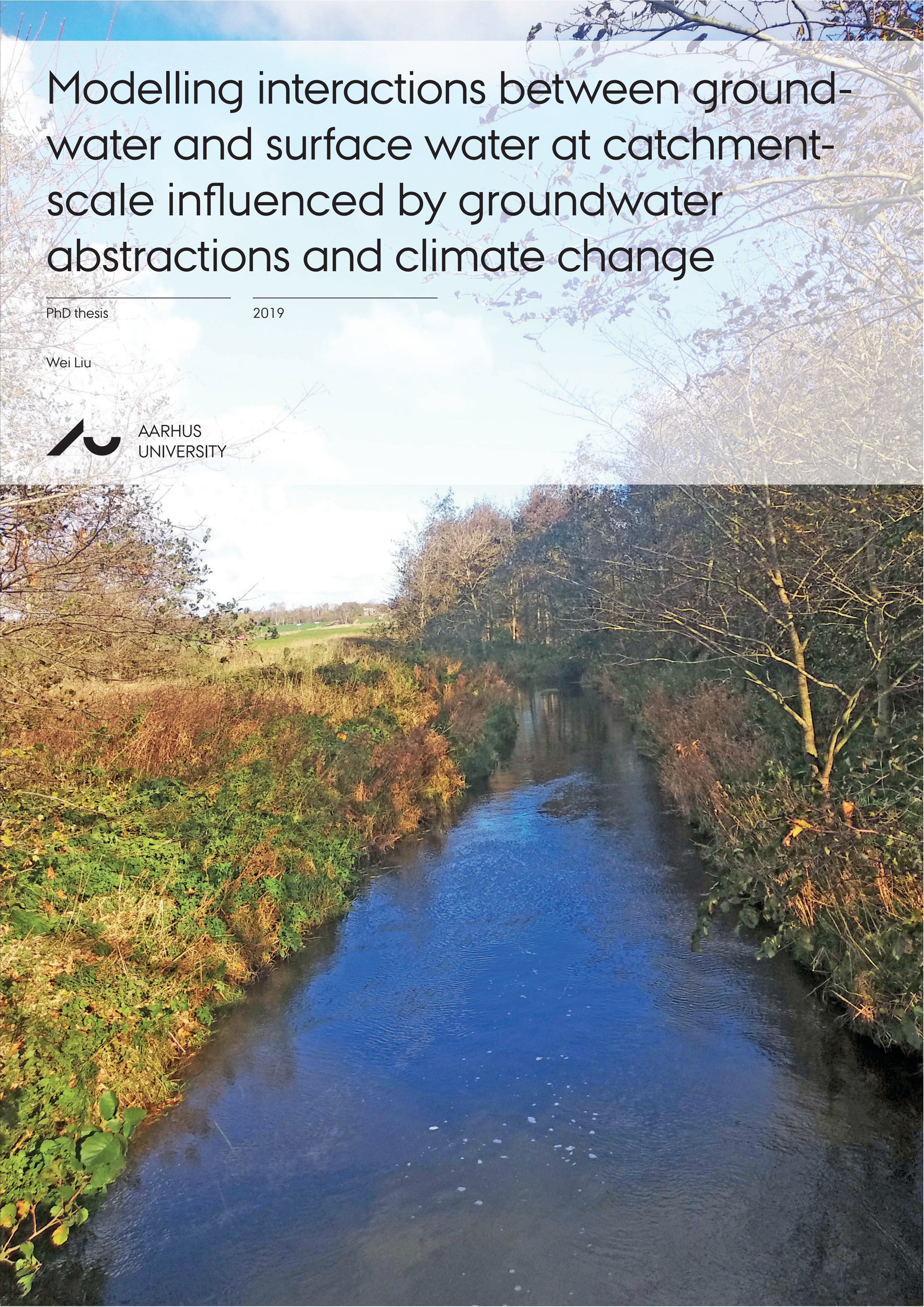

Modelling interactions between groundwater and surface water at catchment-scale influenced by groundwater abstractions and climate change

PhD thesis

2019

Wei Liu

AARHUS
UNIVERSITY

MODELLING INTERACTIONS BETWEEN GROUNDWATER AND SURFACE WATER AT CATCHMENT-SCALE INFLUENCED BY GROUNDWATER ABSTRACTIONS AND CLIMATE CHANGE

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Content

Preface

This dissertation is the outcome of my Ph.D. project conducted during the three years from September 2016 to August 2019, and is submitted to Aarhus University in partial fulfillment of the requirements for achieving a Ph.D. degree. My Ph.D. project was funded by the China Scholarship Council, and included collaboration with a Danish consultant company NIRAS A/S and the SWAT-MODFLOW developer group at Colorado State University (CSU) in the United States. Most of the work was undertaken at the Department of Bioscience, Aarhus University, and a part was conducted during a three-month research stay at CSU.

My Ph.D. project deals with the development and application of a new integrated surface-subsurface model SWAT-MODFLOW that can contribute to a greater understanding of groundwater-surface water interactions and help address pressing challenges in water resources management under the impacts of climate change and groundwater abstractions, particularly in groundwater-dominated catchments.

Most of the work were presented in the three submitted manuscripts, which constitute the main body of this dissertation. The reviewers' comments of two manuscripts have been received. I will further modify the manuscripts based on the reviewers' comments after my thesis submission and expect at least one manuscript to be accepted before the defense. I contributed the majority to all the three studies, including designing the studies, setting up and calibrating the models, developing the PEST-based calibration approach, analyzing results, producing figures, and writing the manuscript, while under the supervision of Dennis Trolle and Erik Jeppesen at the Department of Bioscience, Aarhus University. Dr. Seonggyu Park and Associate Professor Ryan T. Bailey at the Colorado State University contributed to the idea and development of PEST-based calibration approach. Ryan T. Bailey also provided knowledge on application of SWAT-MODFLOW and further developed the SWAT-MODFLOW codes to better represent the cases of my study. The "model lab" in Silkeborg, including Anders Nielsen, Dennis Trolle, Eugenio Molina-Navarro, Hans Estrup Andersen and Hans Thodsen, assisted in providing most of the input data for the models, which for the most part is stored in National databases, and also contributed with their knowledge on setting up and calibrating the models. Jacob Skødt Jensen and Jacob Birk Jensen who previously worked in NIRAS A/S provided a version of a steady-state MODFLOW-NWT set-up and contributed with background knowledge on this application. Kai Peng from the University of Chinese Academy of Sciences (UCAS) helped analyze results and also helped prepare some figures for manuscript 3. All co-authors of the three manuscripts contributed with discussions and revisions to the manuscripts.

Besides the three manuscripts, the dissertation also includes a summary of the dissertation in English and Danish respectively, a review of present state-of-the-art within hydrological modelling, a summary of the objectives and methodologies applied in the manuscripts, and a summary of my main results, perspectives, and conclusions. An additional five papers and two conference abstracts that I have contributed during my Ph.D. study are listed.

In accordance with the rules of GSST (Graduate School for Science and Technology, Aarhus University), parts of this dissertation were also presented in the progress report for my Ph.D. qualifying examination.

Acknowledgements

Looking back on the journey of my Ph.D. study, I have experienced and gained a lot. On the occasion of the completion of this dissertation, I would like to express my sincere gratitude to a great many people, without whose dedication, support and company, this dissertation would not have been possible.

First of all, I would like to express my deep gratitude to my main supervisor Dennis Trolle, who has contributed with insightful guidance, great support on academic resources and network connection, as well as comprehensive feedback throughout my study. Without you, I would never know so much about hydrology, catchment modeling and scientific writing as I do now. Many thanks for your patience and encouragement all the time. I am also very grateful to my co-supervisor Erik Jeppesen, who always returns me his substantial comments and edits on my manuscripts fast. Thank you for inviting me to your house to have dinner or barbecue for so many times. I also appreciate a lot about the good time having hot-pot and beers together with you in Silkeborg. To students, you are absolutely the most approachable and friendly professor I have met.

I owe my special thanks to Dr. Ryan T. Bailey at the Colorado State University, who were always available by E-mail when I encountered difficulties in the set-up and calibration of models, guided me during my three-month stay in the United States, and taught me a lot about the models (e.g. MODFLOW, RT3D, SWAT-MODFLOW-RT3D). I also thank Chenda Deng, Qinghua Li, Jun Li, Xiaolu Wei, Yao Zhang, Zaichen Xiang, and etc., for their incredible hospitality and great help during my research stay at the Colorado State University.

I am grateful to my co-authors for their contributions to my studies, as mentioned in the preface. Thanks to Frankie Zea Henriksen for IT support, to Anne Mette Poulsen for linguistic improvements in all manuscripts and to Tinna Christensen for layout design of this dissertation. Sincere thanks go to my office mates for your kindness and everyday company. I also thank all my colleagues in Silkeborg for organizing unforgettable Christmas parties and activities which make the work environment warm and interesting.

I would like to thank all the friends I met in Denmark, especially the Chinese group in Silkeborg, who helped and supported me a lot both in my daily life and study. I also appreciate all the great parties, group tours and endless entertainment we had together, which left me precious memories.

Finally, I owe my deepest gratitude to my family – my parents, Keyou Liu and Yinju Bi, my younger sister and her husband, Ting Liu and Tao Wang. Thank you for always believing and supporting me, and always giving me great freedom to make my own decision. I cannot wait to go back to China to see you and my newborn nephew (Muyi Wang).

Wei Liu

Publication list

Papers included in dissertation

1. **Liu, W.,** Park, S., Bailey, R.T., Molina-Navarro, E., Andersen, H.E., Thodsen, H., Nielsen, A., Jeppesen, E., Jensen, J.S., Jensen, J.B. and Trolle, D. (2019). Comparing SWAT with SWAT-MODFLOW hydrological simulations when assessing the impacts of groundwater abstractions for irrigation and drinking water, Hydrol. Earth Syst. Sci. Discuss.,1-51, 10.5194/hess-2019-232. In revision.
2. **Liu, W.,** Bailey, R.T., Andersen, H.E., Jeppesen, E., Park, S., Thodsen, H., Nielsen, A., Molina-Navarro, E. and Trolle, D. (2019). Assessing the impacts of groundwater abstractions on flow regime and stream biota: combining SWAT-MODFLOW with flow-biota empirical models, Science of The Total Environment. In revision.
3. **Liu, W.,** Bailey, R.T., Andersen, H.E., Jeppesen, E., Nielsen, A., Kai, P., Molina-Navarro, E., Park, S., Thodsen, H. and Trolle, D. (2019). Quantifying the effects of climate change on hydrological regime and stream biota in a lowland catchment: A modelling approach combining SWAT-MODFLOW with flow-biota empirical models, submited to Science of The Total Environment.

Additional papers

1. **Liu, W.,** Bailey, R.T., Jeppesen, E., Wei, X., Andersen, H.E., Thodsen, H., Nielsen, A. and Trolle, D. (2019). Identifying the the most critical areas of nitrate and total phosphorous losses to groundwater and surface water with SWAT-MODFLOW-RT3D. In preparation.
2. **Liu, W.,** An, W., Jeppesen, E., Ma, J., Yang, M. and Trolle, D. (2019). Modelling the fate and transport of Cryptosporidium, a zoonotic and waterborne pathogen, in the Daning River watershed of the Three Gorges Reservoir Region, China, Journal of Environmental Management, 232, 462-474, https://doi.org/10.1016/j.jenvman.2018.10.064.
3. Mu, X., Lv, X., **Liu, W.,** Qiu, C., Ma, Y., Zhang, S. and Jeppesen, E. (2019). Biofilm attached to Myriophyllum spicatum promote ammonium removal evidenced by 15N tracking, nitrogen budget and metagenomics analysis. Submitted to Water Research.
4. He, H., Li, Q., Han, Y., Cao, Y., **Liu, W.,** Yu, J., Li, K., Liu, Z. and Jeppesen, E. (2019). Turning up the heat: Warming influences plankton biomass and spring phenology in subtropical waters characterized by extensive fish omnivory. Submitted to Limnology and Oceanography.
5. He, H., Jeppesen, E., Bruhn, D., Yde, M., Hansen, J.K., Spanggaard, L., Madsen, N., **Liu, W.,** Søndergaard, M. and Lauridsen, T.L. (2019). Decadal changes in zooplankton biomass, composition and body mass in four temperate shallow brackish lakes subjected to various degrees of eutrophication, Inland Waters. Under review.

Conference abstracts

1. Bailey, R., Park, S., Wei, X., Trolle, D., **Liu, W.,** Flores, L., Nielsen, A. and Ayub, R. SWAT-MODFLOW for Coupled Groundwater/Surface Water Systems: Current Applications, American Geophysical Union, Fall Meeting, December 10-14, 2018, Washington, D.C., the United States.
2. Bailey, R., Molina-Navarro, E., **Liu, W.,** Wei, X. and Trolle, D. SWAT-MODFLOW: Recent Applications and an Introduction to Version 3, July 15-19, 2019, SWAT Conference, Vienna, Austria.

English Summary

With intensifying water crisis, environmental and ecological degradation, as well as ongoing climate change worldwide, integrated water resources management, which considers surface water (SW) and groundwater (GW), is becoming increasingly important. As integrated surface–subsurface hydrological models are capable of simulating water processes in an integrated and holistic fashion, provide spatially and temporally detailed description of the catchment-scale hydrological cycle, enable scenario analysis, and may be coupled with other models (e.g. solute transport model), they are essential and useful tools in integrated water resources management. The SWAT-MODFLOW is such a surface-subsurface model.

Excessive groundwater abstractions can decrease the groundwater table, and thereby affect the aquifer-connected surface water bodies, which may deteriorate the quality of aquatic ecosystems. At the same time, climate change affects inland water ecosystems not only by increasing the water temperatures, but also by influencing hydrological processes (e.g. evapotranspiration) and thereby alter the flow regime. The overall objective of my Ph.D. project was to further develop and apply a newly integrated surface-subsurface model SWAT-MODFLOW in order to improve the understanding of SW-GW interactions, and to assess the impacts of groundwater abstractions and climate change on the hydrological regime and on stream biota.

In the first part of my study (presented in manuscript 1), we further developed the SWAT-MODFLOW complex based on the previous publically available version (v.2) to enable application of a Drain Package and an auto-irrigation routine. To better understand how groundwater pumping wells may influence streamflow patterns, we applied both the semi-distributed SWAT model and the further developed the integrated surface–subsurface hydrological, SWAT-MODFLOW model to a Danish, lowland, groundwater-dominated catchment - the Uggerby River Catchment (357 km2). Both models were calibrated and validated, and an approach based on PEST (Model-Independent Parameter Estimation and Uncertainty Analysis) was developed and utilized to enable simultaneous calibration of SWAT and MODFLOW parameters. The performance of the models when simulating streamflow and the simulated streamflow signals when running four groundwater abstraction scenarios through the two models were analyzed and compared. Both models demonstrated generally good performance of the temporal pattern of streamflow, albeit SWAT-MODFLOW performed somewhat better. In addition, SWAT-MODFLOW generates spatially explicit groundwater-related outputs, such as spatial-temporal patterns of water table elevation. In general, the simulated signals of SWAT-MODFLOW appeared more plausible than those of SWAT, and the SWAT-MODFLOW decrease in streamflow was much closer to the actual volume abstracted. The impact of drinking water abstraction on streamflow depletion simulated by SWAT was unrealistically low, and the streamflow increase caused by irrigation abstraction was exaggerated compared with SWAT-MODFLOW.

To quantitatively assess the effects of groundwater abstractions and climate change on the hydrological regime and on stream biota, we combined the SWAT-MODFLOW model with novel nationwide-scale flow-biota empirical models for three key biological taxonomic identities (fish, macroinvertebrates, and macrophytes). We applied the integrated approach to the Uggerby River Catchment and assessed to what extent the flow regime and key biota in stream segments of different sizes may be altered by groundwater abstractions and climate change. In the second part of my study (presented in manuscript 2), we

therefore analyzed and assessed the impacts of present level of groundwater abstractions and a scenario with extreme groundwater abstraction for three subbasin outlets representing stream segments of different sizes. Current stream biotic indices at the three subbasin outlets. The simulated extreme abstractions, however, led to significant impacts on the smallest stream but had comparatively minor effects on the larger streams. The fish index responded most negatively to the groundwater abstractions, followed by the macrophyte index, decreasing, respectively, by 23.5% and 11.2% in the small stream in the extreme groundwater abstraction scenario. No apparent impact was found on the macroinvertebrate index as in any of the three subbasin outlets.

In the third part of my study (presented in manuscript 3), we analyzed and assessed the effects of predicted climate change towards the end of this century relative to the reference period (1996-2005) in two climate change scenarios of different greenhouse gas emission levels (RCP2.6 and RCP8.5) for all subbasin outlets classified into streams of three size classes. The overall streamflow and groundwater discharge in the catchment decreased slightly in the RCP2.6 scenario, while it increased in the RCP8.5 scenario. The differently sized streams underwent different alterations in flow regime and also demonstrated different biotic responses to climate change as represented by the fish and macrophyte indices. Large and some small streams suffered most from climate change, as the fish and macrophyte quality indices decreased up to 14.4% and 11.2%, respectively, whereas these indices increased by up to 14.4% and 6.0% respectively, in medium and some small streams. The climate change effects were larger in the RCP8.5 scenario than in the RCP2.6 scenario, as expected.

In conclusion, the further developed SWAT-MODFLOW model calibrated by PEST provided a better hydrological simulation performance, wider possibilities for groundwater analysis, and much more realistic signals relative to the semi-distributed SWAT model when assessing the impacts of groundwater abstractions for either irrigation or drinking water on streamflow; hence, it has great potential to be a useful tool in water resources management in groundwater-dominated catchments. The novel approach of combining SWAT-MODFLOW and flow-regime biota models is a useful tool to quantitatively assess the effects of groundwater abstractions on stream biota and thereby support water planning and regulations related to groundwater abstractions. To best of my knowledge, the third part of my study is the first to quantitatively assess the impacts of streamflow alterations induced by climate change on stream biota beyond specific species, which would assist in water planning and regulations in response of the challenges posed by climate change.

Dansk sammenfatning

Med en global forværring af vandressourcer, herunder forringelse den miljømæssige og økologisk integritet af vandsystemer, samtidig med igangværende klimaforandringer, er der stadig større behov for en integreret vandforvaltning, der omfatter både overfladevand og grundvand og deres sampil. Integrerede overflade-grundvands hydrologiske modeller kan anvendes til bidrage til en sådan forståelse. De kan give en rummelig og tidslig detaljeret beskrivelse af den hydrologiske cyklus på oplandsskala, og kan anvendes til scenarieanalyser og hvis de kobles med andre modeller (f.eks. kemiske transportmodeller), kan de være essentielle værktøjer i en integreret forvaltning af vandressourcer. SWAT-MODFLOW modellen er et eksempel på netop sådan en overflade-grundvands-model.

Overdreven grundvandsindvinding kan mindske grundvandsniveauer, og derigennem påvirke tilknyttede vandløb og søer og deres vandkvalitet. Samtidig påvirker klimaforandringer disse økosystemer ikke blot ved at øge vandtemperaturen, men også ved at ændre den hydrologiske cyklus og afstrømningsmønstre. Det overordnede mål med mit ph.d. studie var at videreudvikle og anvende en ny integreret overflade-grundvands-model SWAT-MODFLOW, for derved at skabe en bedre forståelse for interaktionerne mellem overfladevand og grundvand, samt at få indblik i hvordan grundvandsindvindinger samt klimaforandringer indvirker på det hydrologiske regime og vandløbenes økologiske kvalitet.

I første del af mit studie (manuskript 1) videreudviklede vi SWAT-MODFLOW model-komplekset, baseret på den tidligere offentligt tilgængelige version (v.2), ved at inkludere en ”drænings” rutine og en automatisk markvandings-rutine. For bedre at forstå, hvordan indvindinger kan påvirke strømningsmønstrene i vandløb, anvendte vi både den semi-distribuerede SWAT model og den videreudviklede, fuldt distribuerede, SWAT-MODFLOW model på et dansk, fladt, grundvandsdomineret afvandingsområde, Uggerby å (357 km2). Begge modeller blev kalibreret og valideret, og en metode baseret på PEST blev udviklet og anvendt for samtidig kalibrering af SWAT og MODFLOW-model-parametre. Modellernes evne til at simulere vandføring, og de simulerede vandføringssignaler, ved fire forskellige grundvands-indvindingsscenarier, blev analyseret og sammenlignet. Begge modeller demonstrerede generelt en god evne til at simulere vandføring, omend SWAT-MODFLOW præsterede lidt bedre. Generelt forekom de simulerede signaler af SWAT-MODFLOW modellen mere plausible end SWAT-modellen, under indvindingsscenarierne. Reduktionen i afstrømning simuleret af SWAT-MODFLOW var eksempelvis meget tættere på den faktiske ændring i indvindingsvolumen. Påvirkningen af indvinding af drikkevand på vandføringen simuleret med SWAT var urealistisk lav, og forøgelsen af vandføringen i scenarier med øget markvanding var overdrevet sammenlignet med SWAT-MODFLOW simuleringer.

For kvantitativt at kunne vurdere påvirkningerne af grundvandsindvindinger og klimaændringer på det hydrologiske regime og vandløbenes økologi kombinerede vi SWAT-MODFLOW-modellen med nye landsdækkende flow-biotiske empiriske modeller for tre vigtige taksonomiske grupper (fisk, makroinvertebrater og makrofytter). Vi anvendte denne integrerede tilgang for Uggerby å oplandet, som et casestudie, og vurderede, i hvilket omfang vandføringen og vandløbsbiologien i vandløb af forskellige størrelse kan påvirker af grundvandsindvindinger og fremtidige klimaforandringer. I den anden del af mit studie (præsenteret i manuskript 2) analyserede og vurderede vi derfor effekten af det nuværende niveau af grundvandsindvinding samt et scenarie med mere ekstrem indvinding for tre deloplande, der repræsenterer vandløb af forskellige størrelse. makrofytindekset, som faldt med hhv. 23,5%

og 11,2% i det lille vandløb i det ekstreme scenarie. Der blev ikke fundet nogen nævneværdig effekt af indvinding på makroinvertebrat-indekset i nogen af de tre deloplande. I den tredje del af mit studie (manuskript 3) analyserede og vurderede vi effekterne for fremtidige klimascenarier, repræsenteret ved slutning dette århundrede i to klimaforandringsscenarier med forskellige drivhusgasemissioner (RCP2.6 og RCP8.5). Vandløbene i Uggerby å oplandet blev klassificeret i tre størrelses-grupper, og resultaterne blev sammenlignet med referenceperioden (1996-2005). Den samlede vandføring og grundvandsafstrømning til vandløb i afvandingsområdet faldt en smule i RCP2.6-scenariet, mens det steg i RCP8.5-scenariet. Vandløbene med forskellig størrelse gennemgik forskellige grader afændringer i vandføringsregimet og udviste forskellig grad af biologiske respons på klimaforandringer, især ved fiske- og makrofyt-indeksene. De store og nogle små vandløb blev påvirket negativt af klimaforandringer, mens de mellemstore og nogle små vandløb i nogle tilfælde drog fordel af klimaforandringer. Således faldt fiske- og makrofyt-indeksene med op til hhv. 14.4% og 11.2 procent i førstnævnte gruppe, mens de steg med up til 14.4 og 6% i mellemstore og nogle mindre vandløb. Effekterne af klimaforandringerne var e, som forventet, større i RCP8.5-scenariet sammenlignet med RCP2.6-scenariet.

Sammenfattende, har mit studie vist, at den videreudviklede SWAT-MODFLOW-model, der blev kalibreret med PEST metoden, gav en bedre hydrologisk simulering og meget mere realistiske signaler af indvindingsscenarier, i forhold til den semi-distribuerede SWAT-model. SWAT-MODFLOW modellen har derfor potentialet til at blive et særdeles nyttigt værktøj til vandforvaltere i grundvandsdominerede afvandingsområder. Den nye tilgang, hvor vi kombinerede SWAT- MODFLOW modellen med empiriske ligninger for vandløbsbiologi kan være et holistisk og nyttigt værktøj til kvantitativ vurdering af effekterne af indvindinger på vandløbsbiologien. Så vidt jeg ved, er mit studie det første, hvor effekter af klimaforandringer undersøges for mere end ét biologisk kvalitetselement, og illustrerer hvordan vandforvaltere kan vurdere effekter af både indvindinger og et fremtidig klima i deres planlægning.

