filling of data gaps and satellite validation studies.

Synthesis

The general research aim was to show the potential use of soil moisture information as part of operational water resources management systems, in particular hydrological models, using high-resolution remote sensing data. Besides the findings of Chapter 3 and Chapter 4, we have shown possible applications of in situ, remotely sensed and hydrological modelling based soil moisture information for operational water management in Chapter 5. Furthermore, we have identified several means for the integration of new information in water management applications. We expect that, in the near future, the increasing availability of high-resolution soil moisture data and the increasing availability of computational power will lead to promising possibilities for research and practical applications. Therefore, we want to give several recommendations for further research and water management applications in the next section.

6.2 Recommendations

6.2.1 Scientific implications

Estimating soil moisture conditions on various spatiotemporal scales

The various applications in this work show the utility of soil moisture information for hydrological applications. Although the dissertation explored various ways to relate in situ, remote sensing and hydrological modelling estimates, substantial differences exist between the different spatial and temporal scales of these methods. Therefore, research should continue to focus on developing new methods to bridge the gap between field, regional, national and global soil moisture scales. Research should focus on which spatiotemporal scales are needed to solve specific issues related to water management. Also, the relationship between surface soil moisture and deeper soil layers should be extensively studied. As process-based methods are often complex, data-driven methods show great potential to link these spatiotemporal scales.

Explore potential of multivariate data assimilation

Chapter 3 showed that the univariate assimilation of surface soil moisture estimates into an unsaturated zone model improved root zone soil moisture simulations. Section 5.1.2 elaborated on the effect of the soil moisture assimilation on other hydrological variables. Increasing the accuracy of soil moisture simulations had a small effect on actual evapotranspiration simulations, and slightly increased the accuracy of phreatic groundwater level simulations in terms of bias. In particular, multivariate data assimilation approaches seem promising to update multiple hydrological variables in subsurface modelling. We recommend exploring the assimilation of both soil moisture and groundwater observations. Moreover, the opportunities of using field scale remote sensing soil moisture observations for data assimilation schemes should be studied, as we expect that such high-resolution estimates will become increasingly available in the near future.

Improve groundwater modelling using model parameter updating

Updating soil moisture state variables did not lead to a significant increase in accuracy of groundwater simulations. We encourage exploring the value of soil moisture data assimilation for updating of subsurface model parameters used by the saturated zone model MODFLOW as part of the NHI hydrological modelling framework. The OpenDA-MetaSWAP data assimilation framework, developed and introduced in Chapter 3, allows both updating of model state variables and parameters. In particular, we recommend to explore the value of data assimilation for updating subsurface model parameters such as hydraulic conductivity, as such parameters are generally not observable.

Explore possibilities of TFN modelling

As TFN models are fast and easy to develop, they form competent alternatives for process-based models. Section 5.1.3 elaborated on various possible applications of TFN modelling for soil moisture modelling. In particular, it would be valuable to explore the possibilities for predicting soil moisture. As TFN models are fast, combining them with ensemble predictions can help in identifying the uncertainties of soil moisture modelling. Furthermore, the parameters of the IR functions can help water managers to identify regions in their management area which respond either fast or slow on input stresses like precipitation. Such findings would help water managers to adapt water management practices on a local scale. Also, the IR functions of both satellite and in situ soil moisture data can be compared. The similarities or differences in system responses between the IR functions provide valuable information on the overlap of spatiotemporal scales between satellite and in situ data. Next, the SMAP satellite experienced malfunctioning in July 2019. The TFN models can help in filling the data gaps caused by the malfunctioning. Similarly, when long-term datasets of stress series are available, one could develop historical soil moisture time series. KNMI provides precipitation and crop reference evapotranspiration up to tens of years back in time. The long-term historical soil moisture time series can be used to study the effect of the changing climate on subsurface hydrology.

6.2.2 Practical implications

Develop structured methodologies

To integrate both evidence-based and experiential information in decision-making, we encourage the development of structured methodologies for operational water resources management. Structured methodologies will help to take robust and reliable decisions based on both evidence-based and experiential information. The increasing development of decision support systems, including hydrological model forecasting applications, are a good starting point and should be encouraged. We should continue assessing whether such systems provide the correct information in understandable formats to the right people by re-identifying the needs of water managers. Furthermore, we should invest in studies on how we can transfer uncertainty concepts to decision-makers, building on studies like Walker et al. (2003), Morss et al. (2005), Beven and Alcock (2012), and Warmink et al. (2017).

Collect soil moisture data for operational water management settings

As national and regional water authorities show interest in using soil moisture information, we encourage to increase the collection of soil moisture field measurements. Such information would help in interpreting both remote sensing and hydrological model estimates and require relatively small investments. For example, the Dutch National Committee for Water Distribution (*Landelijke Coördinatiecommissie Waterverdeling, LCW*), issues a drought report (*droogtemonitor*) every month. Soil moisture information is a valuable addition to this report. We have to create long-term soil moisture datasets with a length of at least a couple of years to perform anomaly analyses. Also, both process-based and data-driven modelling methods generally need as much input and validation data as possible. Furthermore, the increasing availability of long-term in situ soil moisture data would have great value for satellite validation studies and would increase our understanding of climate change effects on the hydrology of the soil subsurface.