Introduction

The need for surface-subsurface hydrological models

Surface water (SW) and groundwater (GW) are two interconnected components of the hydrological system in all types of landscapes (Winter,1998) and alterations in one will inevitably affect the other (Winter, 1999). Although the interactions between SW and GW were studied and emphasized in early hydrological research, SW and GW resources have long been investigated and managed separately and often treated as two isolated entities and handled in completely different branches of government (Graham and Butts, 2005; Fleckenstein et al., 2010). With the ever-growing demands on water for anthropogenic needs and increasing challenges in water resources management associated with water rights issues and climate change, the awareness and needs to manage GW and SW as an integrated resource has grown steadily over the past three decades, in Europe particularly due to the EU Water Framework Directive. This new perception of water resources management and its operational complexity not only challenges our management structure, but also requires more sophisticated management tools (Graham and Butts, 2005). Additionally, the fact that water resources management not only pertains to the management of water quantity and quality but also involves the preservation of the linked ecosystems poses more challenges to managers and researchers (Fleckenstein et al., 2010).

The exchange between GW and SW largely depends upon the elevation difference between the groundwater table and stream surface. If the groundwater table is higher than the stream surface, stream gains water from inflow of GW through the streambed (gaining stream). If the water table is lower than the stream surface, stream loses water to aquifer by infiltration through the streambed (loosing stream) (Fig. 1). Very often, a stream gains water in some reaches and loses water in others (Sophocleous, 2002).

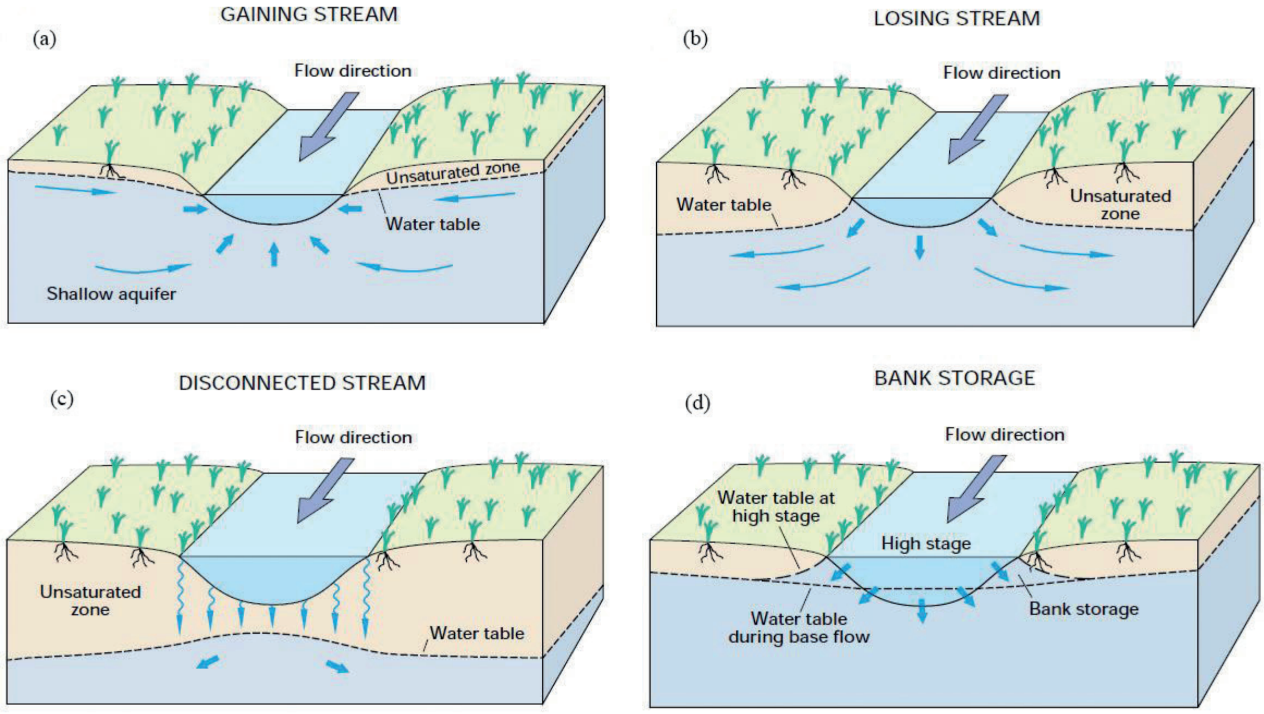


Figure 1. The exchange relationships between SW and GW: (a) fully connected gaining stream; (b) fully connected loosing stream; (c) disconnected loosing stream (d) partly connected loosing stream with bank storage. From Winter (1998).

Besides weather-induced variability, climate change and anthropogenic activities (e.g. GW abstractions and land-use changes) can also cause changes in flow direction and exchange rates between SW and GW, and thereby cause changes in surface runoff. These changes may influence the sustainability of both the water resource itself and also the ecosystems that it supports (Liu et al., 2019d). Since interactions between groundwater and surface water are complicated to observe and measure, it has been a challenge to disentangle the streamflow changes induced by climate change or groundwater abstractions from disturbances caused by weather-induced variability. In this regard, surface-subsurface hydrological models can overcome the above limitation to some extent because of their ability to simulate GW-SW interactions through a holistic approach and also enable scenario analysis (e.g. climate change, groundwater abstractions and land use planning etc.).

Surface-subsurface hydrological models

A blueprint for a physically-based, integrated surface-subsurface hydrological model that was firstly outlined 50 years ago (Freeze and Harlan, 1969) has become a reality in the last two decades. With the rapid growth of computational capabilities, a growing number of integrated surface-subsurface hydrological models of different complexity have been developed and is increasingly applied in integrated water resources management and research (Tian et al., 2016). They include InHm (VanderKwaak, 1999; Loague et al., 2005), CATHY (Bixio et al., 2002; Camporese et al., 2010), ParFlow (Kollet and Maxwell, 2006; Kollet and Maxwell, 2008; Srivastava et al., 2014), MIKE-SHE (Graham and Butts, 2005), SWAT-MODFLOW (Bailey et al., 2016; Guzman et al., 2015; Kim et al., 2008) GSFLOW (Markstrom et al., 2008; Markstrom et al., 2009), PAWS (Shen and Phanikumar, 2010), HydroGeoSphere (Brunner and Simmons, 2012), and etc. The three-dimensional form of Richards equation (Richards, 1931) to simulate unsaturated zones and Darcy's law for the saturated subsurface flow is mostly used in the models. The full Richards equation is the most accurate when the unsaturated flow is dynamic, but also the most computationally intensive (Graham and Butts, 2005).

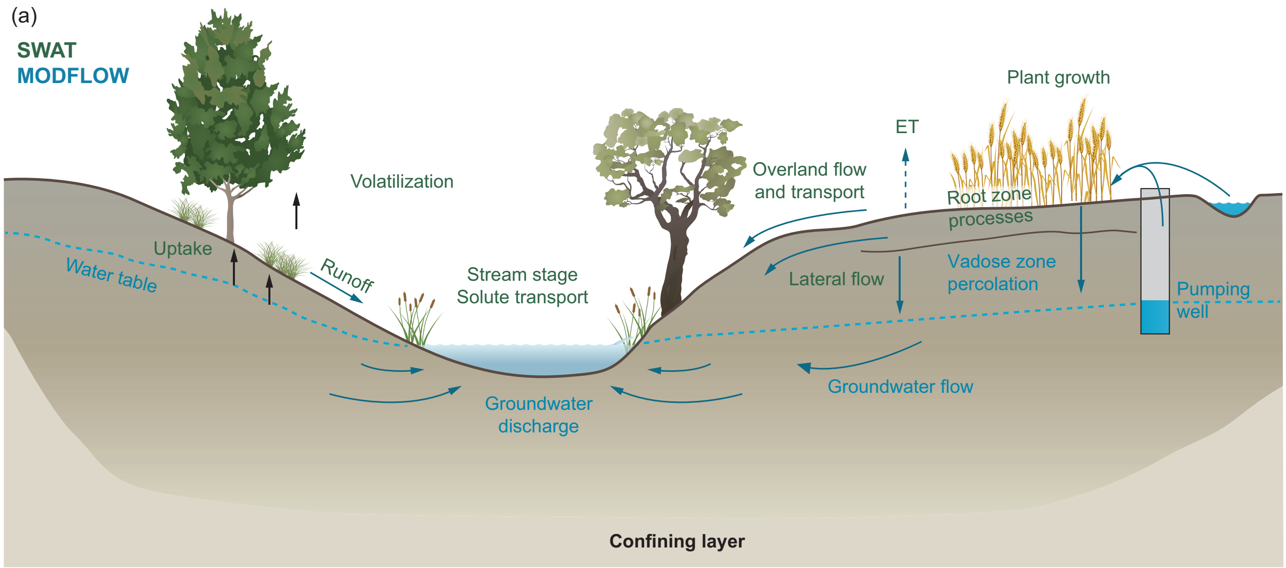
Integrated surface–subsurface hydrological models are capable of simulating water processes in an integrated fashion and provide a spatially and temporally detailed description of a basin-scale hydrologic cycle. In addition, many of these models are being coupled to solute transport models (Heppner et al., 2006; Donn et al., 2012; Wei et al., 2018), ecological process model (Niu et al., 2014), vegetation models (Ivanov et al., 2008a, b), land-energy models (Maxwell and Kollet, 2008) and atmosphere models (Maxwell et al., 2007; Maxwell et al., 2011).

The models are now essential and useful tools in water resources management. They can help us to improve our understanding of SW-GW interactions in different landscapes (Hassan et al., 2014; Tian et al., 2015; Bailey et al., 2016), assess the impacts of climate change and anthropogenic activities on water resources considering both SW and GW (Markstrom et al., 2009; Gilfedder et al., 2012; Chunn et al., 2019; Yu et al., 2019), predict water and solute fluxes exported from water-sheds to receiving water bodies (Shen and Phanikumar, 2010), and manage our water resources (e.g. irrigation management) in an integrated fashion (Condon and Maxwell, 2013; Wu et al., 2015; Wei and Bailey, 2019).

SWAT (Soil and water assessment tool) is a physically-based, basin-scale, continuous-time, semi-distributed hydrological model (Gassman et al., 2007; Neitsch et al., 2011). It has been widely used in catchment management at different geographical locations and scales by simulating hydrology and solute transport (e.g.

sediment, nutrients, waterborne microorganism and pesticide) (Ricci et al., 2018; Liu et al., 2019a; Somaye et al., 2019; Wang et al., 2019) and predicting the influences of anthropogenic activities (e.g. land use planning, management practices) and climate change on water resources (Anand et al., 2018; Molina-Navarro et al., 2018; Wang et al., 2018; Merriman et al., 2019). In SWAT, the basin is divided into subbasins based on topography and each subbasin is further divided into Hydrologic Response Units (HRUs), which are unique combinations of land use, soil type, and surface slope. HRUs are modelled as non-geo-located and lumped (Guzman et al., 2015) within each subbasin, which makes SWAT computationally efficient for long-term simulation, but this comes with the sacrifice of spatial discretization of HRUs within a subbasin. Additionally, groundwater dynamics in SWAT is highly simplified; groundwater from aquifers contributes to streamflow as baseflow through a linear reservoir approximation, ignoring distributed parameters such as hydraulic conductivity and storage coefficients (Kim et al., 2008; Liu et al., 2019d). With this simplified implementation of groundwater dynamics, the SWAT model may mislead evaluation of groundwater resources or perform rather poorly in catchments in groundwater-dominated catchments (Gassman et al., 2014; Liu et al., 2019d).

MODFLOW (Harbaugh 2005) is a physically-based, fully-distributed, three-dimensional groundwater model with Richards equation as the governing equation to simulate subsurface flow. MODFLOW is considered a state-of-the-art international standard for simulating and predicting groundwater conditions and GW-SW interactions (http://water.usgs.gov/ogw/modflow/). It is enabled to simulate sol-



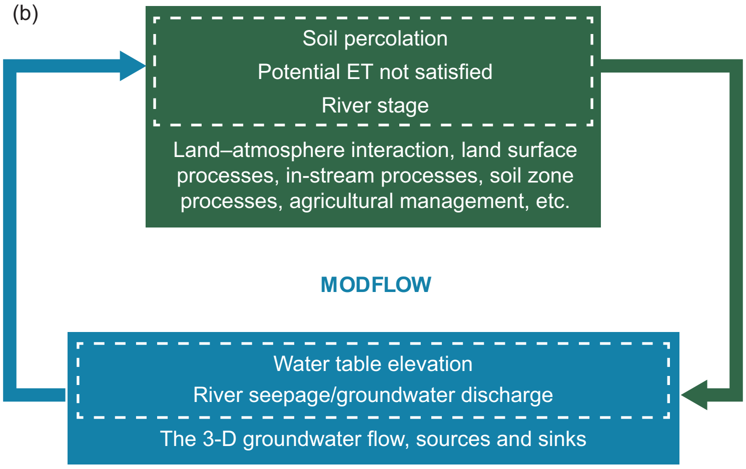


Figure 2. (a). Schematic representation of water processes in stream-aquifer system modelled in the previous published SWAT-MODFLOW (version 2). From Molina-Navarro et al. (2019). (b). SWAT and MODFLOW simulation processes and their linkages in SWAT-MODFLOW.

ute transport in the subsurface when coupled with MT3D (Zheng, 1992) or RT3D (Clement, 1999). MODFLOW has been widely used for groundwater resources management worldwide (Koohestani et al., 2013; Qadir et al., 2016; Jonubi et al., 2018). However, its applications are limited to groundwater-related issues and its performance is highly dependent on the quality of the input data on recharge rates and groundwater-surface water interactions (Liu et al., 2019b).

To overcome the disadvantages of both SWAT and MODFLOW, a few researchers have coupled SWAT and MODFLOW code into one model complex (Kim et al., 2008; Yi and Sophocleous, 2011; Guzman et al., 2015; Bailey et al., 2016). The most recent of these, the SWAT-MODFLOW code developed by Bailey et al. (2016) has several advantages over others: an efficient HRU-grid cell mapping scheme with generation of geographically explicit HRUs, the ability to use SWAT and MODFLOW models of different spatial domain, public availability of the code, and a graphical user interface available for facilitating its application (Bailey et al., 2017; Park et al., 2018). The previous published SWAT-MODFLOW code (Version 2 on the SWAT website) has been applied to catchments of varying sizes worldwide, such as in the USA (Bailey et al., 2016; Wei and Bailey, 2019; Gao et al., 2019), Africa (Blin et al., 2017), Canada (Chunn et al., 2019), Denmark (Molina-Navarro et al., 2019), Iran (Semiromi and Koch, 2019), Japan (Sith et al., 2019) and India (Loukika et al., 2020), for water resources assessment and management. It has also been further developed to be applicable in large-scale mixed agro-urban river basins (Aliyari et al., 2019) and linked to RT3D to simulate nitrate transport in coupled surface and subsurface hydrologic systems (Wei et al., 2018).

Within the coupled SWAT-MODFLOW framework, SWAT simulates surface hydrological processes, whereas MODFLOW-NWT simulates subsurface hydrological processes and all associated sources and sinks (Liu et al., 2019c) (Fig. 4). The HRU-calculated deep percolation from SWAT is passed to the grid cells of MODFLOW as recharge, and MODFLOW-calculated GW-SW exchange fluxes are passed to the stream channels of SWAT (Bailey et al., 2016). Only the domain covered by both SWAT and MODFLOW is coupled, and the original functionality of MODFLOW or SWAT is retained beyond the common domain. Since the model complex ac- counts for two-way interactions between GW and SW, is fully distributed in the groundwater domain, and enables spatially explicit infiltration, the model complex may provide a better representation and thus understanding of the spatial-temporal patterns of groundwater-surface water interactions, relative to alternative open source models (Liu et al., 2019d).

Groundwater abstractions and climate change in Denmark

In regions with large aquifer systems, such as Denmark, groundwater often serves as a key resource to meet the water demands. When groundwater abstractions exceed groundwater recharge, existing groundwater storage depletes and water table decreases, which negatively affect streamflow and ecosystems of groundwater-fed rivers, especially during the dry season when the streamflow is mainly constituted by base flow (Stefania et al., 2018).

Denmark enjoys a temperate marine climate, with mild winters (average temperatures in January and February are 0 °) and cool summers (average temperatures in July and August are around 15 °), and average annual precipitation from 660 to 1160 mm (Stisen et al., 2012). Denmark has few surface water resources with only some small-sized streams, lakes and wetlands compared with the water bodies in many other countries, as it is a lowland country (maximum elevation is 173 m.a.s.l.), which cannot store much water on the surface. Instead, owing to high net precipitation (precipitation minus evapotranspiration) and flat aquifer systems, dominated by sand and limestone, Denmark has abundant groundwater resources (Flindt Jørgensen et al., 2017). For this reason, approximately 100% ofwater used for drinking, irrigation and industry in Denmark is derived from ground-water abstractions, making Denmark the most groundwater- dependent country in the world (Flindt Jørgensen et al., 2017).

The exploitation of groundwater resources in Denmark have traditionally been considered sustainable at the national scale, ensured in part by implementing a groundwater abstraction permit authority system (DEPA, 1992). However, with more economic activities and examples of intermittent events where some wetlands and streams have dried up during the past three decades, concerns about potential over-abstraction have been raised, particularly in Copenhagen and other relatively large cities during summers (Henriksen et al., 2008; Flindt Jørgensen et al., 2017). Henriksen (2014) identified that there remains some places where current groundwater abstraction depletes streamflow to an unacceptable level during dry seasons accord-ing to a national water resource model (DK-model). Thus, assessing the impacts of groundwater abstractions on local streamflow and stream ecosystems in Denmark is necessary, and also crucial for decision making in water resources management and preservation of aquatic ecosystems, particularly in efforts towards compliance with the EU Water Framework Directive (Molina-Navarro et al., 2019).

Globally, unprecedented increase in temperature and markedly changes in precipitation patterns, as well as increases in the frequency of extreme weather events have been recorded and further changes are predicted to occur in the near future, driven by anthropogenic activities (Pachauri et al., 2014; Jeppesen et al., 2015). Through analyzing historical climate data and predicting future climate with an ensemble of 23 global climate models, the Danish Meteorological Institute (DMI) concluded that the temperature trend in Denmark largely follows the trend in the global average annual mean temperature, both in terms of observations since the 1870s and projections of future temperatures up to 2100. The average annual air temperature and precipitation in Denmark has increased by approximately 1.5 °C and 100 mm since 1870, respectively, and the frequency of heavy precipitation events (>100 mm in a few hours) tends to be higher now than in the last century (Olesen et al., 2014; Liu et al., 2019b). Additionally, this tendency is expected to continue in near future; a warmer climate with overall higher precipitation and more extreme weather events is expected. Such changes in climate may cause huge alterations in hydrology and water quality, which are particularly complex in groundwater-dominated catchments, as climate change may cause marked changes in groundwater recharge (Döll, 2009) and enhance the irrigation demand of plants (Diaz et al., 2007; Yano et al., 2007; Liu et al., 2019b).

Climate change affects inland water ecosystems not only by increasing the water temperatures but also by altering the flow regime. Rising temperatures may result in a reduction or even extinction of biota (Eaton and Scheller, 1996) and eutrophication aggravation in inland waters (Trolle et al., 2015; Trolle et al., 2019). Altera-tions in flow regime caused by climate change may lead to a series of negative effects on river ecosystem, such as lower biodiversity and ecological quality, local species extinction, invasion of exotic species (Bunn and Arthington, 2002), damage of habitats by extreme flooding and decrease of habitat availability. However, the flow regime changes may also have some positive effects on aquatic biota, for instance, the streamflow increase could replenish the streamflow during dry season and lead to the increase in connectivity between floodplain and main channel, which could benefit the breeding and survival of fish and other mobile organisms (Arthington et al., 2010; Cui et al., 2018). With more concerns about the consequence of climate change being received, quantifying the effects on flow regime and stream biota is imperative.

Objectives and methods

The overall objective of this Ph.D. project was to further develop and apply the new integrated surface-subsurface model SWAT-MODFLOW to improve the understanding of SW-GW interactions under different scenarios of groundwater abstraction for either drinking water or irrigation. A further objective was to take an integrated ap-proach, where the SWAT-MODFLOW model is combined with empirical flow-biota models to assess the impacts of groundwater abstractions and climate change on hydrological regime and stream biota. This work can help address pressing challenges in water resources management under the influence of groundwater abstractions and climate change in groundwater-dominated catchments.

We further developed the SWAT-MODFLOW complex based on the previous publically available version (v.2) (https://swat.tamu.edu/software/swat-modflow/) to enable application of the Drain Package and an auto-irrigation routine. In addition, a PEST-based approach (Fig. 3) was developed to calibrate the coupled SWAT-MODFLOW by adjusting SWAT and MODFLOW parameters simultaneously, using observations of both streamflow and groundwater table in the objective function. To better understand how pumping wells for drinking water or irrigation may influence nearby streamflow patterns, we applied both SWAT and the further developed SWAT-MODFLOW to a Danish, lowland, groundwater-dominated catchment, the Uggerby River catchment (357 km^2, Fig. 4) (manuscript 1). By linking SWAT-MODFLOW with the flow-regime models, we assessed the impacts of groundwater abstractions and climate change on the hydrologic regime and on stream biota (manuscript 2 and 3).

In manuscript 1, we hypothesize that, the integrated surface-subsurface model SWAT-MODFLOW will perform better relative to the semi-distributed catchment model SWAT when assessing the impacts of groundwater abstractions (for either irrigation or drinking water) on streamflow patterns.

To test the hypothesis, firstly, we set up a SWAT model for the catchment with a Digital Elevation Model (DEM), land use, soil, climate, agricultural management, wells, and wastewater discharge as the input data. Secondly, we calibrated the discharge in SWAT against the daily discharge records at two hydrologically connected monitoring stations by implementing the sequential Uncertainty Fitting

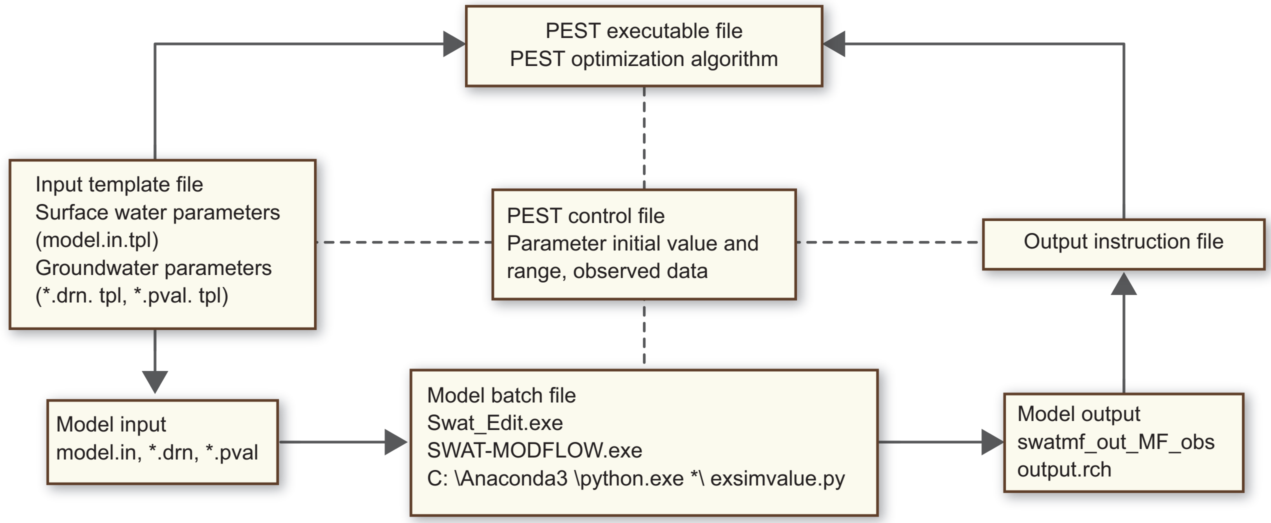


Figure 3. Schematic diagram of the PEST optimization process. The "*" means file name or file path. Modified from (Zhulu, 2010).

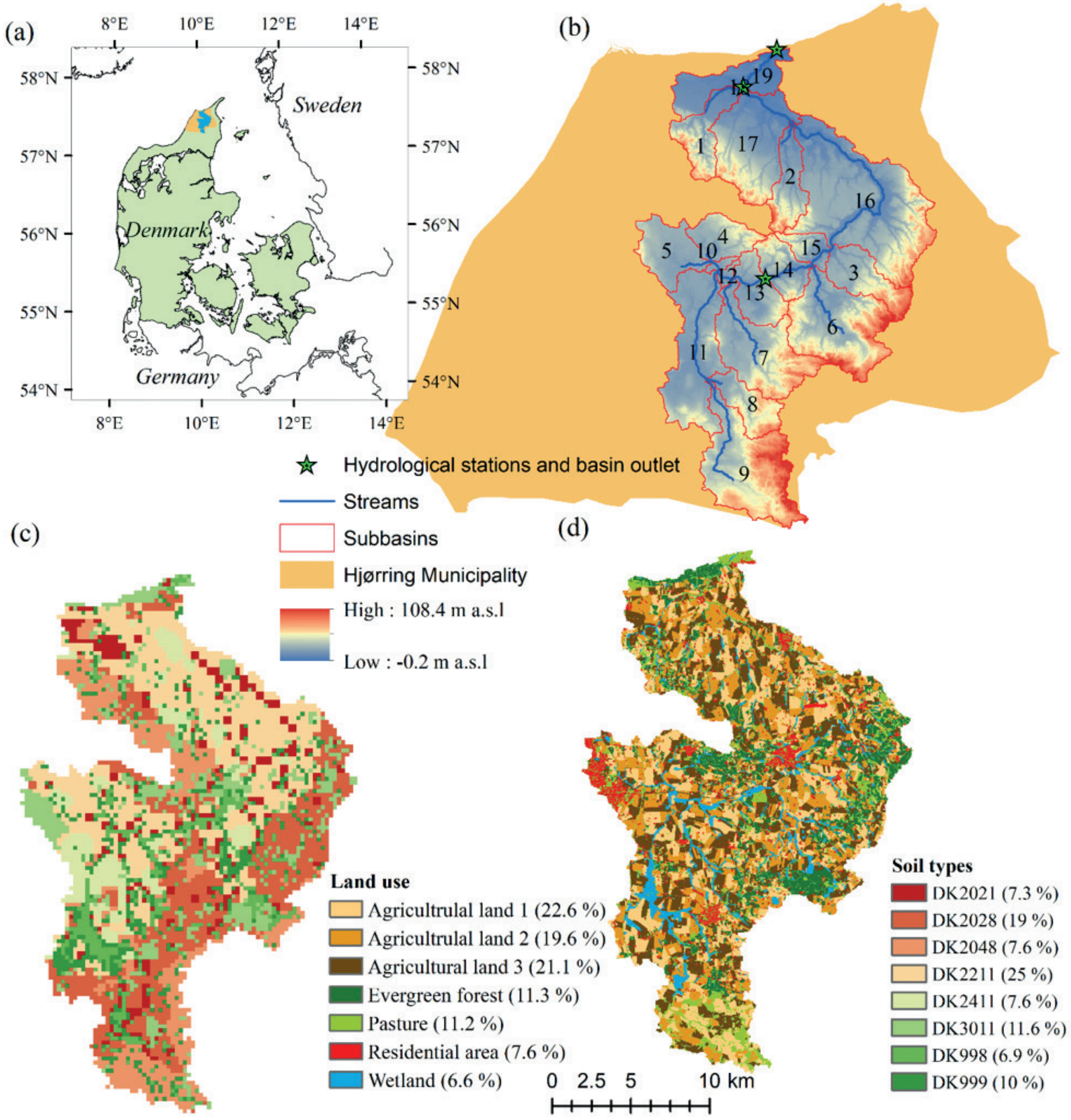


Figure 4. Location of the Uggerby River Catchment and Hjørring Municipality in Denmark (a) and their delineation in SWAT and MODFLOW, respectively (b). The distribution and proportion of each land use (c), soil type (d), after reclassification for HRU definition in SWAT.

gorithm (SUFI2) in the SWATCUP software. Thirdly, we transformed a calibrated steady-state MODFLOW-NWT set-up (obtained from the water consultant company NIRAS/A) for Hjørring Municipality covering the Uggerby River catchment to the transient state with storage coefficient values of each cell assigned. For facilitating the posterior SWAT-MODFLOW calibration, we reduced the number of specific hydraulic conductivities in the original steady-state model from 18 to 5. The modified calibrated steady-state MODFLOW performance was evaluated by visualization of the proximity of simulated and observed groundwater head contours and three summary statistics. Fourthly, we coupled the calibrated SWAT and the transient MODFLOW by using the coupling framework developed by Bailey et al. (2016), but with further developments to enable the application of the Drain package and an auto-irrigation routine. Fifthly, we calibrated the coupled SWAT-MODFLOW based on a PEST-based approach (Fig. 3) against both the streamflow and groundwater table. At last, we conducted four groundwater abstraction scenarios by applying both the calibrated SWAT and calibrated SWAT-MODFLOW models. The performance of the two models on hydrological simulation and the simulated streamflow signals of each model when running four groundwater abstraction scenarios were assessed and compared.

To quantitatively assess the effects of groundwater abstractions and climate change on hydrological regime and stream biota, we combined the SWAT-MODFLOW model with novel nationwide-scale flow-biota empirical models. The flow-biota empirical models refer to the empirical relationships between flow regime variables and the ecological quality ratio of DFFVa (fish index), DVPI (macrophytes index), and DVFI (macroinvertebrate index) according to (Gräber et al., 2015). We applied the integrated approach to the Uggerby River Catchment, as a case study, and assessed to what extent the flow regime and key biota in stream segments of different sizes may be altered by groundwater abstractions and climate change. We analyzed and assessed the impacts of the present level of groundwater abstractions and a scenario with more extreme groundwater abstraction on streamflow, groundwater discharge to streams, flow regime variables and stream biota (the three biotic indices) for three subbasin outlets representing stream segments of different sizes (manuscript 2). We then analyzed and assessed the effects of predicted climate change towards the end of this century relative to the reference period 1996-2005 in two climate change scenarios of different greenhouse gas emissions (RCP2.6 and RCP8.5) on hydrological components, streamflow, groundwater discharge, flow regime variables and biota for all subbasin outlets classified into streams of three sizes (manuscript 3).

Main findings of the study

Three manuscripts were included in this dissertation. Manuscript 1 focused on comparing the performance of SWAT and SWAT-MODFLOW on hydrological simulations, particularly when assessing the impacts of groundwater abstractions for irrigation and drinking water on streamflow. A PEST-based approach to further calibrate SWAT-MODFLOW was developed. The SWAT- MODFLOW used was further developed based on the previously published version to allow the application of Drain Package and an auto-irrigation routine. Manuscript 2 focused on assesing the impacts of groundwater abstractions on flow regime and stream biota by combining SWAT-MODFLOW with flow-biota empirical models. Manuscript 3 focused on assessing the impacts of climate change on hydrological regime and stream biota with the same modelling approach as used in the manuscript 2.

SWAT and SWAT-MODFLOW performance on hydrological simulation

Model results showed that both the SWAT and SWAT-MODFLOW model reproduced streamflow temporal patterns generally well at the two hydrological stations during the calibration and validation periods. However, SWAT-MODFLOW performed visually better in the streamflow hydrograph, especially during recession curves and low flow periods, implying a better simulation of SW-GW interaction (Fig. 5). Accordingly, the corresponding summary performance statistics were also some-what better for SWAT-MODFLOW (Table 1). The parameter sensitivity analysis results revealed that groundwater processes parameters played an important role in SWAT-MODFLOW, while they were less impo-

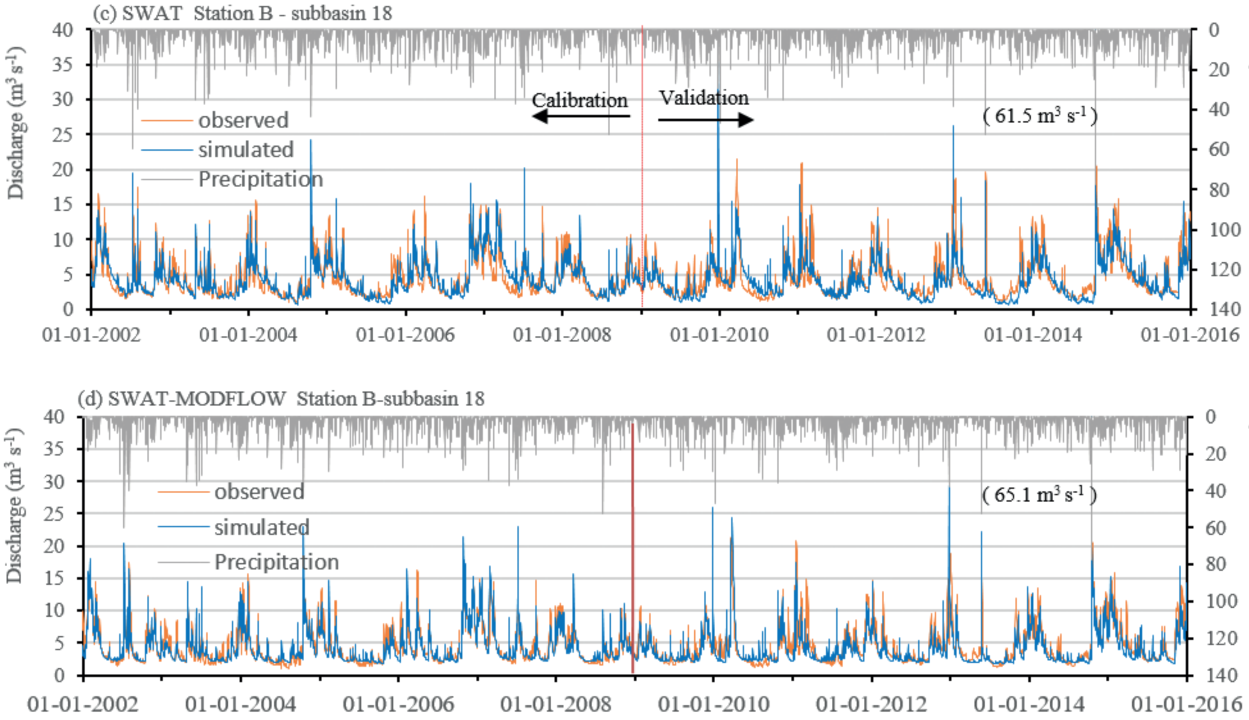


Figure 5. Temporal patterns of precipitation observed and best simulated daily streamflow at station B during the calibration period (2002-2008) and the validation period (2009-2015) based on SWAT and SWAT-MODFLOW. The value in bracket is the discharge on 16 October 2014, which is outside the range of the plot area. From manuscript 1.

Table 1. Performance statistics indices for daily runoff at station A and station B during the calibration and validation (in brackets) periods by SWAT, SWAT-MODFLOW without PEST calibration, and SWAT-MODFLOW with PEST calibration. From manuscript 1.

Outlets	Used models	N_{SE}	R^2
Station A	SWAT	0.66 (0.50)	0.67 (0.53)
	SWAT-MODFLOW without PEST calibration	0.72 (0.51)	0.75 (0.60)
	SWAT-MODFLOW with PEST calibration	0.78 (0.54)	0.78 (0.61)
Station B	SWAT	0.74 (0.47)	0.74 (0.53)
	SWAT-MODFLOW without PEST calibration	0.77 (0.46)	0.79 (0.57)
	SWAT-MODFLOW with PEST calibration	0.81 (0.53)	0.82 (0.60)

rtant in SWAT for improving the streamflow simulation performance. This reflects the shortcoming of the highly simplified SWAT groundwater module, implying that the discharge 19WAT cannot be optimized to the same extent as in SWAT-MODFLOW (manuscript 1).

Relative to SWAT, the SWAT-MODFLOW model not only produced output for streamflow but also provides fully distributed groundwater-related outputs such as spatial water table elevation on any given day, distributed aquifer recharge, and GW-SW exchange rates at a cell or subbasin level, permitting detailed analysis of groundwater and its interaction with surface water. These data may be an important input to groundwater resources management (e.g. groundwater abstraction) and to obtain solution of surface water rights issues.

Models ability to simulate effects of groundwater abstractions on streamflow

In manuscript 1, we found that the SWAT simulations underestimated the impacts of groundwater abstractions for both drinking water and irrigation water on streamflow depletion, while SWAT-MODFLOW provided more realistic assessments. As discussed in manuscript 1, apart from due to the simple representation of groundwater dynamics in SWAT, is that the impact of groundwater removal by abstractions on water table fluctuation is not taken fully into account in the groundwater discharge calculation in current SWAT source code. By contrast in the SWAT-MODFLOW model, the exchange rate between groundwater and surface water is based on the head difference between the river stage (or drain cell stage) and the head of its surrounding groundwater grid cells. This model can therefore account for the temporally dynamic hydrological processes and also the impacts from all the external stressors (e.g. temporally and spatially varying recharge and groundwater abstractions) on water table fluctuations Naturally, this should also allow SWAT-MODFLOW to provide more realistic assessments of the impacts of groundwater abstractions on streamflow relative to SWAT.

Our finding are generally consistent with the previous studies which showed the ability of SWAT-MODFLOW to evaluate the impacts of groundwater abstraction on streamflow or GW-SW interactions (Guzman et al., 2015; Molina-Navarro et al., 2019; Chunn et al., 2019), though all of the studies only considered the groundwater abstractions for drinking water without considering irrigation and based on assumed drinking water pumping wells. Additionally, in the previous SWAT-MODFLOW version published by Bailey et al. (2016), the River Package in the MODFLOW model was the only package used for simulating GW-SW interaction, ignoring potential drain flow processes. The SWAT-MODFLOW complex used in our study was further developed to allow application of the Drain Package and an auto-irrigation routine to extract water from groundwater grid cells; in this way the impacts of groundwater abstraction for both drinking water and irrigation could be assessed.

The PEST-based approach for further calibrating SWAT-MODFLOW

In previous studies, after coupling a calibrated SWAT and calibrated MODFLOW model, the SWAT-MODFLOW model complex was applied either without further calibration (Chunn et al., 2019; Bailey et al., 2016), with calibration against only streamflow observations (Molina-Navarro et al., 2019), with separated calibration for streamflow and groundwater head (Guzman et al., 2015), or with simple manual calibration by graphically comparing the simulated and observed streamflow and groundwater head (Sith et al., 2019). Since both the SWAT and MODFLOW supporting software can use inverse modeling (IM) methods for calibration, and parameter non-uniqueness is an inherent property of IM (Abbaspour, 2015), the coupling of a calibrated SWAT and a calibrated MODFLOW cannot guarantee a proper or sufficiently optimized parameter set for the integrated SWAT-MODFLOW model. Because groundwater and surface water interact with each other, calibrating the simulation of one part does not guarantee proper simulation of the other part. In this study, as discussed in manuscript 1, application of a combined calibration approach based on PEST allowed us to calibrate the SWAT- MODFLOW model by adjusting simultaneously SWAT and MODFLOW parameters and using observations of both streamflow and groundwater table when deriving the objective function. After calibration by PEST, the summary statistics of SWAT-MODFLOW performance on streamflow simulation were slightly improved (Table 1), and the weighted residuals between simulation and observation considering both streamflow and groundwater head were reduced, with the reduced residuals mainly for streamflow simulation.

Impacts of groundwater abstractions on flow regime and stream biota

In manuscript 2, we found that the current groundwater abstractions in the catchment has generally caused minor decreases in groundwater discharge and streamflow throughout the catchment, compared with the scenario with no drinking water wells. Consequently, the flow regime variables and the biotic indices for stream ecology quality only showed modest or no changes (Fig. 6). In contrast, the simulated extreme abstraction scenario in an upper-stream subbasin (subbasin 7 where the abstraction rates were enhanced by 20-times relative to the current groundwater abstractions), caused larger streamflow decrease at all three subbasin outlets representing stream segments of different sizes along the main channel, compared with the current groundwater abstractions. However, only for subbasin 7 (small-sized stream) there was considerable impacts on the flow regime variables and the biotic indices despite the larger streamflow decreases in the outlets of subbasin 13 (medium-sized stream) and 18 (large-sized stream). The cause of this, we believe, is because the impacts of extreme abstraction in subbasin 7 on larger streams downstream subbasin 7 are buffered by the water contribution from the other subbasins in the catchment. Our results indicate different responses to groundwater abstractions by streams of different sizes, and also highlights the importance of resolving these differences in a model set-up to advance today's water management and render groundwater abstraction permit confirmation taken into account basin heterogeneities (manuscript 2).

Among the three biotic indices, the fish index responded most negatively to the groundwater abstractions, followed by the macrophyte index, decreasing, respectively, by 23.5% and 11.2% in the small stream in the extreme groundwater abstraction scenario. No apparent impact was found on macroinvertebrate index in any of the three subbasin outlets (Fig. 6). Groundwater abstractions affect streamflow mainly through reducing the baseflow, thereby lowering the BFI, which is highly dependent on the baseflow. As discussed in manuscript 2, according to the regression coefficients related to each flow regime variable, the BFI, of which the coefficient is 0.811 and much larger than the coefficients of the other flow regime variables, has the strongest influence on the ecological state, making the DEFVa the most vulnerable index to groundwater abstractions.

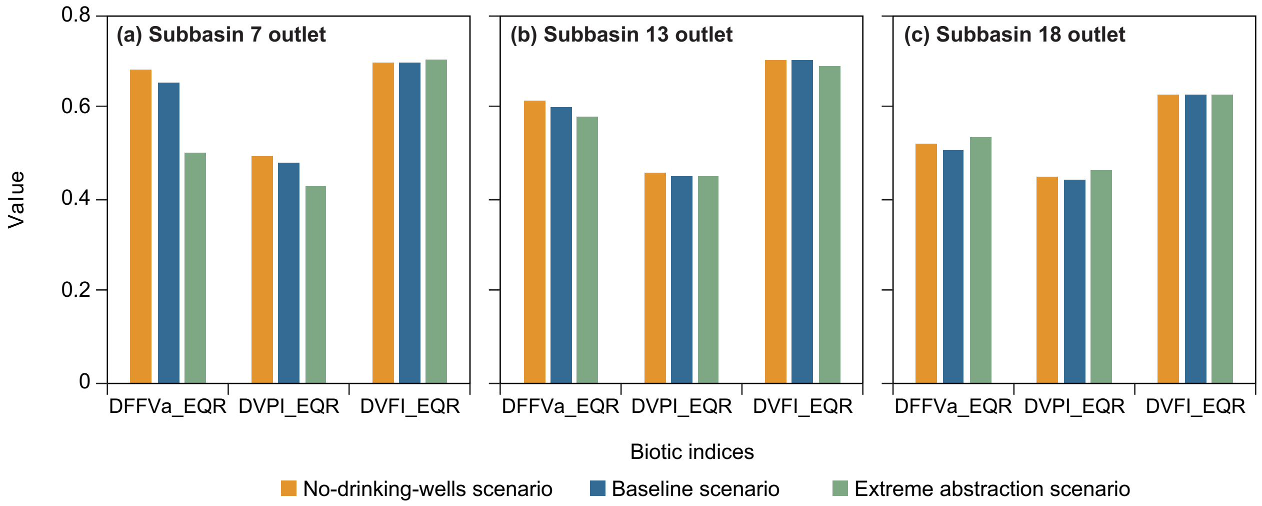


Figure 6. Comparison of the biotic indices (DFFVa: fish index; DVPI: macrophyte index; and DVFI: macroinvertebrate index) at subbasin outlet 7, 13, and 18, respectively, during 2002-2015 between the three different scenarios (no drinking water abstraction, baseline, and extreme abstraction). From manuscript 2.

Impacts of climate change on flow regime and stream biota

Former studies (Kim et al., 2011; Mittal et al., 2016; Pradhanang et al., 2013; Yang et al., 2017) investigating the effect of climate change revealed large regional differences in flow regime alterations – some areas will experience an overall increase in runoff while others will exhibit a decrease (Goudie, 2006; Pachauri et al., 2014). Besides regional differences, we also found that the overall increase or decrease of runoff depends on the climate change scenario; the total flow in the study area decreased by 0.26% in the RCP2.6 scenario but increased by 2.4% in the RCP8.5 scenario (manuscript 3). Yano et al. (2007) predicted an increase of 15–22% in the irrigation demand for a wheat–maize crop rotation in Turkey, while Rodriguez Diaz et al. (2007) estimated an increase of 15–20% in the seasonal irrigation demand in a basin in Spain by 2050 (Jeppesen et al., 2015). In this study, the predicted climate change will raise the irrigation demand for agriculture and pastures in the irrigated areas, with an average annual increment of 2% in the RCP2.6 scenario and of 31% in the RCP8.5 scenario.

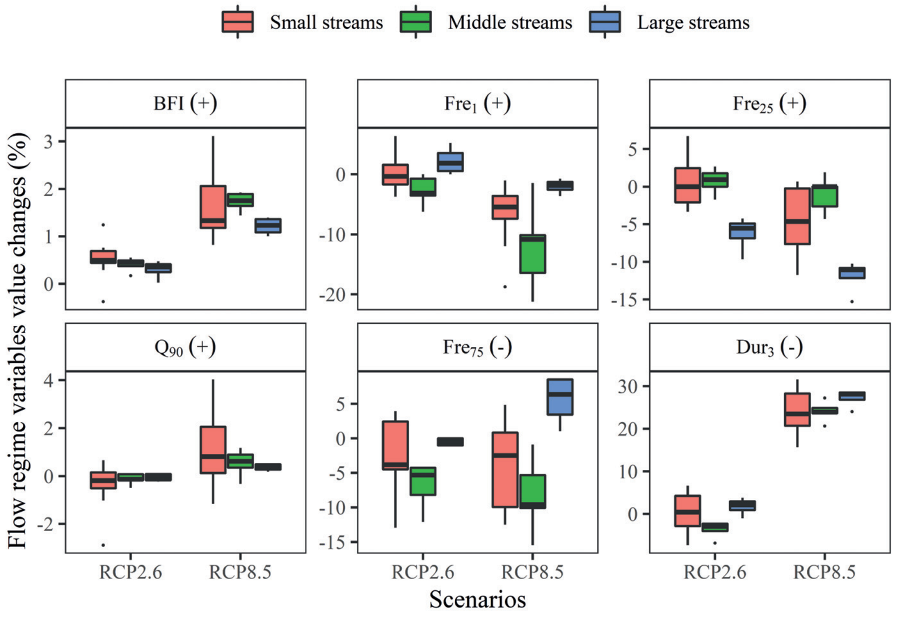


Figure 7. Changes in flow regime variable values from the baseline in the two climate change scenarios (RCP2.6, RCP8.5) in the three differently sized streams (small, medium and large). "+" and "-" indicate, respectively, a positive and a negative effect on stream biotic indices as predicted by the flow-biota empirical models. From manuscript 3.