Apply new remote sensing data in operational settings

Analogous to the research framework (Figure 1.9), we recommend testing various applications of soil moisture remote sensing data for operational water management. Dutch water authorities are already investing in remote sensing by buying tailor-made remote sensing data. Also, the Netherlands Space Office maintains an online database consisting of already processed remote sensing data which can be freely downloaded and used: `https://www.spaceoffice.nl/nl/satellietdataportaal`. Additionally, the European Union and ESA developed Copernicus, the European Earth Observation Programme. A primary aim of Copernicus is the development of the Sentinel satellite family, which provide satellite data for various applications in the earth sciences. The Sentinel DataHub allows easy access to the Sentinel data: `https://scihub.copernicus.eu/dhus`. Subsequently, water managers are encouraged to use the data in their daily practices to discover the utilization possibilities. This work shows that such remote sensing data have value in data assimilation procedures (Chapter 3) and data-driven modelling approaches (Chapter 4). We invite water managers to continue executing such ideas and see great potential in participatory approaches to merge the knowledge of scientists, businesses, and decision-makers.

Enable easy access of soil moisture data and other relevant datasets

Various initiatives exist to publicly share soil moisture data, like the International Soil Moisture Network. Both national and regional water authorities should support these initiatives. Furthermore, we encourage the inclusion of relevant datasets, for example, indicators based on soil moisture data.

Invest in innovative information technology (IT) infrastructure

The increasing availability of high-resolution remote sensing data and hydrological modelling leads to increasing requirements for data storage and processing facilities, high-capacity computational environments, decision support systems, and many other IT applications. Water authorities and institutes should not underestimate the need to invest in required infrastructural developments. As such systems are still quite expensive, it might be helpful to seek collaborations, e.g. to start national, supranational, or even global initiatives for developing IT infrastructure.

Educate water managers

During the execution of this research, we often found that operational water managers in the Netherlands are not very familiar with the concepts of soil moisture processes. Also, they are often either not familiar with or interested in new scientific developments. Consequently, water managers might take the opinion-based bypass (Figure 2.1), which leads to sub-optimal decisions. To increase the understanding of water managers and to inform them about recent developments, water managers must be encouraged to embrace new technological advances and have to be educated accordingly. New ways of presenting scientific findings, like innovative ways of presenting information in decision support systems, can help in educating water managers. Not only researchers, but also business firms can help to improve this aspect. Hydrologists, operational water managers as well as policy makers should be included in this process. Finally, a better understanding of the physical concepts and processes by water managers would help the integration of soil moisture information in operational water management.

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About the author

Michiel Pezij was born in Almelo, the Netherlands, on the 2nd of August 1992. After graduating from CSG 't Noordik in Almelo, he started the bachelor of Civil Engineering at the University of Twente in 2010. He visited the National Institute of Water and Atmospheric Research (NIWA) in Christchurch, New Zealand, as an intern. The internship focused on the morphological development of the Hororata river, which course was significantly altered by the 2010 Canterbury earthquake. Michiel started the master programme Civil Engineering and Management at the University of Twente in 2013, focusing on the Water Engineering and Management track. His MSc. thesis project was conducted at the research institute Deltares in Delft, the Netherlands, where he studied the evolution of a sand nourishment in the Eastern Scheldt estuary.

Michiel started as a PhD candidate at the Water Engineering and Management (WEM) department of the University of Twente in October 2015. Simultaneously, he was invited as a guest researcher at Deltares. Michiel presented his research at international conferences in Bonn, Reading, San Francisco, and Vienna. After finishing his PhD thesis in October 2019, he continued as a postdoc at the University of Twente.

List of publications

Peer-reviewed journal publications

1. Benninga, H.F., Carranza, C.D.U., **Pezij, M.**, Van Santen, P., Van der Ploeg, M.J., Augustijn, D.C.M., Van der Velde, R. 2018. The Raam regional soil moisture monitoring network in the Netherlands. Earth System Science Data 10, 61-79. doi:10.5194/essd-10-61-2018.

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4. **Pezij, M.**, Augustijn, D.C.M., Hendriks, D.M.D., Hulscher, S.J.M.H. *Submitted.* Applying transfer function-noise modelling to characterize soil moisture dynamics: a data-driven approach using remote sensing data.

5. Van der Velde, R., Colliander, A., **Pezij, M.**, Benninga, H. F., Bindlish, R., Chan, S. K., Jackson, T. J., Hendriks, D. M. D., Augustijn, D. C. M., and Su, Z. 2019. Validation of SMAP L2 passive-only soil moisture products using in situ measurements collected in Twente, The Netherlands. Hydrology and Earth System Sciences Discussions, doi:10.5194/hess-2019-471, in review.

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1. **Pezij, M.**, Augustijn, D.C.M., Hendriks, D.M.D., Hulscher, S.J.M.H. 2016. Optimizing operational water management with soil moisture data from Sentinel-1 satellites. EGU2016-8226. EGU General Assembly 2016.
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3. **Pezij, M.**, Augustijn, D.C.M., Hendriks, D.M.D., Hulscher, S.J.M.H. 2019. Transfer Function-Noise Modeling Using Remote Sensing Data to Characterize Soil Moisture Dynamics: a Data-driven Approach. AGU Fall Meeting 2019.

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2. **Pezij, M.**, Augustijn, D.C.M., Hendriks, D.M.D., Hulscher, S.J.M.H. 2017. Optimizing operational water management with a Sentinel-1 satellite soil moisture product. Course on advanced data assimilation methods. ECMWF, Reading, United Kingdom.
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Datasets

1. Benninga, H.F., Carranza, C.D.U., **Pezij, M.**, Van der Ploeg, M.J., Augustijn, D.C.M., Van der Velde, R. 2017. Regional soil moisture monitoring network in the Raam catchment in the Netherlands. University of Twente. Dataset. doi:10.4121/uuid:2411bbb8-2161-4f31-985f-7b65b8448bc9.
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