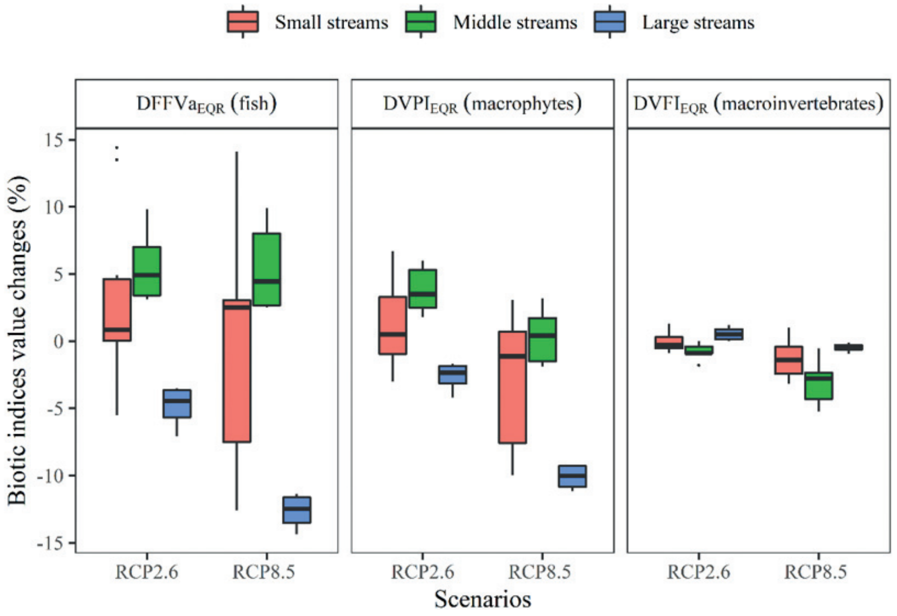


Figure 8. Changes in flow regime variable values from the baseline in the two climate change scenarios (RCP2.6, RCP8.5) in the three differently sized streams (small, medium and large). "+" and "-" indicate, respectively, a positive and a negative effect on stream biotic indices as predicted by the flow-biota empirical models. From manuscript 3.

The differently sized streams underwent different alterations in flow regime (Fig. 6) and also demonstrated different biotic responses to climate change, notable the fish and macrophyte indices (Fig. 7). Large and some small streams suffer ed most from climate change, as the fish and macrophyte quality indices decreased up to 14.4% and 11.2%, respectively, whereas these indices increased by up to 14.4% and 6.0% respectively, in medium and some small streams. The climate change effects were, as expected, larger in the RCP8.5 scenario than in the RCP2.6 scenario (Fig. 7).

Through summarizing the related literatures, Cui et al. (2018) concluded that flow regime shifts induced by climate change could have both positive and negative influence on river ecosystems depending on the degree of flow regime alteration as well as the hydromorphological characteristics of rivers. In correspondence with their conclusion, we found that the predicted flow regime shifts caused by climate change generally improves the ecological state in some small and medium streams but reduces it in the large and in some small streams.

Perspectives and further work

Managing groundwater and surface water as an integrated resource is imperative to meet the growing water use for anthropogenic needs and increasing challenges in water resources management associated with water rights issues, ecological degradation and ongoing climate change. Surface -subsurface models are essential and useful tools in integrated water resources management. A growing number of surface-subsurface hydrological models of different complexity have been developed in the past decades. When modellers choose a model for application, the balance between scientific accuracy and the computational burden as well as the available input data should be defined relative to the study goal. For instance, as shown in the manuscript 1, even though SWAT-MODFLOW can produce more reliable results and more outputs on hydrological simulation than SWAT, SWAT-MODFLOW requires more effort and data to be set up and for calibration, and longer time to run. As the purpose of this study was to investigate effect of groundwater abstraction on stream and further on stream biota, clearly, efforts should be focused on setting up and applying a model, which is fully-distributed in the groundwater domain, such as SWAT-MODFLOW.

All the scenario analysis and hydrological impact assessments in this study through the models were based on the “best” parameter combination achieved through calibration. We deemed this method as satisfactory for the purpose of this study. However, in practical water resources management, uncertainties of hydrological simulations by models should ideally be considered. To meet this demand, the developed PEST-based approach in this study for SWAT-MODFLOW calibration needs to be further explored and adapted to allow model uncertainty analysis in the future.

The approach of combining SWAT-MODFLOW and the flow-biota empirical models demonstrated many advantages, as outlined in manuscript 2. Our study gave an example of how to quantify the effect of groundwater abstractions and climate change on stream biota through scenario simulations, which could have potential implications for local water resources management. Broader application of this combined modelling approach to other catchments would assist in water planning and regulations regarding groundwater management and in response of the challenges posted by climate change in Denmark or other countries (if similar flow-biota empirical model in those countries are developed).

However, even though the flow-biota empirical models used in this study were developed based on a number of stream sites with varying characteristics (e.g. temperature, stream size and nutrient concentration), the application scope of the empirical models is still limited. With further development of the flow-biota empirical models based on a larger number of streams of different sizes and in cluding more factors affecting ecological quality status than flow regime variables, for instance temperature and nutrient concentrations, the overall predictions of the coupled model complex may become more reliable.

Besides the studies presented in the three manuscripts, I also conducted initial studies on nutrients transport simulation. The management of nutrients (nitrogen and phosphorus) is complex due to GW-SW interactions, geographical variability in land cover, anthropogenic activities, soil types, geological properties, and the ongoing climate change. I focused on applying the model SWAT-MODFLOW-RT3D presented by Wei et al. (2018) to help identifying the most critical areas of nitrate and total phosphorous losses to groundwater and surface water. Preliminary simulation results of nitrate and total phosphorus transport by SWAT-MODFLOW-RT3D have been obtained. Further calibration by PEST and analysis should be done, after which critical areas could potentially be identified and a series of scenario analysis of best management practices could be carried out. Such a study could benefit the management of nutrient runoff, particularly in groundwater-dominated catchments.

Conclusions

Generally, both SWAT and MODFLOW simulated well the temporal streamflow hydrographs at two hydrological stations in the Uggerby River catchment during the calibration and validation periods. However, the further developed SWAT-MODFLOW model calibrated by PEST provided a somewhat better hydrological simulation performance, wider possibilities for groundwater analysis, and much more realistic signals relative to the semi-distributed SWAT model when assessing the impacts of groundwater abstractions for either irrigation or drinking water on streamflow; hence, SWAT-MODFLOW has great potential to be a useful tool in waterresources management, particularly in groundwater-dominated catchments.

The novel approach of combining SWAT-MODFLOW and flow-regime biota models is a useful tool to quantitatively assess the effect of groundwater abstractions and climate change on stream biota and thereby support water planning and regulations related to groundwater abstractions and in response of the challenges posed by climate change. However, further developing the flow-biota models based on a larger number of streams of different sizes and including more factors affecting ecology quality status (e.g. nutrients concentration and temperature) may enhance the reliability of the models.

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MANUSCRIPT 1

COMPARING SWAT WITH SWAT-MODFLOW HYDROLOGICAL SIMULATIONS WHEN ASSESSING THE IMPACTS OF GROUNDWATER ABSTRACTIONS FOR IRRIGATION AND DRINKING WATER

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Key Points:

- We compared the performance of SWAT and SWAT-MODFLOW and assessed the simulated streamflow signals in response to a range of groundwater abstraction scenarios targeted for irrigation and drinking water.
- The SWAT-MODFLOW complex was further developed to enable application of the Drain Package and an auto-irrigation routine.
- A PEST-based approach was developed to calibrate the coupled SWAT-MODFLOW.
- The SWAT-MODFLOW model produced more realistic results on groundwater abstraction effects on streamflow.

Abstract

Being able to account for temporal patterns of streamflow, the distribution of groundwater resources, as well as the interactions between groundwater and surface water is imperative for informed water resources management. We hypothesize that, an integrated surface-subsurface model SWAT-MODFLOW performs better relative to a lumped semi-distributed catchment model SWAT when assessing the impacts of groundwater abstractions (for either irrigation or drinking water) on streamflow patterns. We applied the widely used SWAT model and the recently developed SWAT-MODFLOW model, which allows full distribution of the groundwater domain, to a Danish, lowland, groundwater-dominated catchment. We compared the performance of the two models based on the observed streamflow and assessed the simulated streamflow signals of each model when running four groundwater abstraction scenarios. The SWAT-MODFLOW model complex was further developed to enable the application of the Drain Package of MODFLOW and an auto-irrigation routine. Both models were calibrated and validated, and a PEST-based approach was developed and utilized to enable simultaneous calibration of SWAT and MODFLOW parameters. Both models demonstrated generally good performance for the temporal pattern of streamflow, albeit SWAT-MODFLOW performed somewhat better. In addition, SWAT-MODFLOW generates spatially explicit groundwater-related outputs, such as spatial-temporal patterns of water table elevation. In the abstraction scenarios analysis, the impact of drinking water abstraction on streamflow depletion simulated by SWAT was unrealistically low, and the streamflow increase caused by irrigation abstraction was exaggerated compared with SWAT-MODFLOW. We conclude that the further developed SWAT-MODFLOW model calibrated by PEST had a better hydrological simulation performance, wider possibilities for groundwater analysis, and much more realistic signals relative to the semi-distributed SWAT model when assessing the impacts of groundwater abstractions for either irrigation or drinking water on streamflow; hence, it has great potential to be a useful tool in the management of water resources in groundwater-affected catchments. However, this comes at the expense of higher computational demand and more time consumption.

1 Introduction

The interaction between groundwater and surface water is an important aspect of the water cycle, and the management or use of one often impacts the availability and temporal patterns of the other. Improper management and over-exploitation of these water resource components influence the sustainability of both the water resource itself and also the ecosystems that it supports. Groundwater abstraction can cause a decline of the water table, and it thereby directly affects surface water bodies connected to the aquifer (Jeppesen et al., 2015; Vainu and Terasmaa, 2016; Stefania et al., 2018). For rivers in which a considerable portion of the streamflow is base flow, this can have a strong influence on the general flow and deteriorate the function of river ecosystems (Johansen et al., 2011; Pardo and Garcia, 2016). However, interactions between groundwater and surface water are difficult to observe and measure, and it is, therefore, difficult to determine how much of the reduced streamflow recorded in some rivers is due to abstractions and how much is due to natural weather-induced variability in water table elevation.

For quantitative assessment of the impacts of pumping wells on streamflow, a hierarchy of modeling tools has been developed, ranging from simple water balance calculations to regional, three-dimensional numerical models, depending on the complexity and available data source of the site (Chen and Yin, 2001; Parkin et al., 2007; May and Mazlan, 2014). The analytical solutions generally require less data for parameter identification and may therefore be applied when available data are sparse, thus offering water managers a simple approach for estimating streamflow depletion with less time, expertise, and financial costs (Glover and Balmer, 1954; Hunt, 1999; Huang et al., 2018; Zipper et al., 2018). Nevertheless, as they do not simulate many of the physical processes and ignore the real-world complexity, they may render results far away from reality. In contrast, numerical, process-based models consider more about the complexity and heterogeneity of river-aquifer systems. Such models can simulate the regional groundwater dynamics as well as the interactions between groundwater and surface water. They are therefore part of local water management applications including estimation of streamflow depletion, although they are generally more time-consuming and costly to set up, calibrate, test, and apply.

MODFLOW is a physically-based, fully-distributed, numerical and three-dimensional (3D) finite-difference ground-water model. It can be used to simulate both steady state and transient conditions. MODFLOW outputs include groundwater hydraulic head or drawdown at the cent-er of each grid cell as well as groundwater flow rates to/from each stream segment if the River (RIV) Pack-age or the Streamflow Routing Package (SFR) is used (Wei et al., 2018). A number of studies have applied MODFLOW to assess the impact of groundwater abstraction on surface water resources (Sanz et al., 2011; May and Mazlan, 2014; Shafeeque et al., 2016; Stefania et al., 2018). However, MODFLOW does not simulate surface processes such as land-atmosphere interactions, agricultural management practices, and surface runoff (Lachaal et al., 2012; Surinaidu et al., 2014). To obtain spatial-temporal varying recharge rates, MODFLOW is therefore often linked with land-surface models such as the Precipitation-Runoff Modelling system (Markstrom et al., 2008; Markstrom et al., 2015) and the Soil and Wa-ter Assessment Tool (SWAT) (Izady et al., 2015; Wei et al., 2018).

The SWAT model is a semi-distributed catchment-scale model and has been widely used to simulate surface runoff, sediment erosion, pesticide and microorganism transport, and nutrient cycling in catchments at different geographical locations and scales (Nielsen et al., 2013; Fukunaga et al., 2015; Malago et al., 2017; Liu et al., 2019). In SWAT, the basin is divided into subbasins through a topography-based delineation, each subbasin containing a tributary of the river. Each subbasin is further divided into Hydrologic Response Units (HRUs), which are unique combinations of land use, soil type, and surface slope. When simulating hydrological dynamics, the areas of the HRUs are lumped within each subbasin, which makes SWAT computationally very efficient, but this comes at the expense of losing the spatial discretization of HRUs within a subbasin. SWAT has been utilized to simulate and quantify the groundwater resources (Ali et al., 2012; Cheema et al., 2014; Shafeeque et al., 2016) or the effects of drinking water or irrigation pumping on streamflow (Güngör and Göncü, 2013; Lee et al., 2006). However, the SWAT model has tradition-ally emphasized surface processes as the model only includes a relatively simple representation of ground-water dynamics, and its output does not give any spa-tially explicit information on the groundwater table. In the most recent version of SWAT (v. 670), groundwater is represented by a lumped module in individual subba-sins divided into a shallow and a deep aquifer. Both the shallow and the deep aquifer may contribute to stream-flow as baseflow through a linear reservoir approxima-tion, ignoring distributed parameters such as hydraulic conductivity and storage coefficients (Kim et al., 2008). With this simplified implementation of groundwater dynamics in SWAT, the model can mislead evaluation of groundwater resources or perform rather poorly in catchments where the streamflow is strongly dependent on groundwater discharge (Gassman et al., 2014).

To the best of our knowledge, there are two main approaches for making SWAT perform better in groundwater-dominated catchments. One approach is to modify the SWAT groundwater module code itself. For example, (Zhang et al., 2016) modified the subroutines in the SWAT source code by converting the shallow aquifer water storage change into water table fluctuation with three groundwater parameters added, namely specific yield, the bottom bed burial depth, and shallow aquifer porosity. The modified SWAT could then simulate both water table fluctuations and water storage of the shallow aquifer in time and space. However, it still applied a lumped, linear reservoir approach to simulate groundwater storage and derive the water table at HRU level, which could give rise to errors as the HRUs are not spatially explicit within a subbasin. (Pfannerstill et al., 2014) implemented a three-storage concept in the groundwater module by splitting the shallow aquifer into a fast and a slow contributing aquifer. (Nguyen and Dietrich, 2018) replaced the deep aquifer in the original SWAT model with the multicell aquifer model. In both of these studies, the modified SWAT model achieved a better prediction of baseflow than the original SWAT model. However, both models only improved a part of aquifer system simulation, either the shallow aquifer or the deep aquifer. In addition, they maintained the semi-distributed approach.

The other approach for improving the performance of SWAT in groundwater-dominated catchments is to couple SWAT with a physically based, spatially distributed numerical groundwater model, such as MODFLOW. There are a few studies that have integrated SWAT and MODFLOW code into one model complex (Kim et al., 2008; Yi and Sophocleous, 2011; Guzman et al., 2015; Bailey et al., 2016). The most recent of these, the SWAT-MODFLOW code developed by (Bailey et al., 2016) couples the most recent SWAT code with the MODFLOW-NWT code (a Newton-Raphson formulation for MODFLOW-2005 (Niswonger et al., 2011), which improves the solution of unconfined groundwater-flow problems). This coupled version has several advantages over others: an efficient HRU-grid cell mapping scheme (including generation of geographically explicit HRUs), the ability to use SWAT and MODFLOW models of different spatial coverage, public availability, and a graphical user interface that has been recently developed for its application (Bai-ley et al., 2017; Park et al., 2018). Recently, the current published SWAT-MODFLOW code (Version 2 on the SWAT website) has been applied to catchments in the USA (Bailey et al., 2016; Abbas et al., 2018; Gao et al., 2019), Canada (Chunn et al., 2019), Denmark (Molina-Navarro et al., 2019), Iran (Semiromi and Koch, 2019), and Japan (Sith et al., 2019). It has also been further de-veloped for application in large-scale mixed agro-urban river basins (Aliyari et al., 2019). Within the coupled SWAT-MODFLOW framework, SWAT simulates surface hydrological processes, whereas MODFLOW-NWT simulates groundwater flow processes and all associated sources and sinks on a daily time step. In addition, the HRU-calculated deep percolation from SWAT is passed to the grid cells of MODFLOW as recharge, and MODFLOW-calculated groundwater-surface water interaction fluxes are passed to the stream channels of SWAT. Hence, the model complex accounts for two-way interactions between groundwater and surface waters and thereby enables a potentially much better representation and thus understanding of the spatial-temporal patterns of groundwater-surface water interactions, which are of key importance to catchment management in groundwater-dominated catchments.

In Denmark, approximately 800 million m^3 of water are abstracted annually and used for irrigation or drinking water (GEUS, 2009), making the country highly dependent on groundwater. Since the very dry summers in 1975 and 1976 led to dry out of many watercourses around some cities in Denmark, the national government has endeavored to regulate the abstraction of surface and groundwater to a level preventing negative impacts on in-stream biota. Gradually, direct abstraction from surface waters has been prohibited and groundwater abstraction is regulated to secure a certain minimum flow in all Danish rivers, mainly by moving the abstraction wells away from riverbanks and wetlands and implementing a groundwater abstraction permit authority system. However, there still remains some areas where groundwater exploitation is above the sustainable yield and causes streamflow depletion according to the national water resource model (Henriksen et al., 2008).

To better understand how abstraction wells used for drinking water or irrigation may influence nearby streamflow, we applied both SWAT and SWAT-MODFLOW to a lowland catchment in Northern Denmark – the Uggerby River Catchment. We hypothesize that, the SWAT-MODFLOW performs better relative to SWAT when assessing the impacts of groundwater abstractions (for either irrigation or drinking water) on streamflow patterns. We compared the performance of the two models and assessed the simulated signals of streamflow in a range of groundwater abstraction scenarios with real wells and abstraction rates for either drinking water or irriga-tion with both models. The SWAT-MODFLOW complex used in this study was further developed based on the publically available version (https://swat.tamu.edu/software/swat-modflow/) to enable application of the Drain Package of MODFLOW and to allow auto-irriga-tion. In addition, an approach based on PEST (Doherty, 2018) was developed to calibrate the coupled SWAT-

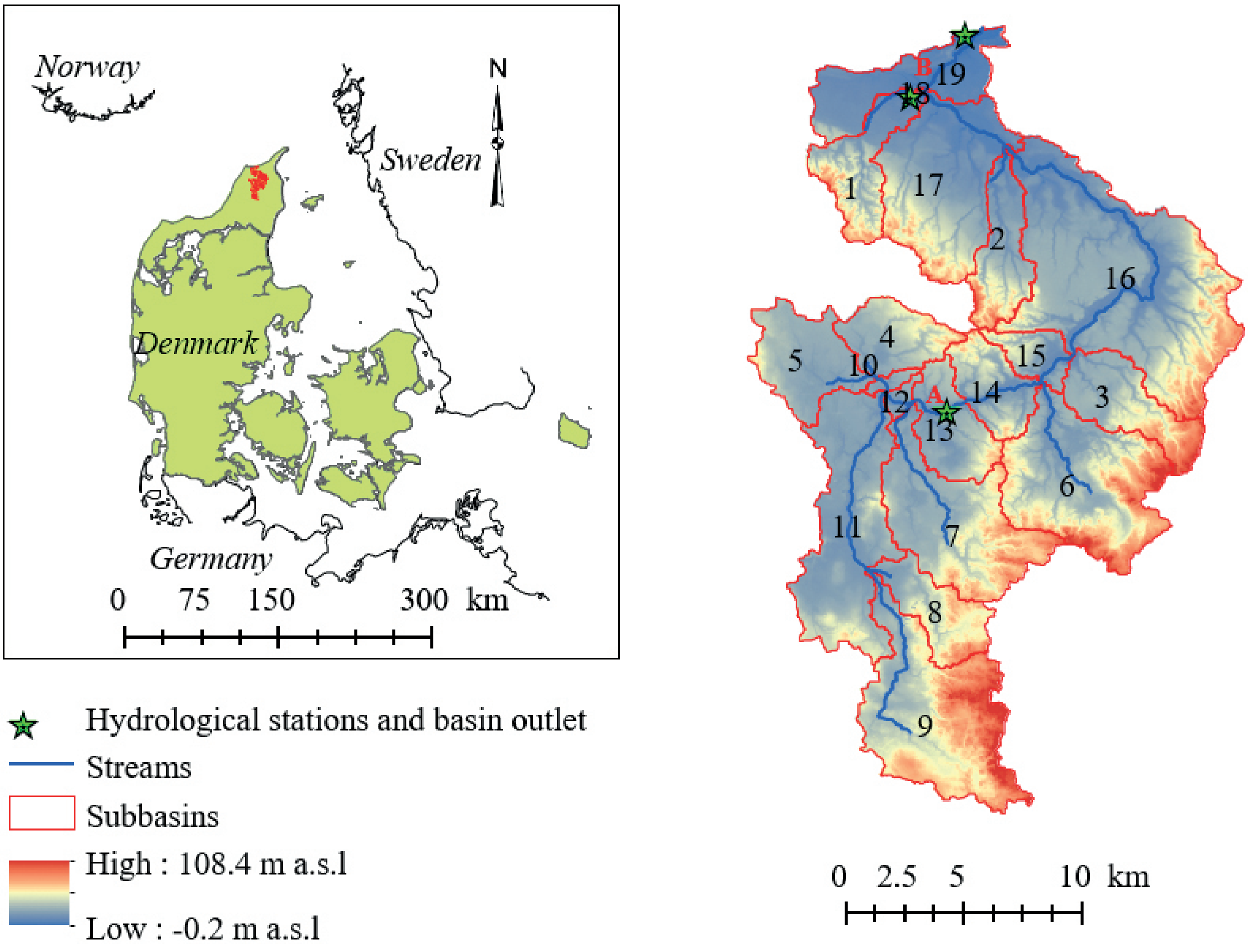


Figure 1. Location of the Uggerby catchment and its delineation in SWAT, including subbasins division, stream network definition based on the digital elevation model (DEM), hydrological monitoring stations, and basin outlet.

MODFLOW by adjusting SWAT and MODFLOW parameters simultaneously against the observations of both streamflow and groundwater table.

2 Materials and methods

2.1 Study area

The Uggerby River Catchment lies between latitude 57°17′10″ - 57°35′25″ N and longitude 9°58′47″ - 10°19′55″ E. It covers an area of 357 km2 and is located in the Municipality of Hjørring, which is situated in the northern part of Jutland, Denmark (Fig. 1). The Uggerby River originates from the southern part of Hjørring in Sterup and winds its way through the area of Hjørring, Sindal, Mosbjerg, Bindslev, and Uggerby and then discharges into the bay Tannisbugten at the coast of the North Sea. The study area has a typical Atlantic climate, which is temperate with an average annual temperature around 8 °C, being warmest in August (17 °C average) and coldest in January (0.5 °C average). The average annual precipitation during the study period 2002-2015 was approximately 933 mm with no obvious distinctions among seasons.

The mean catchment elevation is 34.5 m a.s.l and ranges from 0 to 108 m. Land cover in the catchment is dominated by agricultural land, and the other land use types include evergreen forest, pasture, wetland, and urban areas. The soil types are loamy sand, sandy loam, and sand. The main crops grown in the area include winter wheat, winter rape, barley, corn, and grass. Artificial tile drains have been installed in parts of the agricultural land in the catchment, although the precise drainage locations are somewhat uncertain (Olesen, 2009). According to an investigation carried out by Hjørring Municipality in 2009, there are 101 drinking water pumping wells registered within the catchment and 57 irrigation pumping wells placed on pasture and agricultural land. Generally, irrigation only occurs from April to October. The average annual irrigation amount varies from 80 to 200 mm depending on the types of crop and soil conditions (Aslyng, 1983).

2.2 Model set-up and coupling

2.2.1 SWAT model set-up

We used the QSWAT 1.5 interface (George, 2017), which works with the latest SWAT Editor version 2012.12.19 and is integrated into a QGIS 2.8.1 interface. The input

Table 1. Farm types and crop rotations used to describe agricultural management in the Uggerby River Catchment (W: winter, S: spring).

				Rotation scheme				
Rotation type	**Farm Type**	**Manure N (kg N/ha)**	**% Farm area**	**Year 1**	**Year 2**	**Year 3**	**Year 4**	**Year 5**
Agricultural land 1	Mixed and horticulture	<50	31.0	W. wheat	W. wheat	S. barley	W. rape	S. barley
Agricultural land 2	Dairy/Cattle	85-170	35.7	S. barley	Grass	S. barley	Grass	Grass
Agricultural land 3	Dairy/Cattle	85-170	33.3	S. barley	S. barley	W. wheat	Corn silage	Corn silage

data for the SWAT model in this study include topography, land use, soil, climate, agricultural management, wells, and wastewater discharge as point sources.

The catchment was divided into 19 subbasins (Fig. 1) based on the 32 m pixel size Digital Elevation Model (DEM), which has resampled from a 1.6 m LIDAR DEM (Knudsen and Olsen, 2008). For the creation of HRUs, we used the land use map based on the Danish Area Information System (NERI, 2000) and the soil map based on a national three-layer soil map with a 250 m grid resolution (Greve et al., 2007), and surface slope type was classified into three classes (<2%, 2-6%, >6%). To reduce the number of HRUs and facilitate the posterior model linkage process, land use for range-grasses and range-brush, which covered only 1.3% and 1.9% of the total catchment area, respectively, were merged into pasture, and water (0.9%) was merged into wetland areas. In order to represent the agricultural management practices in detail, the agricultural area was split into three equally sized types with different five-year crop rotation schedules (Table 1) based on the real contour of agricultural field plots and the land use map. Similar to land use, soil types covering a minor part of the catchment (1% or less) were merged into similar soil types. The distribution and proportion of each land use, soil type, and slope band after reclassification are shown in Fig. 2. Based on the combination of land use, soils, and slope, the catchment was discretized into 2620 HRUs.

Climate data used in the model comprised the 10 km-grid national daily precipitation data (six stations inside the catchment), 20 km-grid daily solar radiation and wind speed data (five stations inside or near the catchment), gauged-level daily maximum and minimum temperatures, and relative humidity data (one station, 27 km from the catchment) during 1997-2015 from the Danish Meteorological Institute (Lu et al., 2016).

Farm type and manure/mineral fertilizer application of each agricultural rotation as well as dates of sowing, harvesting, and tillage were assigned based on reported statistics for 2005 available from http://www.dst.dk/en (Table 1). We do not know the specific tile drain distribution with-

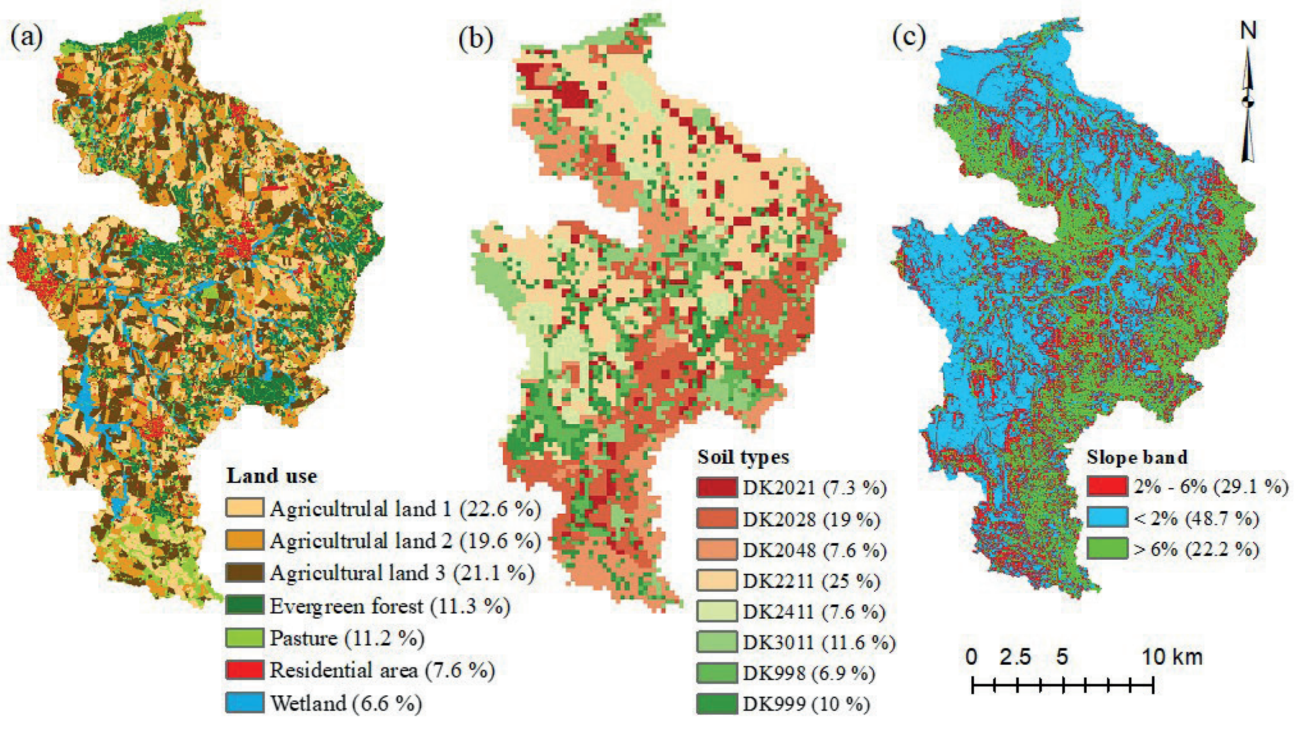


Figure 2. The distribution and proportion of each land use (a), soil type (b), and slope band (c) after reclassfication for HRU definition in SWAT.

in the entire catchment. In general, loamy soils in relatively flat areas are known to be tile drained in Denmark (Olesen, 2009). To represent this situation, tile drains were set up in agricultural land with a slope less than 2% and for soil types with a clay content above 8% (Thodsen et al., 2015), representing 27% of the agricultural land in the catchment.

We assumed that irrigation only occurs in the HRUs where irrigation pumping wells exist (based on a MODFLOW model created by NIRAS A/S). It is difficult to know the exact dates and water amount used for irrigation. Thus, to simulate the irrigation, auto-irrigation management was set up based on heat unit scheduling for the HRUs containing irrigation pumping wells. For the auto-irrigation of crops, the water resource used for pumping was defined as the shallow aquifer, and the soil water content, commonly used as an indicator in actual field irrigation (Chen et al., 2017), was selected as the water stress identifier with 70 mm as the initial water stress threshold. With the number and location of pumping wells as well as their pumping rates obtained from the Well Package in the MODFLOW model, the water abstraction amounts from drinking water wells were added up in each subbasin and set as the water use pumped from the shallow aquifer in SWAT.

The only significant point source of the study area is the discharge from the wastewater treatment plant in Sindal located in subbasin 16. With a few other minor sources aggregated to a total discharge from the wastewater treatment plant, a total of 2768.8 m^3 of water was discharged into the stream per day (data is based on an average for the period 2007-2010).

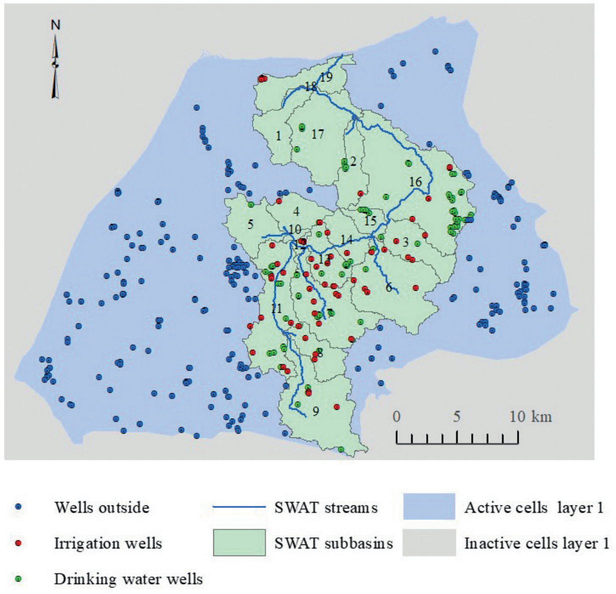


Figure 3. SWAT and MODFLOW set-up coverage and the well locations distributed inside or outside the Uggerby River Catchment.

2.2.2 MODFLOW-NWT model set-up

A steady-state version of the MODFLOW-NWT model has previously been set up for the entire Hjørring Municipality, covering an area of 930 km^2, in which the Uggerby River Catchment is situated (Fig. 3). The model set-up was firstly established in 2011 and then updated in 2016 by the consultant company NIRAS A/S and Hjørring Water Supply Company, and has been applied for water resources management in the Hjørring Municipality. In the model set-up, the geology is represented by 5 hydro-stratigraphic layers, discretized into 183,112 grids (376 rows and 487 columns) with a discretization of 100 × 100 meters. The uppermost layer is unconfined and the remaining four layers are confined. The Upstream Weighting (UPW) Package for MODFLOW, which contains hydraulic properties of each cell, was used as the internal flow package, and a number of boundary condition packages, including Time-variant specified-head Package, Drain Package, River Package, Well Package, and Recharge Package, were employed in the model to simulate external stresses. The steady-state model was calibrated using 1,063 head observations sampled during the period 1996-2010 at 1,006 well locations distributed within the first, third, and fifth layer by a combination of manual calibration and auto-calibration through PEST (http://www.pesthomepage.org/).

Eighteen different hydraulic conductivity values exist in the originally calibrated MODFLOW model. In order to facilitate the posterior SWAT-MODFLOW calibration, we reclassified and grouped the specific hydraulic conductivities into five groups. The grouping was made for grid cells of similar specific hydraulic conductivities, representing the sedimentary materials of clay, silt, silty sand, mixture of silty sand and clean sand, and clean sand, respectively. Each group was assigned a unique specific hydraulic conductivity, which could be targeted for calibration.

For the SWAT-MODFLOW set-up, we converted the modified calibrated steady-state model into a transient model by assigning values to the specific yield (only for the unconfined layer) and specific storage of each cell according to the type of sedimentary materials of the cell and representative values of storage coefficients. The simulated heads generated by the steady-state model were used as the initial head conditions for the transient model.

2.2.3 SWAT-MODFLOW coupling

SWAT and MODFLOW were combined using the coupling framework developed by (Bailey et al., 2016) and following the procedures described in the instructions available from the SWAT website (http://swat.tamu.edu/software/swat-modflow/).

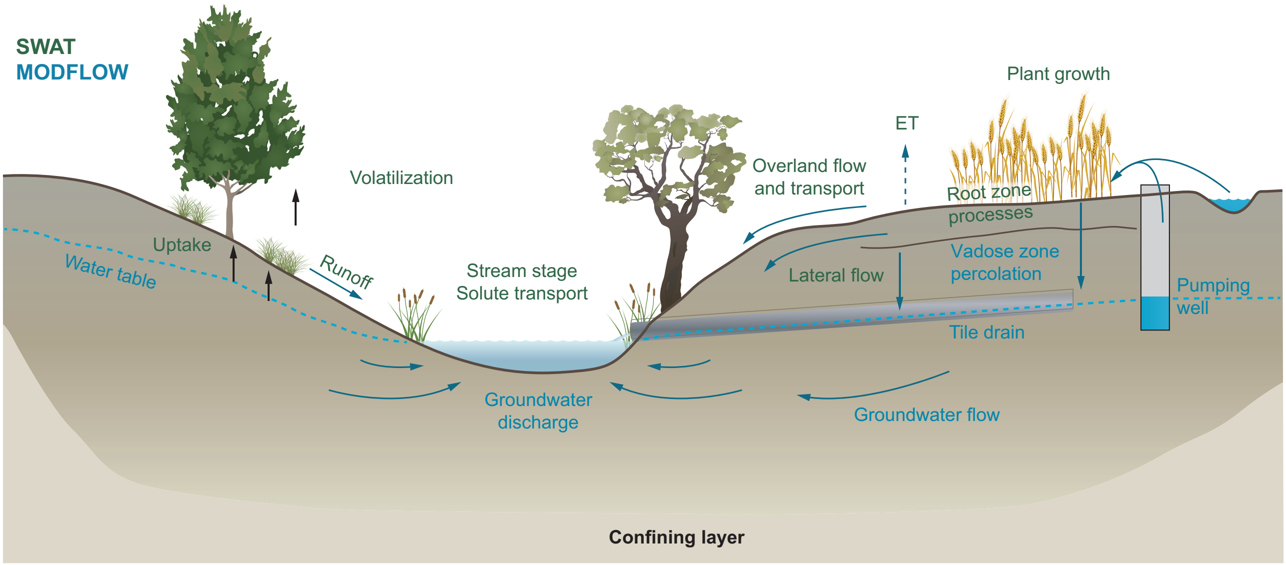


Figure 4. Schematic representation of water transport routes in stream-aquifer system as simulated by SWAT-MODFLOW, showing SWAT (green) and MODFLOW (blue) simulation processes. Adapted from (Molina-Navarro et al., 2019).

For this study, the following changes were made to the original SWAT-MODFLOW code: (1) the grid cells in the Drain Package were linked with SWAT subbasins so that groundwater removed from subsurface drains is routed to stream channels; and (2) groundwater pumping in agricultural areas or pastures is dictated by irrigation applied to HRUs through SWAT's auto-irrigation routines. For the latter, this is achieved by calculating the daily volume of applied irrigation water (irrigation depth * HRU area) and then extracting this volume from the underlying grid cells using MODFLOW's Well Package (Fig. 4). When applying the Drain Package of MODFLOW, the original tile drain routine in SWAT was disabled. The steps in the coupling procedure included: 1) disaggregation of HRUs to disaggregated hydrologic response units (DHRUs) through GIS processing to make the model spatially explicit; and 2) creation of six linking text files (HRUs to DHRUs, DHRUs to MODFLOW grids, MODFLOW grids to DHRUs, MODFLOW river cells to SWAT subbasin rivers, MODFLOW drain cells to subbasin rivers, irrigation pumping wells in HRUs to MODFLOW grids) through GIS processing. All related files (MODFLOW input files, original SWAT model files, linkage files) were stored in one working directory for SWAT-MODFLOW execution.

2.3 Model calibration

2.3.1 SWAT calibration

The Sequential Uncertainty Fitting Algorithm (SUFI2), which is implemented in the SWAT-CUP software (Abbaspour, 2015), was used to calibrate discharge performance in SWAT. The latest SWAT-CUP version (5.1.6.2) was used. Calibration was performed based on daily discharge records from 1 Jan. 2002 to 31 Dec. 2008, with a previous 5-year model warm-up period and using Nash-Sutcliffe efficiency (NSE) as the objective function. Five parameters at basin-wide level and 17 parameters at subbasin level related to streamflow were selected and assigned initial calibration value ranges based on expert judgement and previous SWAT applications in Danish catchments (Lu et al., 2015; Molina-Navarro et al., 2017).

In the study area, two hydrologically connected monitoring stations are found, located at the outlet of subbasin 13 (station A) and subbasin 18 (station B), respectively (Fig. 1). The two stations represent a small (average discharge 1.95 m^3 s^{-1}) and relatively large (average discharge 4.56 m^3 s^{-1}) stream in Denmark, and both were used for calibration and validation in this study. Station A is located upstream from station B and its flow therefore has an influence on station B. Thus, the simulated discharge of station A was preliminarily calibrated first (initial range of related parameters are shown in Table 2), running 3 iterations with 500 simulations each. After the final iteration for station A, the subbasin level parameters for the area upstream station A were fixed, while the final ranges of the basin-wide parameters were used in the subsequent calibration of station B. As the basin-wide parameter values can impact the hydrology of the entire catchment, for the calibration of station B, discharge data from both station A and B were included in the objective function. An additional three iterations with 500 simulations were run, where the subbasin level parameters for the remaining area upstream station B were calibrated using the same initial parameter range as for station A (Table 2), while the basin-wide parameter ranges from the final calibration step for station A were used as initial ranges. By this approach, we attempted to make the basin-level parameters representative for both upstream and downstream areas. Afterwards, the water stress threshold was calibrated manually to ensure proper simulation of the annual irrigation amount, which ranges from 80 to 120 mm yr^{-1} and occurs in the period April to October (Aslyng,

Table 2. Initial ranges and calibrated values of the selected parameters for SWAT calibration.

Parameter	Description	Initial range	Calibrated values	
			Subbasins: 4,5,7-13 (upstream)	Subbasins: 1,3,6,14-19 (downstream)
v_SFTMP.bsn	Snowfall temperature (°C)	-1 – 1	0.175	
v_SMFMN.bsn	Melt factor for snow on December 21 (mm H_2O °C^{-1} d^{-1})	1 – 2	1.287	
v_SMFMX.bsn	Melt factor for snow on June 21 (mm H_2O °C^{-1} d^{-1})	1.6 – 3.5	2.467	
v_SMTMP.bsn	Snow melt base temperature (°C)	-2.3 – 1	-1.342	
v_SURLAG.bsn	Surface runoff lag coefficient	1 – 10	6.379	
v_ALPHA_BF.gw	Baseflow alpha factor for shallow aquifer (l d^{-1})	0 – 1	0.453	0.639
v_ALPHA_BF_D.gw	Baseflow alpha factor for deep aquifer (l d^{-1})	0 – 1	0.756	0.913
v_ALPHA_BNK.rte	Baseflow alpha factor for bank storage (l d^{-1})	0 – 1	0.912	0.533
v_CH_K2.rte	Effective hydraulic conductivity in main channel alluvium (mm h^{-1})	0 – 75	57.068	45.018
r_CN2.mgt	Initial SCS runoff curve number for moisture condition II	-0.3 – 0.3	-0.279	0.137
r_DDRAIN.mgt	Depth to subsurface drain (mm)	-0.3 – 0.3	0.066	-0.129
v_EPCO.hru	Plant uptake compensation factor	0.01 – 1	0.163	0.254
v_ESCO.hru	Soil evaporation compensation factor	0 – 1	0.466	0.931
r_GDRAIN.mgt	Drain tile lag time (h)	-0.3 – 0.3	0.052	-0.021
v_GWQMN.gw	Threshold depth of water in the shallow aquifer required for return flow to occur (mm)	0 – 2000	1435.04	960.32
v_GW_DELAY.gw	Groundwater delay time (d)	0 – 200	116.28	123.40
v_GW_REVAP.gw	Groundwater "revap" coefficient	0.02 – 0.1	0.092	0.0313
r_OV_N.hru	Manning´s "n" value for overland flow	-0.2 – 0.2	-0.037	-0.025
v_REVAPMN.gw	Threshold depth of water in the shallow aquifer for "revap" or percolation to the deep aquifer to occur (mm)	1000 – 2000	1633.81	1521.80
r_SOL_AWC().sol	Available water capacity of the soil layer (mm H_2O mm soil^{-1})	-0.8 – 0.8	-0.674	0.786
r_SOL_BD().sol	Moist bulk density (g cm^{-3})	-0.2 – 0.2	-0.067	0.156
r_SOL_K().sol	Saturated hydraulic conductivity (mm h^{-1})	-0.8 – 2	1.290	1.831
r_TDRAIN.mgt	Time to drain soil to field capacity (h)	-0.3 – 0.3	-0.097	-0.210
v_RCHRG_DP.gw	Deep aquifer percolation fraction	0 – 0.4	0.296	0.219
AUTO_WSTRS	Water stress threshold that triggers irrigation (mm)	70	30, 40, 60	

Note: v_ means that the existing parameter value is to be replaced by a given value; r_ means that an existing parameter value is multiplied by (1+ a given value).

1983). Once the calibration was completed and the parameters were fixed, we validated the model by running one simulation from 1 Jan. 1997 to 31 Dec. 2015 using the first 12-years as a warm-up period.

To analyze parameter sensitivity and make the sensitivity analysis comparable with SWAT-MODFLOW, an additional iteration with 500 simulations was run for the calibration period. In this iteration, the ranges of basin level parameters and subbasin level parameters for the area upstream station A were the same as those in the final calibration step for station A, while the ranges of subbasin level parameters for the area upstream station B were identical with the final calibration step for station B.

2.3.2 SWAT-MODFLOW calibration

After model coupling, the SWAT-MODFLOW was calibrated by adjusting SWAT and MODFLOW parameters simultaneously against the observations of both streamflow and groundwater table through a combination of manual calibration and auto-calibration by the widely used PEST approach (Doherty, 2018). The periods used for model warm-up, calibration, and validation were identical to those used for SWAT. SWAT-MODFLOW can also be run through SWAT-CUP, whereby the summary statistics of model performance can be derived and directly compared between SWAT and SWAT-MODFLOW. In addition, model.in and Swat_Edit.exe, which are included in the creation of the SWAT-CUP project folder, can be used to adjust SWAT parameters within the PEST routine.

Table 3. Initial values, ranges, and calibrated values of the selected parameters for SWAT-MODFLOW calibration using PEST.

Parameter	Description	Initial value	Parameter ranges	Calibrated values
v_SFTMP.bsn	---	0.175	-0.946 – 0.351	0.351
v_SMFMN.bsn	---	1.287	1.117 – 1.424	1.424
v_SMFMX.bsn	---	2.467	2.387 – 3.129	2.387
v_SMTMP.bsn	---	-1.342	-1.687 – -0.46	-0.46
v_SURLAG.bsn	---	6.379	4.452 – 8.151	4.964
v_ALPHA_BNK.rte[a]	---	0.912	0.7 – 1	0.7
v_ALPHA_BNK.rte[b]	---	0.533	0.206 – 0.617	0.231
v_CH_K2.rte[a]	---	57.068	29.322 – 59.779	59.779
v_CH_K2.rte[b]	---	45.018	30.246 – 60.088	41.182
r_CN2.mgt[a]	---	-0.279	-0.3 – -0.106	-0.3
r_CN2.mgt[b]	---	0.137	-0.019 – 0.175	0.0004
v_EPCO.hru[a]	---	0.163	0.077 – 0.436	0.436
v_EPCO.hru[b]	---	0.255	0.01 – 0.334	0.304
v_ESCO.hru[a]	---	0.466	0.227 – 0.681	0.227
v_ESCO.hru[b]	---	0.931	0.684 – 1	0.943
r_OV_N.hru[a]	---	-0.037	-0.2 – -0.02	-0.02
r_OV_N.hru[b]	---	-0.025	-0.155 – -0.005	-0.023
r_SOL_AWC().sol[a]	---	-0.675	-0.8 – -0.316	-0.508
r_SOL_AWC().sol[b]	---	0.786	0.344 – 0.8	0.8
r_SOL_BD().sol[a]	---	-0.067	-0.187 – -0.05	-0.185
r_SOL_BD().sol[b]	---	0.156	0.077 – 0.2	0.172
r_SOL_K().sol[a]	---	1.29	0.902 – 2	0.902
r_SOL_K().sol[b]	---	1.831	1.012 – 2	1.012
COND_1	Drain conductance	0.00467	0.00311 – 0.00622	0.00543
COND_2	Drain conductance	0.02487	0.01658 – 0.03316	0.03316
HK_CLAY	Hydraulic conductivity of clay (m s^{-1})	3.84E-08	1E-09 – 4.4E-08	2.2E-08
HK_SILT	Hydraulic conductivity of silt (m s^{-1}1)	5.00E-07	1E-07 – 9E-07	1E-07
HK_SS	Hydraulic conductivity of silty sand (m s^{-1})	6.70E-06	1.51E-06 – 7.50E-06	7.5E-06
HK_SSCS	Hydraulic conductivity of silty sand and clean sand (m s^{-1})	1.79E-05	1E-05 – 8E-05	1.79E-05
HK_CS	Hydraulic conductivity of clean sand (m s^{-1})	0.000327	1E-04 – 5E-04	3.15E-04
SS_CLAY	Specific storage of clay (m^{-1})	0.001099	9.19E-04 – 1.28E-03	1.28E-03
SS_SILT	Specific storage of silt (m^{-1})	0.000755	4.92E-04 – 1.02E-03	1.02E-03
SS_SAND	Specific storage of sand (m^{-1})	0.000166	1.28E-04 – 2.03E-04	2.03E-04
SY_CLAY	Specific yield of clay (%)	0.06	0.04 – 0.08	0.04
SY_SILT	Specific yield of silt (%)	0.2	0.15 – 0.25	0.22
SY_SAND	Specific yield of sand (%)	0.32	0.25 – 0.35	0.35
AUTO_WSTRS	---	30, 40, 60	30, 40, 60, 80	

Notes: “a” means that the parameter applies to the upstream areas, including subbasins: 4, 5, 7-13, while “b” applies to downstream areas, including subbasins 1, 3, 6, 14-19. “---” indicates that the corresponding parameters can be found in Table 2.

The framework using PEST to calibrate SWAT-MODFLOW was firstly introduced by (Park, 2018). We applied this framework to this study as well but with BEOPEST (Doherty, 2018) instead of PEST as the PEST executable file. Five types of files are required to run PEST: PEST control file, PEST executable file, model batch file, model input template files, and model output instruction files. The PEST control file is a master file that contains control variables, initial values and ranges of model parameters, observations and their weights for deriving the value of the objective function, as well as names of all input and output files related to calibration. BEOPEST was used as the PEST executable file that enables parallelization of model runs on multiple computer cores, thereby shortening the calibration time considerably. After each iteration of a PEST run, the PEST optimization algorithm adjusts the model parameter values to optimize the value of the objective function. The newly updated model parameter values are then written to model input files using input template files and Swat_Edit.exe. Next, the SWAT-MODFLOW executable is called by a batch file and generates a set of output files if the model runs successfully. A python script (exsimvalue.py) extracts the simulated values from the streamflow output file (output.rch) and the groundwater table output file (swatmf_out_MF_obs). The extracted simulated data are read by PEST using information from the model output instruction file and then compared against the corresponding observations. Each iteration includes a number of model runs according to the control variable set in the PEST control file to allow adjustment of parameter values. After each iteration, the objective function and a Jacobian matrix are calculated, based on which the PEST will make its decision for the next iteration until one of its stopping criteria, specified in the PEST control file, is met. More detailed information about the optimization process and principles of PEST can be found in (Zhulu, 2010) and the PEST manual (Doherty, 2018).

As shown in Table 3, 26 parameters from SWAT related to surface hydrological processes and 13 parameters from MODFLOW were selected and calibrated through PEST. For SWAT parameters, with the parameters related to tile drains and groundwater excluded, the final calibrated parameter values used in SWAT were applied as the initial values in PEST, and the parameter ranges used in the iteration for SWAT parameter sensitivity analysis were employed as the parameter ranges in PEST. By manually adjusting MODFLOW parameter values to test their impacts on model outputs, storage coefficients (SY and SS), horizontal hydraulic conductivity (HK), and two drain conductance (COND) were deemed as the potential sensitive parameters, with the value of HANI (the ratio of hydraulic conductivity along columns to hydraulic conductivity along rows) always being 1 and the values of VKA (the ratio of horizontal to vertical hydraulic conductivity) fixed as the values in the original MODFLOW set-up. For MODFLOW parameters, the originally calibrated and modified parameter values in the steady-state MODFLOW version were used as the initial parameter values in PEST, and a small range around the initial values was assigned as the parameter range according to the experience from manual calibration and representative values (derived from http://www.aqtesolv.com/aquifer-tests/aquifer_properties.htm).

The observed streamflow used for calibrating SWAT-MODFLOW was identical to that used for calibrating SWAT. Relatively continuous observations of the groundwater table were available at the location of two grid cells, and these were used for calibrating the variation of the groundwater table simulated by SWAT-MODFLOW. Because station A is located upstream from station B and its flow thus has an influence on station B, the weight for deriving the objective function for station A, which represents a small stream, was set to 2, and the weight for station B was set to 1. The weights for the two grid cells were set to 1.

In order to establish template files and facilitate the process of modifying parameter values (HK, SS, SY) in the UPW Package while running PEST, the parameter value file (PVAL) and Zone file (https://water.usgs.gov/ogw/modflow-nwt/MODFLOW-NWT-Guide/) were first established based on the original UPW Package through running a code file in FORTRAN.

Ten iterations were specified as the stop criteria in the PEST control file. Due to the large number of grid cells (183,112) in the MODFLOW set-up and the amount of disaggregated HRUs (DHRUs, 66,765) compared with the case study conducted by (Bailey et al., 2017), it takes the coupled SWAT-MODFLOW model complex around 4 hours to run a single simulation (12 years' simulation) when MODFLOW runs with a daily interval. To shorten the calibration time, 11 BEOPEST slaves were created on three computers with BEOPEST as the pest executable file so that 11 simulations could be run simultaneously. A total of 638 simulations were run before the stop criteria was achieved. With the calibrated parameters fixed, the water stress threshold was calibrated manually to ensure proper simulation of the annual irrigation amount (ranging from 80 to 120 mm yr^{-1}, occurring in the period between April to October) and make the simulated average annual irrigation amount in the irrigated HRUs (mm yr-1) comparative with that in the calibrated SWAT model. Finally, the SWAT-MODFLOW model performance was validated following a procedure equivalent to that used for SWAT.

2.4 Water abstraction scenarios

Besides the 158 wells registered within the Uggerby River Catchment, another 256 wells exist outside the catchment but inside Hjørring Municipality (Fig. 3). All these wells were included in the Well Package in the SWAT-MODFLOW set-up. In SWAT-MODFLOW, the irrigation pumping source was defined as the third layer. For drinking water wells, 7 of the 101 drinking water wells were placed in the first layer, 91 in the third layer and 3 in the fifth layer. In order to evaluate the impacts of both irrigation and drinking water abstractions on streamflow for streams of difference sizes, four abstraction scenarios were designed and applied to the Uggerby River Catchment using both models: 1) the no-wells scenario, where all abstractions are terminated; 2) the irrigation-wells-stop scenario, where all abstractions in irrigation wells are terminated, while abstractions in drinking water wells remain; 3) the drinking-wells-stop scenario, where all abstractions in drinking water wells are terminated, while abstractions in irrigation wells remain; and 4) the baseline scenario, where abstractions in all wells are included, which represents the current level of abstraction. We assumed that the point source discharge to the stream in subbasin 16 would remain the same in all scenarios. Once the scenarios were simulated, their impacts on streamflow were analyzed by assessing the average annual runoff amount, the contribution of water balance components, and the temporal dynamics of streamflow. The simulated signals of SWAT and SWAT-MODFLOW in the abstraction scenarios were then compared.

Table 4. The summary statistics for the calibrated MODFLOW performance.

Layer number	The number of observed heads	M_E (Mean error)	M_{AE} (Mean absolute error)	R_{MSE} (Root mean squared error)
Layer 1	453	-0.59	1.94	2.84
Layer 3	572	-0.54	2.36	3.15
Layer 5	38	-1.24	3.44	5.00
All	1063	-0.59	2.22	3.11

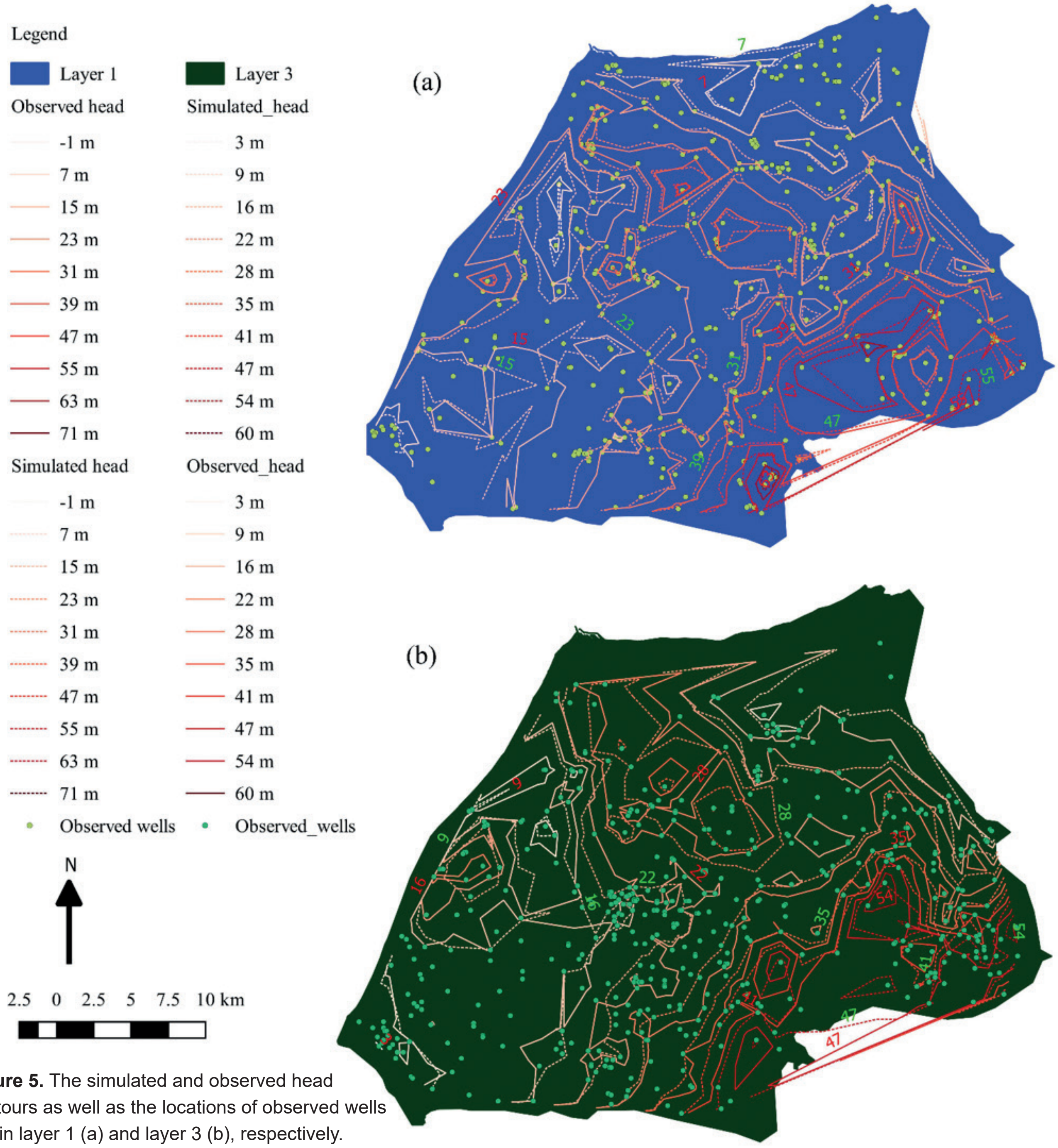


Figure 5. The simulated and observed head contours as well as the locations of observed wells within layer 1 (a) and layer 3 (b), respectively.

3 Results

3.1 Steady-state MODFLOW performance

Visualization of the proximity of simulated and observed head contours (Fig. 5) was used to evaluate how well the modified calibrated MODFLOW model performed at steady state and three summary statistics were used as indicators for goodness of model fit (Table 4). The simulated heads and summary statistics have changed little compared with the original calibrated MODFLOW setup. Thus, the modified calibrated MODFLOW model was satisfactory and suitable as a basis for coupling to SWAT in transient mode.

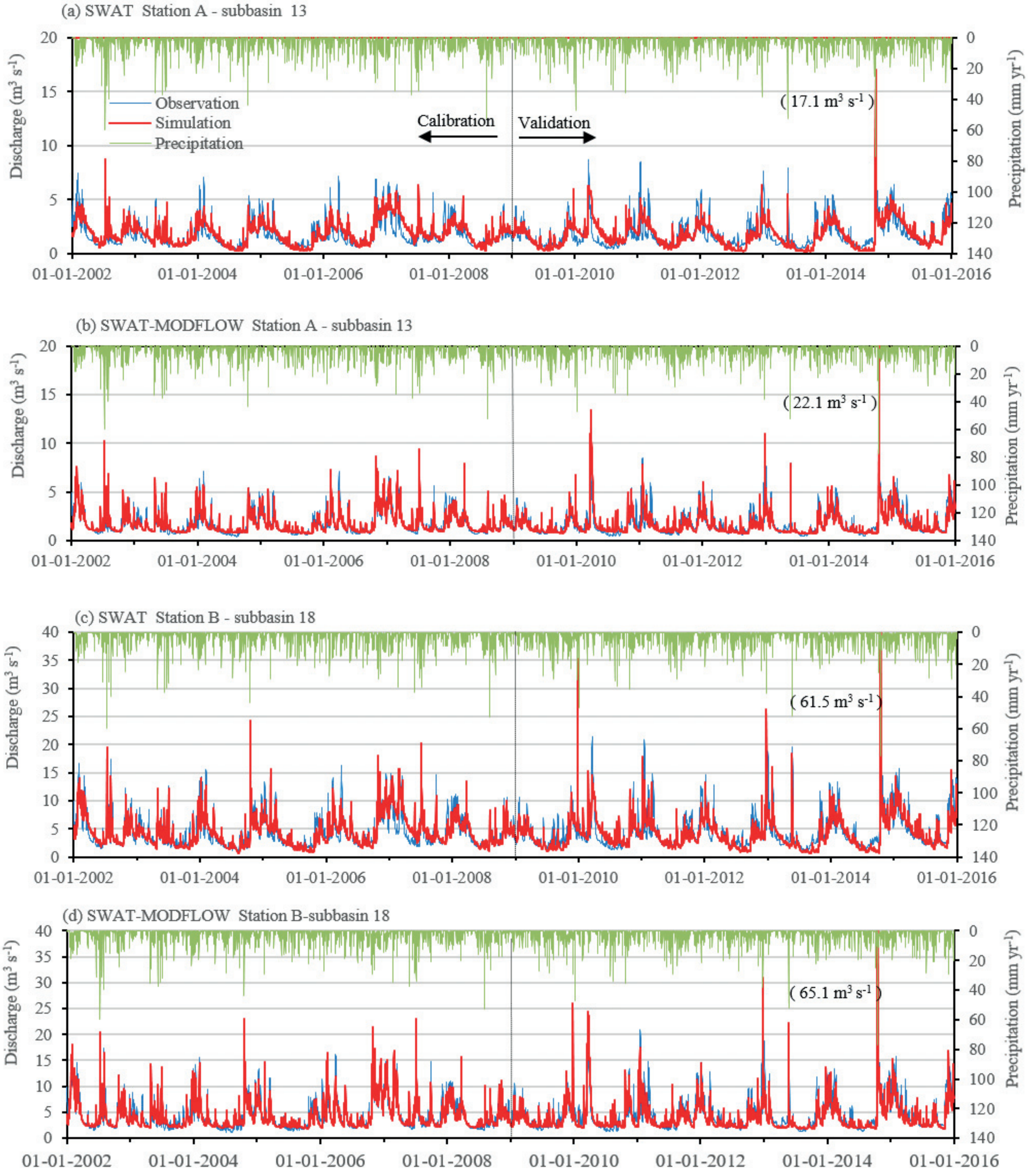


Figure 6. Hydrographs of precipitation, observed and best simulated daily streamflow at the outlets of subbasin 13 (station A) and subbasin 18 (station B) during the calibration period (2002-2008) and the validation period (2009-2015) based on SWAT and SWAT-MODFLOW. The value in bracket is the discharge on 16 October, 2014, which is outside the range of the plot area.

Table 5. Performance statistics indices for daily runoff at the outlets of subbasin 13 and subbasin 18 during the calibration (2001-2008) and validation (2009-2015, in brackets) periods by SWAT, SWAT-MODFLOW without PEST calibration, and SWAT-MODFLOW with PEST calibration.

Outlets	Used models	N_{SE}	R^2
Subbasin 13 outlet	SWAT	0.66 (0.50)	0.67 (0.53)
	SWAT-MODFLOW without PEST calibration	0.72 (0.51)	0.75 (0.60)
	SWAT-MODFLOW with PEST calibration	0.78 (0.54)	0.78 (0.61)
Subbasin 18 outlet	SWAT	0.74 (0.47)	0.74 (0.53)
	SWAT-MODFLOW without PEST calibration	0.77 (0.46)	0.79 (0.57)
	SWAT-MODFLOW with PEST calibration	0.81 (0.53)	0.82 (0.60)

Table 6. Summary statistics for the SWAT-MODFLOW calibration result.

Observation group	Number of observed data	Weight of observed data	Contribution to squared weighted residuals before calibration by PEST	Contribution to squared weighted residuals after calibration by PEST
Streamflow A	2557	2	4410.3	3479.7
Streamflow B	2557	1	4911.7	4025.3
Well A	570	1	113	154.9
Well B	961	1	946.6	908.6
Sum	6645	---	10381	8568.5

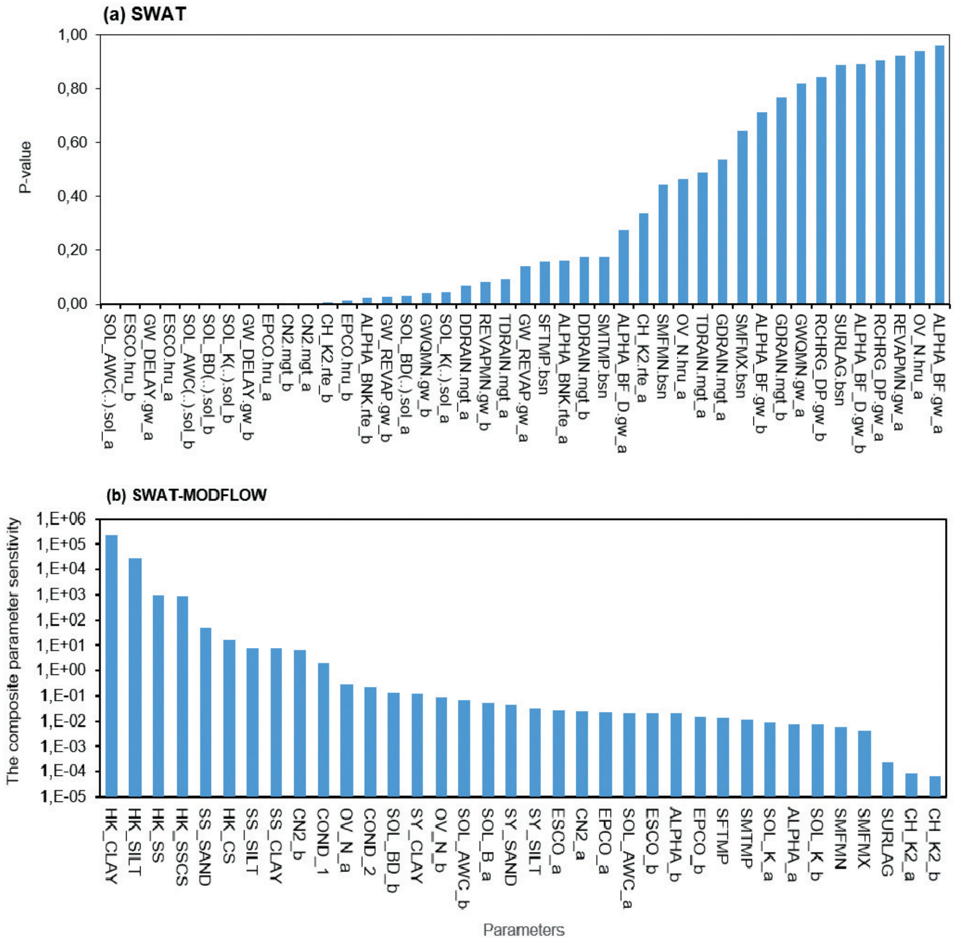


Figure 7. The sensitivity ranking of parameters in SWAT (a) and SWAT-MODFLOW (b) during calibration. The composite sensitivity of parameters was calculated based on the Jacobian matrix and the weight matrix after each PEST iteration and generated as an output once the PEST calibration was finished. The composite sensitivity values vary a little among the different iterations. The average value of each parameter among the 10 iterations for calibration is shown in the figure. More details regarding composite parameter sensitivity can be found in (Doherty, 2018). The "a" indicates that the parameter applies to the upstream areas, including subbasins: 4, 5, 7-13, and "b" indicates that the parameter applies to downstream areas, including subbasins 1, 3, 6, 14-19.

3.2 SWAT and SWAT-MODFLOW transient model performance

The SWAT and SWAT-MODFLOW models both represented well the streamflow hydrographs during the calibration period, while during the validation period, one high peak flow event occurred in the SWAT and SWAT-MODFLOW simulations but not in the observations (Fig. 6). The baseflow was generally reproduced well by both models, but the SWAT-MODFLOW visibly performed better.

Compared with the recommended evaluation criteria by (Moriasi et al., 2015), for NSE values, the performance was "very good" for SWAT-MODFLOW calibration at station B, "good" for SWAT-MODFLOW calibration at station A, "satisfactory" for SWAT calibration and SWAT-MOD-FLOW validation at both stations and SWAT validation at station A, but "unsatisfactory" for SWAT validation at station B. For R^2 values, the performance was "good" for SWAT-MODFLOW calibration, "satisfactory" for SWAT calibration and SWAT-MODFLOW validation, but "unsatisfactory" for SWAT validation.

The statistical performances of SWAT-MODFLOW with and without PEST calibration were compared. After calibration by PEST, the summary statistics of SWAT-MODFLOW were improved, especially for the validation period at station B where the performance increased from "unsatisfactory" to "satisfactory" according to NSE values (Table 5). In addition, the weighted residuals between simulation and observation were reduced after calibration by PEST, with the reduced residuals mainly coming from streamflow simulation (Table 6).

In SWAT, almost all the top 12 sensitive parameters (Fig. 7) were surface process parameters (Table 2) except for the groundwater parameter GW_DELAY. In contrast, for SWAT-MODFLOW (Table 3), all the top 12 sensitive parameters were groundwater parameters with the exclusion of only one surface process parameter OV_N.

Compared with SWAT, the SWAT-MODFLOW model not only produced output for streamflow but also for the groundwater table of each cell on any given day. The variation of groundwater heads across the simulation period was minimal for layer 1, while there was some, albeit small, variation in layer 3 (Fig. 8). There was generally a good agreement between the groundwater head level and dynamics simulated by SWAT-MODFLOW and that was recorded at the two observation wells within the catchment (Fig. 9).

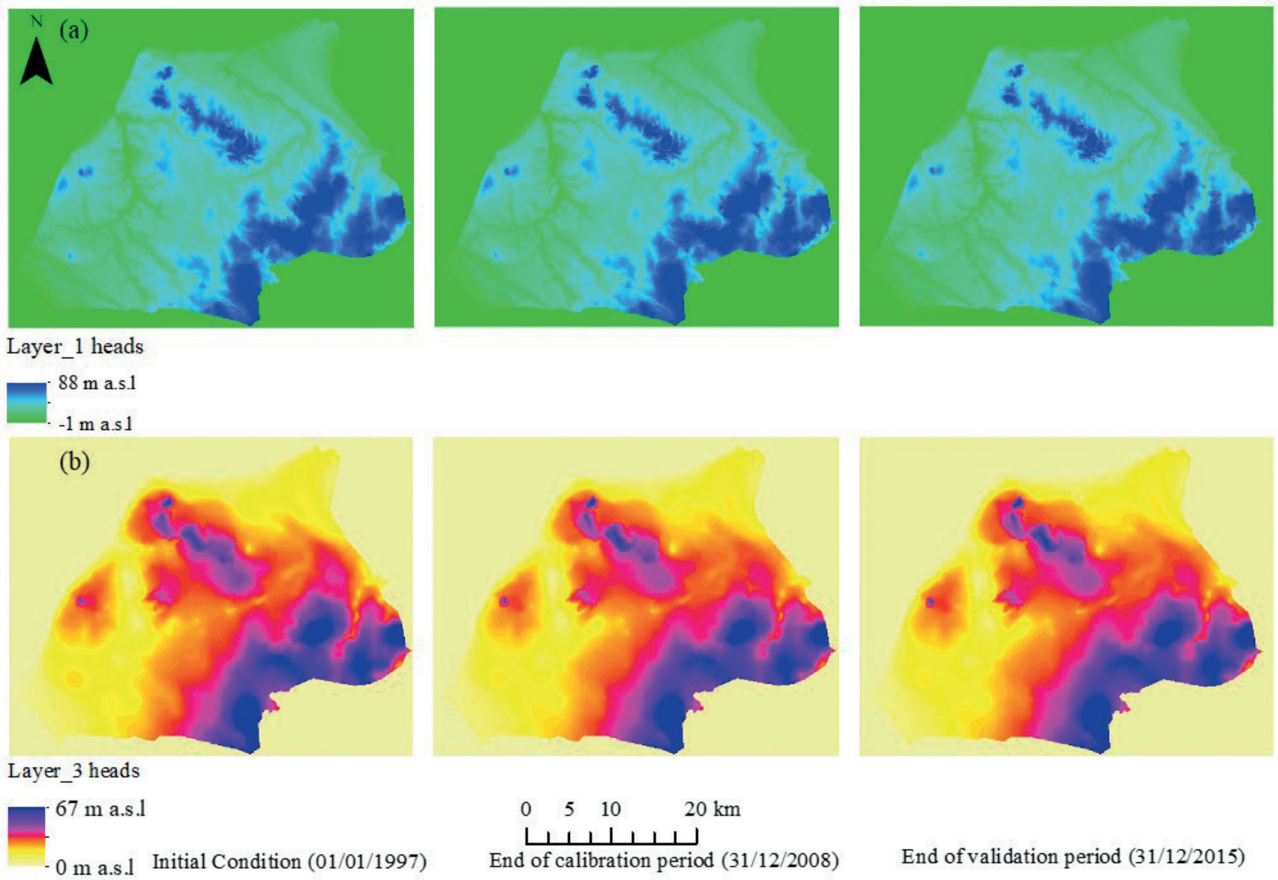


Figure 8. The simulated groundwater heads for the first layer (a) and third layer (b) at initial conditions, end of calibration period, and end of validation period by the calibrated SWAT-MODFLOW.

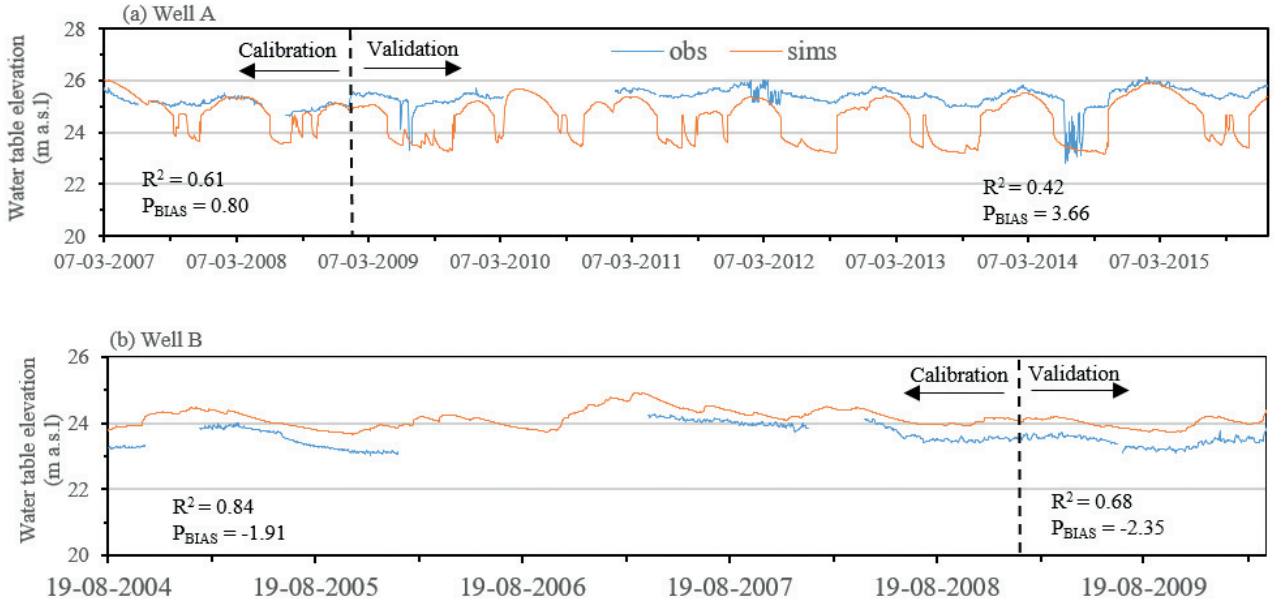


Figure 9. Hydrograph of daily simulated and observed groundwater heads (m a.s.l) of the two wells located in layer 1 used for calibrating the variation of groundwater heads simulated by SWAT-MODFLOW where relatively continuous observed data is available. Also shown are summary performance statistics.

Table 7. Average annual summary of the main components in the hydrological cycle of the Uggerby River Catchment during the study period (2002-2015) simulated by SWAT and SWAT-MODFLOW, respectively.

Components	SWAT	SWAT-MODFLOW
Precipitation (mm yr^{-1})	923	923
Surface flow (mm yr^{-1})	22	30
Lateral subsurface flow (mm yr^{-1})	89	64
Tile drain flow (mm yr^{-1})	20	0
Drain (MODFLOW, mm yr^{-1})	0	268
Groundwater flow (mm yr^{-1})	257	22
Total water yield (mm yr^{-1})	388	384
Actual evapotranspiration (mm yr^{-1})	503	516
Potential evapotranspiration (mm yr^{-1})	727	726
Soil storage (mm yr^{-1})	32	22
Average annual irrigation amount in the irrigated HRUs (mm yr^{-1})	137	133

For the water balance, the evaporation simulated by SWAT-MODFLOW was a little higher (13 mm yr^{-1}) than that simulated by SWAT, while the total water yields (total stream flow) simulated by SWAT and SWAT-MODFLOW were almost equal (Table 7). The water balance components, however, differed substantially. Compared with SWAT, the surface runoff simulated by SWAT-MODFLOW was a little higher, while the lateral subsurface flow and groundwater flow (simulated by the River Package) were much lower. In SWAT-MODFLOW, the largest contributor to streamflow was the drain flow simulated by the Drain Package (constituting 70% of the streamflow). Conceptually, however, this can also be viewed as a surface-near groundwater contribution. Hence, when lumping the contribution from drains and groundwater, these are clearly the dominant sources for streamflow in both the SWAT and SWAT-MODFLOW model.

3.3 Water abstraction scenarios simulation

The annual abstrations by drinking water wells or irrigation wells set up in the two models were approximately equivalent (Table 8). In the SWAT simulations, compared with the no-wells scenario (scenario 1), a decrease in the average annual stream flow was observed in scenario 2 (only drinking water wells), while an increase was recorded in scenario 3 (only irrigation wells) and scenario 4 (both drinking water and irrigation wells). In the SWAT-MODFLOW simulations, the average annual streamflow decreased not only in scenario 2, but also in scenario 4, and at subbasin 18 outlet in scenario 3, while a slight increase occurred at subbasin 13 outlet in scenario 3. The decrease in scenario 2 simulated by SWAT-MODFLOW was much larger than that by SWAT and also closer to the abstracted amount, and the increase

Table 8. Average annual stream flow change (2002-2015) at subbasin 13 outlet and subbasin 18 outlet for each abstraction scenario from no-wells scenario and the corresponding annual abstraction simulated in SWAT and SWAT-MODFLOW.

Scenarios		**Scenario 2 (Only drinking water wells)**		**Scenario 3 (Only irrigation wells)**		**Scenario 4 (Both drinking water and irrigation wells)**	
Model		**SWAT**	**SWAT-MODFLOW**	**SWAT**	**SWAT-MODFLOW**	**SWAT**	**SWAT-MODFLOW**
Average annual stream flow decrease(-) or increase(+) (106 m^3 yr^{-1})	Subbasin 13 outlet	-0.024	-1.10	0.61	0.24	0.59	-0.73
	Subbasin 18 outlet	-0.12	-2.53	1.60	-0.55	1.48	-1.79
Annual abstraction (106 m^3 yr^{-1})	Subbasins 4-5, 7-13	1.10	1.28	17.86	19.45	18.96	20.73
	The entire catchment excluding subbasin 19	4.01	3.96	40.54	39.26	44.55	43.22

Notes: Subbasin 13 outlet receives streamflow from subbasins 4-5, 7-13; Subbasin 18 outlet receives streamflow from the entire catchment excluding subbasin 19.

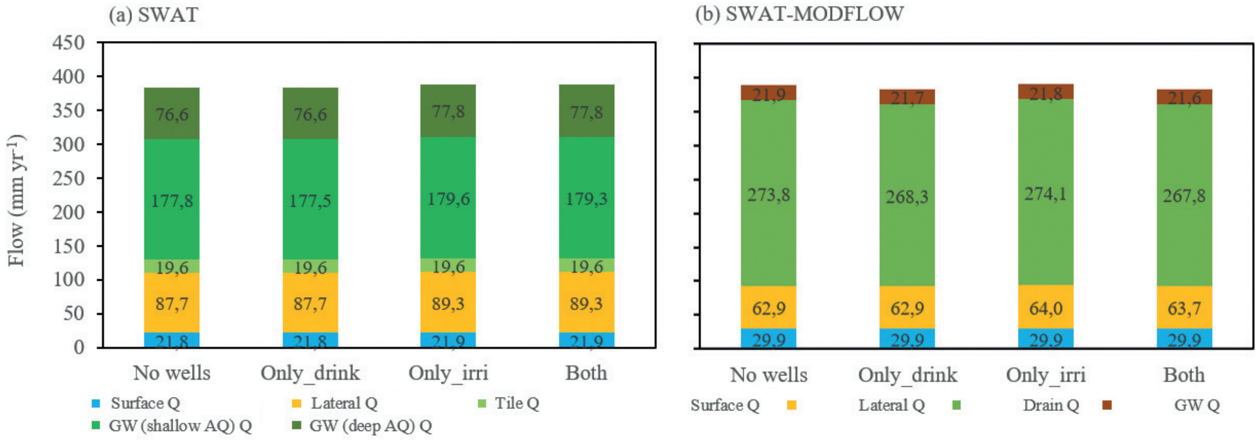


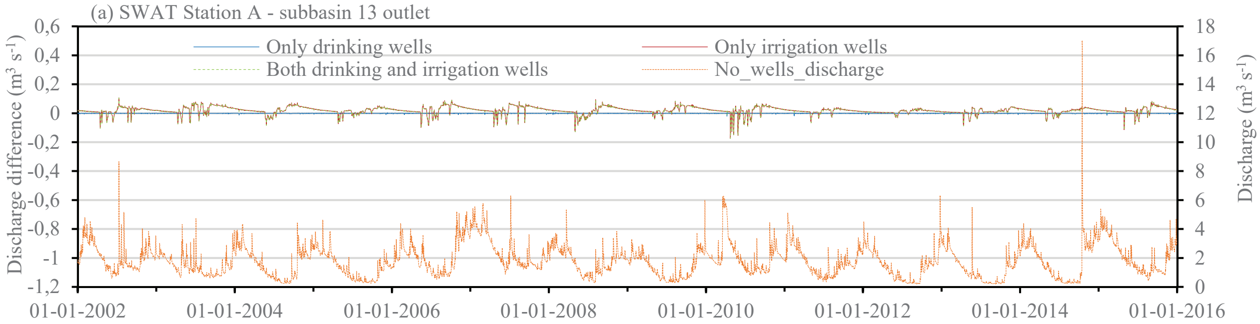
Figure 10. Average annual water yield (total flow) (2002-2015) simulated for the scenarios (no wells, scenario 1; only drinking water wells, scenario 2; only irrigation wells, scenario 3; both drinking water and irrigation wells, scenario 4) with SWAT (a) and SWAT-MODFLOW (b) and divided into flow components (Q = flow; GW = groundwater; AQ = aquifer).

at subbasin 13 outlet in scenario 3 simulated by SWAT-MODFLOW was apparently lower than that simulated by SWAT (Table 8).

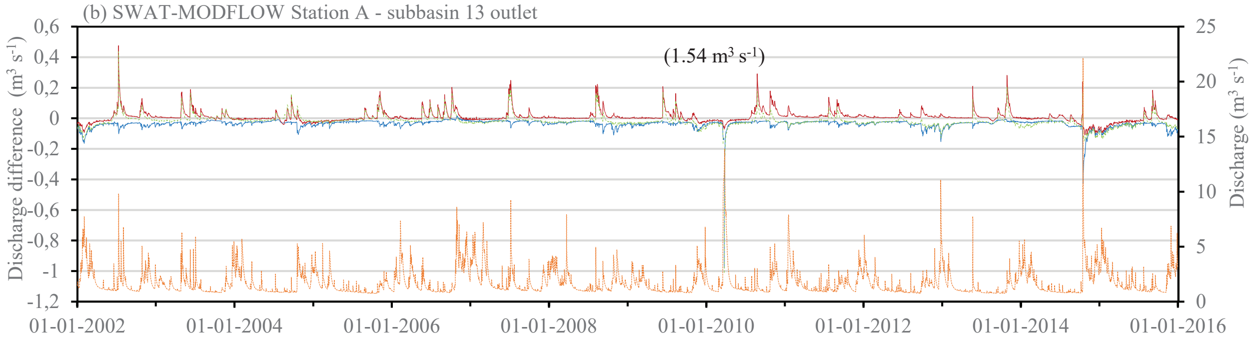
In SWAT, the decrease of average annual total flow in scenario 2 was minimal as a result of a tiny decrease in the groundwater return flow (Fig. 10a). In scenario 3 and scenario 4, with unchanged tile flow, all the other flow components rose, especially groundwater and lateral soil discharge. In SWAT-MODFLOW, the decrease of average annual total flow in scenario 2 also resulted from a decreased groundwater return flow, but the decrease was much larger than that simulated by SWAT. In scenario 3, the lateral soil runoff and drain flow increased in SWAT-MODFLOW similar to SWAT, while in scenario 4, reduced drain flow was recorded (Fig. 10b). Compared with the no-wells scenario, the amount of evapotransportation remained unchanged in scenario 2, whereas it increased by 5 mm yr^{-1} in the sceanarios with irrigation wells in both the SWAT and SWAT-MODFLOW simulations. In the scenario with only irrigation, evaportransportation and total flow increased in both the SWAT and SWAT-MODFLOW simulations, but the soil or aquifer water storage decreased according to the water balance.

When comparing the temporal patterns of streamflow with the no-wells scenario (scenario 1), we found the daily discharge difference in scenario 2 (only drinking water wells) to be almost always negative (sometimes zero), while in scenario 3 (only irrigation wells) and scenario 4 (both drinking water and irrigation wells) it fluctuated around zero in simulations by both SWAT and SWAT-MODFLOW (Fig. 11). Thus, the daily flow in the scenario with drinking water wells was almost always lower than the scenario without drinking water wells, and the daily flow in the scenario with only irrigation wells or the scenario with both irrigation and drinking

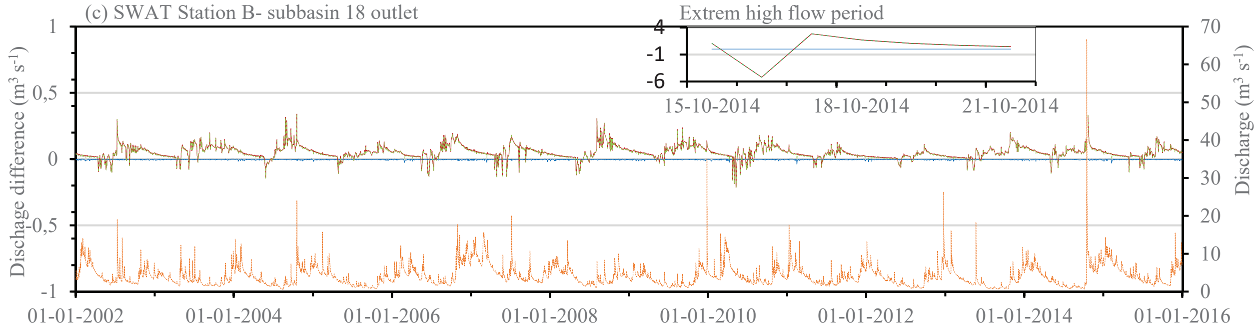
(a) SWAT Station A - subbasin 13 outlet



(b) SWAT-MODFLOW Station A - subbasin 13 outlet



(c) SWAT Station B- subbasin 18 outlet



(d) SWAT-MODFLOW Station B - subbasin 18 outlet

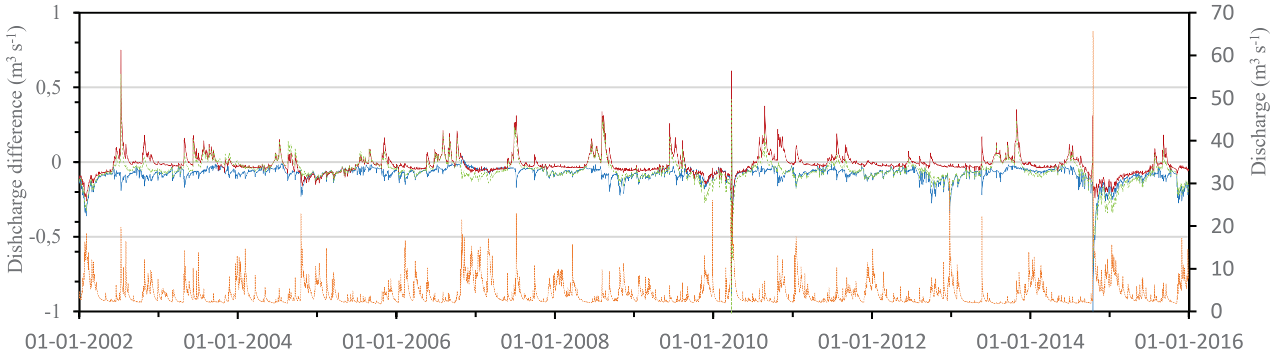
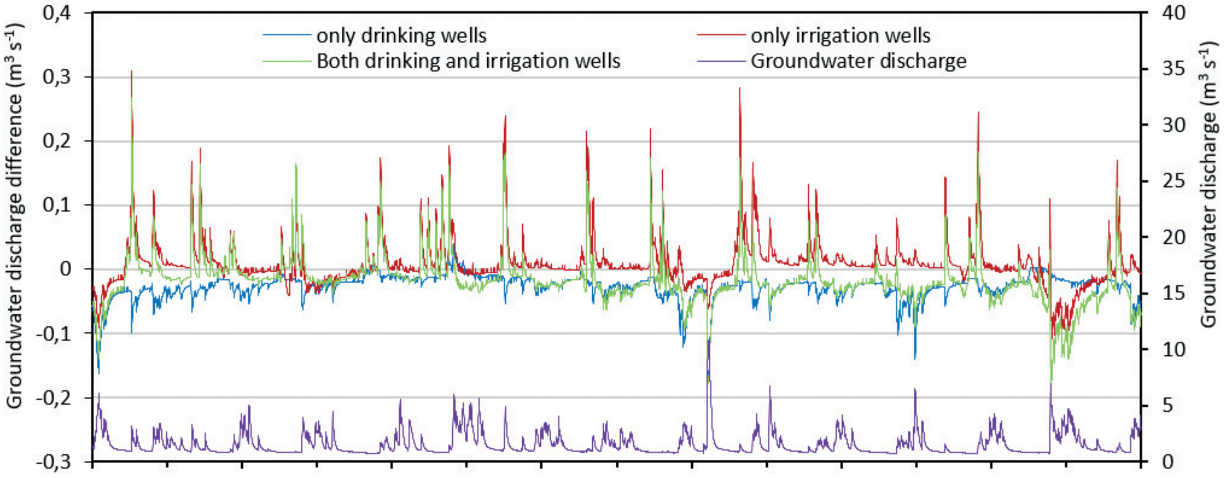
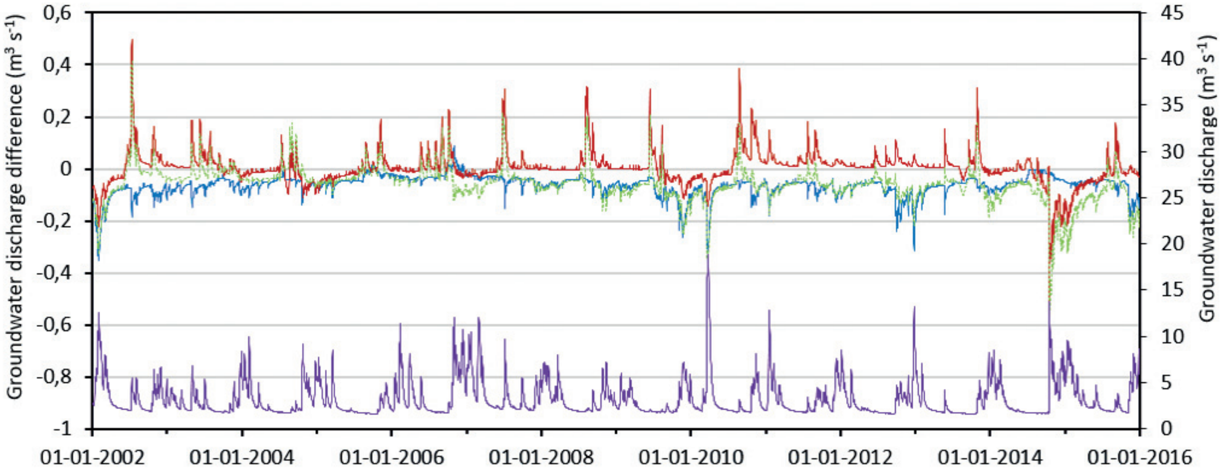


Figure 11. The simulated daily streamflow in the no-wells scenario and daily discharge differences between the abstraction scenarios (only drinking water wells, scenario 2; only irrigation wells, scenario 3; both drinking water and irrigation wells, scenario 4) and the no-wells scenario (scenario 1) at the outlets of subbasin 13 (station A) and subbasin 18 (station B) during the entire study period (2002-2015) based on SWAT and SWAT-MODFLOW, respectively. The value 1.54 $m^3 s^{-1}$ in brackets is the streamflow difference between the no-wells scenario and the scenario with only drinking water wells on 24 March, 2010, which is outside the range of the plot area.

water wells could be higher or lower than the scenario without wells. The daily discharge difference between scenario 2 and the no-wells scenario simulated by SWAT-MODFLOW was obvious, but the difference using SWAT was minimal. In the comparison of scenario 3 with the no-wells scenario, when the discharge difference was positive after an irrigation event, it descended smoothly in the SWAT simulation and more sharply in the SWAT-MODFLOW simulations.



(a) SWAT - MODFLOW Station A - subbasin 13 outlet



(b) SWAT - MODFLOW Station B - subbasin 18 outlet

Figure 12. The hydrograph of simulated daily groundwater discharge to the stream network in the no-wells scenario and daily groundwater discharge differences between the abstraction scenarios (only drinking water wells, scenario 2; only irrigation wells, scenario 3; both drinking water and irrigation wells, scenario 4) and the no-wells scenario (scenario 1) in the upstream area of station A (a) and upstream area of station B (b), respectively, during the entire study period (2002-2015), based on SWAT-MODFLOW.

In the SWAT-MODFLOW set-up, the water exchange between aquifer and streams occurs between each MODFLOW river/drain cell and its surrounding cells. The newly developed SWAT-MODFLOW model complex can output the daily rate of water exchange between aquifer and streams for each subbasin. When the water exchange is positive, it is indicative of water flow from the aquifer to the stream. The temporal pattern of groundwater discharge was the same as for the stream flow, and the temporal patterns of the differences in groundwater discharge between the abstraction scenarios and the no-wells scenario were similar to the differences in streamflow, except for some peak flow days (Fig. 12), which indicates that the abstraction-induced streamflow change followed the groundwater discharge change.

4 Discussion

4.1 Performance and parameter sensitivity of SWAT and SWAT-MODFLOW

Both the SWAT and SWAT-MODFLOW model simulated the temporal patterns of streamflow generally well at the two hydrological stations during the calibration and validation periods. However, visually SWAT-MODFLOW performed better, especially during recession curves and low flow periods, suggesting a better simulation of the interaction between surface water and groundwater. Accordingly, the corresponding summary performance statistics were also better for SWAT-MODFLOW. The simulated peak flow on 16 October 2014 by both models was much higher than the observed data (Fig. 6). This discrepancy may be attributed to a high record of precipitation on that day based on a 10 by 10 km grid, which may not be representative for the wider catchment. Additionally, it is also likely that the observed streamflow was underestimated as it is calculated from the Q-h relation, which typically does not adequately cover peak flow events (Poulsen, 2013).

In the parameter sensitivity analysis, the surface process parameters of the two models shared the same ranges, while the models had different groundwater modules and parameters. While the SWAT-MODFLOW calibration was based on an objective function that took into account not only streamflow but also groundwater heads at the location of two wells, the calibration by PEST mainly improved the streamflow simulation performance (Table 4). According to the parameter sensitivity ranking, the parameters regarding groundwater processes in SWAT-MODFLOW played an important role in the streamflow simulation performance, while in SWAT, the impact of groundwater module parameters on streamflow simulation was generally insignificant. This reflects the shortcoming of the SWAT groundwater module, which ignores the variability in distributed parameters such as hydraulic conductivity and storage coefficients, represents groundwater by a lumped module in individual subbasins, and contributes to the stream network as baseflow based on a linear reservoir approximation. With this simplified implementation of groundwater dynamics and water exchange between surface water and groundwater in SWAT, the discharge simulated by SWAT cannot be optimized to the same extent as that simulated by SWAT-MODFLOW.

The availability of spatial-temporal patterns of the groundwater head in SWAT-MODFLOW could significantly benefit groundwater resources management and provide yet another level of understanding of water resources dynamics within a catchment. The outputs of SWAT-MODFLOW in this study showed that the model performed well, not only in streamflow simulations but also with respect to the spatial-temporal patterns of the simulated groundwater head. In contrast, since no information of groundwater table output is provided by SWAT, its goodness in streamflow simulation may potentially be based on an improper groundwater simulation where its performance on groundwater simulation is unknown.

4.2 Models ability to simulate effects of groundwater abstractions on streamflow

In scenario 2 where only drinking water wells are active according to the water balance where there is no change in evaporation compared with the no-wells scenario, we expected that the streamflow depletion simulated by SWAT would be approximately equivalent to the abstracted water volume, taking into account a possible small change in the aquifer or soil storage. However, results in this study showed that the impact of drinking water abstractions on streamflow in the SWAT simulation was negligible. In the SWAT-MODFLOW set-up, because the aquifer in the Uggerby River Catchment is connected to and interactive with an area outside of the topographical catchment (Fig. 3), the abstraction from an aquifer located in the Uggerby River Catchment not only impacts the hydrology inside but potentially also outside the catchment. According to the water balance, we expected that the SWAT-MODFLOW simulated streamflow depletion in the catchment would be lower at a level somewhat equivalent to the abstracted water volume. With equivalent abstraction for drinking water, the annual flow decrease simulated by SWAT-MODFLOW was much larger than that by SWAT and closer to the abstracted volume. Therefore, we conclude that SWAT simulations underestimate the impacts of groundwater abstraction for drinking water on streamflow depletion, while SWAT-MODFLOW provided more realistic assessments.

The simulated irrigation operation abstracts water from an aquifer and then applies the water onto the surface of agricultural land or pasture. Most of the water infiltrates back into the soil and is then utilized by the vegetation and partly lost through evapotranspiration or infiltrates deeper to the aquifer, and a small part of the water might flow to streams directly as a small increase in surface runoff. Though the abstraction causes groundwater depletion, the recharge from the irrigated water can partly refill the aquifer and produce groundwater discharge. Since in the SWAT-MODFLOW set-up the aquifer in the Uggerby River Catchment was connected and interactive with an outside area, after each event of groundwater abstraction for irrigation, the aquifer storage would be recharged not only from the irrigated land area but also by the groundwater flowing from the outside area. If the recharge rate is larger than the abstracted water amount, the groundwater discharge to the stream will presumably increase. Hence, the irrigation events also brought about a slight increase of average annual stream flow at the subbasin 13 outlet (Table 8), and a slight total flow increase within the catchment (Fig. 10b). The subbasin aquifers in the SWAT set-up are closed and have no interaction with areas outside a subbasin. Meanwhile, the abstracted amount of water from aquifers for irrigation is larger than the amount of returning aquifer recharge from irrigated water, and we would therefore expect decreasing groundwater discharge to streamflow in SWAT simulations. However, the SWAT simulations also showed that irrigation led to enhanced streamflow (Table 8, Fig. 10a), which apparently was even higher than the increase simulated by SWAT-MODFLOW. This supports the point mentioned above that SWAT under-estimates the abstraction effect on streamflow depletion. SWAT simulations can, therefore, lead to incorrect assessments of the impacts of groundwater abstractions for irrigation on streamflow, while SWAT-MODFLOW provided more realistic assessments.

Upon inspecting the SWAT source code, it appears that the groundwater discharge calculation equation used in SWAT does not take into account the impact of water abstraction from shallow aquifers on water table fluctuations. Thus, the groundwater removal by abstractions in the SWAT simulation does not have a direct effect on the groundwater discharge, which may explain the somewhat surprising simulation signals of SWAT. In addition, in the equation, the groundwater discharge on the current day is highly related to the groundwater discharge on the previous day, and the increase of the groundwater discharge resulting from each irrigation application could then lead to enhanced groundwater discharge for several days in a row. This may explain why the increased discharge following an irrigation event descended more smoothly in SWAT than in SWAT-MODFLOW (Fig. 11).

In the SWAT-MODFLOW model, the exchange rate between groundwater and surface water is based on the head difference between the river stage (or drain cell stage) and the head of its surrounding groundwater grid cells. This can reflect the temporally dynamic hydrological processes and also the impacts from all the external stressors (e.g. temporally and spatially varying recharge and groundwater abstractions) on water table fluctuations. Naturally, this should also allow SWAT-MODFLOW to provide more realistic assessments of the impacts of groundwater abstractions on streamflow in comparison with SWAT.

While setting up the drinking water abstraction in SWAT, three limitations were identified, also reported in (Molina-Navarro et al., 2019). The first is that SWAT only allows one decimal point for abstraction numerical inputs with a unit of 104 m^3 day^{-1} for each month. This means that pumping rate variations within one month cannot be simulated by SWAT and that the accuracy of abstraction dynamics thus cannot be guaranteed. As a result of this limitation, the abstraction amount in SWAT and SWAT-MODFLOW was not completely identical. The second limitation is that the abstraction from deep aquifer did not result in any streamflow change. Therefore, all the abstraction sources had to be defined as the shallow aquifer in SWAT to achieve a signal in streamflow despite that we had at least three wells receiving water from a deep aquifer (the fifth layer according to the MODFLOW-NWT set-up). The last limitation is that the abstraction rates of all wells in each subbasin in SWAT have to be summed up to one input value, thereby ignoring the specific location of wells within individual subbasins.

SWAT-MODFLOW overcomes the limitations in SWAT by exploiting the spatial explicitness of MODFLOW where groundwater abstraction can be simulated using the Well Package, which allows many decimal points for abstraction inputs as well as user-defined units, pumping rates at potentially daily intervals, and wells located in any vertical layer and any grid cell within a subbasin. In addition to the outputs from SWAT, SWAT-MODFLOW also provides fully distributed groundwater-related outputs such as spatial-temporal patterns of water table elevation, distributed aquifer recharge, and groundwater-surface water exchange rates at a cell level, permitting detailed analysis of groundwater and its interaction with surface water. This may be an important input to groundwater resources management (e.g. groundwater abstraction) and the solving of surface water rights issues. These capabilities demonstrate the advantage of SWAT-MODFLOW over modifying the SWAT groundwater module codes to improve groundwater flow simulation (Nguyen and Dietrich, 2018; Pfannerstill et al., 2014; Zhang et al., 2016), which remains a semi-distributed way to simulate subsurface hydrologic processes and does not generate detailed groundwater outputs. This point supports the findings about the advantages of SWAT-MODFLOW over SWAT in (Molina-Navarro et al., 2019) but using a much more complex set-up.

4.3 Performance of SWAT-MODFLOW and SWAT relative to other recent studies

In previous studies, after coupling a calibrated SWAT and calibrated MODFLOW model, the SWAT-MODFLOW model complex was applied without further calibration (Bailey et al., 2016; Chunn et al., 2019), with calibration against only streamflow observations (Molina-Navarro et al., 2019), with separated calibration for streamflow and groundwater head (Guzman et al., 2015), or with simple manual calibration by graphically comparing the simulated and observed streamflow and groundwater head (Sith et al., 2019). Since both the SWAT and MODFLOW supporting software can use the inverse modeling (IM) method for calibration, and parameter non-uniqueness is an inherent property of IM (Abbaspour, 2015), the coupling of a calibrated SWAT and a calibrated MODFLOW cannot guarantee a proper or sufficiently optimized parameter set for the integrated SWAT-MODFLOW model. Because groundwater and surface water interact with each other, calibrating the simulation of one part does not guarantee proper simulation of the other part. Application of a combined calibration approach based on PEST allowed us to calibrate the SWAT-MODFLOW model by adjusting simultaneously SWAT and MODFLOW parameters and using observations of both streamflow and groundwater table when deriving the objective function. The calibration results demonstrated that the summary statistics of the SWAT-MODFLOW performance were improved by this approach (Table 6).

The ability of SWAT-MODFLOW to evaluate the impacts of groundwater abstraction on streamflow or groundwater-surface water interactions has been tested in the previous studies (Guzman et al., 2015; Chunn et al., 2019; Molina-Navarro et al., 2019). (Molina-Navarro et al., 2019), for example, also found that the SWAT model showed almost no impact of groundwater abstraction on streamflow depletion. Besides due to the simple representation of groundwater dynamics, the other cause of this, we believe, is that same as suggested above, that the impact of groundwater water removal by abstractions on water table fluctuations is currently not accounted for in the groundwater discharge calculation in the SWAT source code. Our findings are generally consistent with those of these previous studies, although all of the studies tested the effects of groundwater abstraction only by drinking water without considering irrigation and based on assumed drinking water pumping wells. In addition, in all the previous SWAT-MODFLOW studies, the River Package in the MODFLOW model was the only package used for simulating groundwater-surface water interaction, ignoring the potential drain flow processes. The SWAT-MODFLOW complex used in our study was further developed to allow application of the Drain Package and to allow also an auto-irrigation routine to extract water from groundwater grid cells; in this way the impacts of groundwater abstraction for both drinking water and irrigation could be assessed.

4.4 Limitations and future research

Several limitations to this study need to be acknowledged. The simulated head generated by the steady-state model was used as the initial head conditions for the transient model, as also suggested in other studies (Anderson et al., 2015; Doherty et al., 2010). The ideal simulated initial heads should be calibrated with the observed initial heads. However, we did not have enough observed heads at the beginning of the simulation period (1997), so we used the observed heads covering the period 1996-2010 for calibrating the original steady-state MODFLOW-NWT to obtain the simulated initial heads. Fortunately, the groundwater heads of the study area did not change much during the study period (Fig. 8, Fig. 9) and the difference inherently exists between the observed and simulated heads, indicating that the error between the ideal simulated initial heads and the actually used simulated initial heads was small.

An approach based on PEST was utilized to calibrate streamflow and groundwater table variation simultaneously in our SWAT-MODFLOW simulation, which improved the model performance and enabled parameter sensitivity analysis for the model. However, only two wells with relatively continuous time series of observed groundwater head were available and used to calibrate the groundwater variation. Ideally, calibration would involve more wells with continuous time series of observed head, but this limitation is anticipated to be minor in our study as the groundwater head did not change much in our simulations and the change mainly followed the variation of recharge with precipitation as its source.

The average annual streamflow difference and the regular pattern of daily streamflow difference between the abstraction scenarios and the no-wells scenario were generally explained well, but, surprisingly and unexpectedly, the streamflow difference between the scenario with only drinking water wells and the no-wells scenario on 24 March, 2010, simulated by SWAT-MODFLOW at two stations, were positive, being 1.54 and 0.55 m3 s-1, respectively (Fig. 11). The streamflow difference between the scenario with only irrigation wells and the no-wells scenario at station B on the extreme peak flow day (16 October, 2014) simulated by SWAT was -5.2 m3 s-1 but then became positive next day, which cannot be explained well to our best of knowledge so far. However, we found that the general results of this study were not influenced when modifying the value of these two unexpected points to be expected.

Both the SWAT and SWAT-MODFLOW simulations were based on the “best” parameter combination achieved through calibration, which was deemed to be satisfactory for the purpose of this study. However, complex models such as SWAT and SWAT-MODFLOW are subject to non-uniqueness (i.e. more than one parameter combination may yield satisfactory results), so future studies may need to consider the uncertainty due to, for example, parameter uncertainty. The calibration tool SWAT-CUP has already been able to evaluate SWAT parameter uncertainty, whereas the new approach based on PEST to calibrate SWAT-MODFLOW needs to be further explored to adapt for model uncertainty analysis.

Our results support our original hypothesis that SWAT-MODFLOW can produce more reliable results in the simulation of the effects of groundwater abstraction for either drinking water or irrigation on streamflow patterns. In addition, SWAT-MODFLOW can produce more outputs than SWAT. However, SWAT-MODFLOW also requires more effort and data to be set up and calibrated, and longer time to run (around 6 hours for a 19-year simulation in SWAT-MODFLOW by a desktop with an Intel® Core™ Processor i7-6700 CPU and 16 GB installed RAM versus 6 minutes for a SWAT simulation). Therefore, the balance between scientific accuracy and the computational burden should be defined relative to the study goal when choosing between SWAT and SWAT-MODFLOW in a future study. But clearly, if the purpose of a study is to investigate effects of groundwater abstraction on streams, the efforts should be focused on setting up and applying a fully-distributed model in groundwater domain, such as SWAT-MODFLOW. A graphical user interface has also been developed to couple SWAT and MODFLOW based on the publically available version of the SWAT-MODFLOW complex (Park et al., 2018). Since the SWAT-MODFLOW complex used in this study was newly developed and allowed use of the Drain Package and auto-irrigation, a new graphical user interface based on the new SWAT-MODFLOW complex could ensure that a study such as that presented here is repeated with less effort and technical challenges.

5 Conclusions

SWAT and SWAT-MODFLOW models with relatively complex set-ups were applied to a lowland catchment, the Uggerby River Catchment in Northern Denmark. Model performance and the outcome of four groundwater abstraction scenarios (with real wells and abstraction rates) were analyzed and compared.

Generally both models simulated well the temporal patterns of streamflow at the two hydrological stations during the calibration and validation periods. SWAT-MODFLOW, however, showed superior performance when visualizing time series results and when comparing summary statistics. Furthermore, SWAT-MODFLOW generates many additional outputs for groundwater analysis, such as spatial-temporal patterns of water table elevation and groundwater-surface water exchange rates at cell or subbasin level, improving water resources management in a groundwater-dominated catchment.

Abstraction scenarios simulated by SWAT and SWAT-MODFLOW showed different signals in streamflow change. The simulations by both models indicated that drinking water abstraction caused streamflow depletion and that irrigation abstraction caused a slight total flow increase (but decreased the soil or aquifer water storage, which may influence the hydrology outside the catchment). However, the impact of drinking water abstraction on streamflow depletion by SWAT was minimal and underestimated, and the streamflow increase caused by irrigation abstraction was exaggerated compared with the SWAT-MODFLOW simulation, which produced more realistic results.

Overall, the new SWAT-MODFLOW model calibrated by PEST, which included the Drain Package and a new auto-irrigation routine, presented a better hydrological simulation, wider possibilities for groundwater analysis, and more realistic assessments of the impact of groundwater abstractions (for either irrigation or drinking water purposes) on streamflow compared with SWAT. Thus, SWAT-MODFLOW can be used as a tool for managing water resources in groundwater-affected catchments, taking into account its higher computational demand and more time consumption.

5.4.1 Code and data availability

The land use map based on the Danish Area Information System is freely available from (https://www.dmu.dk/1_viden/2_miljoe-tilstand/3_samfund/ais/3_Metadata/metadata_en.htm). Climate data is available from the Danish Meteorological Institute (https://www.dmi.dk/). QGIS is freely available from https://qgis.org/en/site/. QSWAT, SWATCUP, and the SWAT-MODFLOW as well as its source codes are publicly available from https://swat.tamu.edu/software. The steady-state MODFLOW set-up was provided by NIRAS upon request. The PEST utilities and tutorial are freely downloadable from http://www.pesthomepage.org/Home.php. The source code, executable, and tutorial for the further developed SWAT-MODFLOW are available on the SWAT website (https://swat.tamu.edu/software/swat-modflow/). The two code files used for SWAT-MODFLOW calibration by PEST will be available through repository on https://www.re3data.org/ when the paper is accepted.

Author contributions. DT and WL designed the study. WL undertook all practical elements of the study, including setting up and calibrating the models, analyzing results, producing figures, and writing the manuscript. SP and RTB contributed the idea and developed the codes for use of the PEST approach to calibrate the SWAT-MODFLOW model. RTB provided the knowledge to set up SWAT-MODFLOW and further developed the SWAT-MODFLOW complex codes. DT, EMN, HEA, HT, and AN provided most of the data and contributed with their knowledge to setting up and calibrating the models. DT and EJ helped to analyze the results and contributed to the discussion. JSJ and JBJ provided the original steady-state MODFLOW-NWT set-up and contributed with relative knowledge. All co-authors contributed to the manuscript writing.

Competing interests. The authors declare that they have no conflict of interest.

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MANUSCRIPT 2

ASSESSING THE IMPACTS OF GROUNDWATER ABSTRACTIONS ON FLOW REGIME AND STREAM BIOTA: COMBINING SWAT-MODFLOW WITH FLOW-BIOTA EMPIRICAL MODELS

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Abstract

Assessing the impacts of groundwater abstractions on stream ecosystems is crucial for developing water planning and regulations in lowland areas that are highly dependent on groundwater, such as Denmark. To assess the effects of groundwater abstractions on flow regime and stream biota in a lowland groundwater-dominant catchment, we combined the SWAT-MODFLOW model with flow-biota empirical models including indices for three key biological taxonomic identities (fish, macroinvertebrates, and macrophytes). We assessed the effects of the current level of abstractions and also ran a scenario for assessing the effect of extreme groundwater abstractions (pumping rates of the drinking water wells were increased by 20 times in one subbasin of the catchment). Three subbasin outlets representing stream segments of different sizes were used for this evaluation. Current groundwater abstraction level had only minor impacts on the flow regime and stream biotic indices at the three subbasin outlets. The extreme abstractions, however, led to significant impacts on the small stream but had comparatively minor effects on the larger streams. The fish index responded most negatively to the groundwater abstractions, followed by the macrophyte index, decreasing, respectively, by 23.5% and 11.2% in the small stream in the extreme groundwater abstraction scenario. No apparent impact was found on macroinvertebrate index as in any of the three subbasin outlets. We conclude that this novel ap-proach of a combined modelling system is a useful tool to quantitatively assess the effects of ground-water abstractions on stream biota and thereby support water planning and regulations related to groundwater abstractions. We highlight the need for developing improved biotic models that target specifically small headwater streams, which are often most affected by water abstraction.

Key words: SWAT-MODFLOW; SWAT; Flow regime; Groundwater abstraction; Ecology quality; Stream biota; Flow-biota empirical models.

1 Introduction

The flow regime, i.e. the temporal pattern of stream and river flow, has been shown to be the key driver of river ecosystems as it fundamentally controls many physical processes (e.g. the movement of water and sediment within the channel) that have a major influence on the biotic composition and dictates the evolutionary adaptations and viability of many river biota (Bunn and Arthington, 2002; Carlisle et al., 2011). Because the flow regime is critical in shaping stream or river habitats, streamflow alterations due to anthropogenic activities, such as dam operations (Tonkin et al., 2018), water withdrawals (Arroita et al., 2017), land-use activities (Stein et al., 2017), and inter-basin water transfers (Petts, 2018), can heavily impact the structure and function of riverine ecosystems.

Formulating flow regime alteration-ecological response is a critical step in using ecological indicators to develop environmental flow standards at the regional scale (Poff et al., 2010). A number of studies have endeavored to develop relationships between flow regime and ecological integrity. In general, five critical components of the flow regime (magnitude, frequency, timing, duration, and rate of change) have been used to characterize flow alteration (Poff et al., 1997). Taxonomic identity (e.g., macroinvertebrates, fish, and macrophytes) and type of response (abundance, diversity, demographic parameters, and ecological quality ratio) are often used to characterize ecological responses (Poff and Zimmerman, 2010). The links between flow regime alteration and ecological response developed in previous studies have shown different degrees of success and serviceability (Poff and Zimmerman, 2010; Belmar et al., 2013). Most of these studies reported relationships at specific stream segments or watershed scale and have often focused on only one taxonomic identity (Kennen et al., 2009; Stromberg et al., 2010; Falke et al., 2011; Domisch et al., 2017; Perkin et al., 2017).

Since groundwater aquifers contain about 30% of the global freshwaters (Shiklomanov, 1998), groundwater abstractions from aquifers are a prevalent activity all over the world. Abstractions are rapidly increasing worldwide as a result of escalating demands of water use for irrigation, household, indus-try, and recreation (Foster et al., 2013; Wada et al., 2014). However, groundwater abstraction can cause a decline of the groundwater table and thereby directly alter the flow regime of streams connected to the aquifer. Ample literatures describing quantitative assessments of the ef-fects of water withdrawals from streams on stream eco-system have been published (Arroita et al., 2017; Bene-jam et al., 2010; Carolli et al., 2017; Pardo and Garcia, 2016), but only few studies have attempted to assess the effects of groundwater abstraction on stream ecosystems (Falke et al., 2011; Perkin et al., 2017), partly because it has been difficult to assess the effects of groundwater abstraction on flow regime.

SWAT-MODFLOW developed by Bailey et al. (2016) is a comprehensive coupled watershed model that combines the Soil and Water Assessment Tool (SWAT) (Neitsch et al., 2011), simulating the land surface and stream hydrologic processes, and MODFLOW-NWT (Niswonger et al., 2011), simulating the groundwater hydrologic processes and groundwater-surface water exchange. Since the model complex in the groundwater domain is fully distributed and accounts for two-way interactions between groundwater and surface waters, it enables a potentially better representation of hydrological dynamics relative to other hydrological models, such as the lumped semi-distributed SWAT model alone. The ability of SWAT-MODFLOW to evaluate the impacts of groundwater abstraction on streamflow or groundwater-surface water interactions has been tested in several studies (Guzman et al., 2015; Chunn et al., 2019; Molina-Navarro et al., 2019) and has been observed to produce more realistic results in terms of groundwater abstraction effects on streamflow than the widely used catchment model SWAT (Liu et al., 2019; Molina-Navarro et al., 2019).

The water consumption in Denmark comes almost entirely from groundwater abstractions (Jørgensen and Stockmarr, 2009). To provide a sufficient and persistent flow to support in-stream biota, Denmark has endeavored to regulate groundwater abstraction to a certain threshold level, mainly through a system of licenses. Nevertheless, there are still some areas where groundwater exploitation is above the sustainable yield and causes relatively severe streamflow depletion, which may impair the stream ecosystem (Henriksen et al., 2008). Therefore, quantitative assessment of the impact of pumping wells on streamflow and the ecosystems they support now and under potential abstraction and future climate scenarios is imperative for maintaining the integrity of stream ecosystems.

In this study, we take an integrated approach that we combine the SWAT-MODFLOW model with novel nationwide-scale flow-biota empirical models (Gräber et al., 2015) describing key biological taxonomic identities (fish, macroinvertebrates, and macrophytes) to quantitatively assess the effects of groundwater abstraction on stream ecology qualities. Results can therefore help guide management of water abstraction. We used a Danish, lowland, groundwater-dominated catchment, the Uggerby River Catchment, as a case study and assessed to what extent the flow regime and key biota in stream segments of different sizes may be altered by the present level of groundwater abstraction and in a scenario with extreme groundwater abstraction.

2 Methods

2.1 Study area

The Uggerby River Catchment, located in the northernmost part of Jutland (Fig. 1) in Denmark, drains an area of 357 km² and has an elevation ranging from - 0.2 m to 108 m. The catchment is administratively covered by the Municipality of Hjørring, which has an area of 930 km². A SWAT-MODFLOW model for the Uggerby River Catchment was set up with data for the period 2002 to 2015 (Liu et al., 2019). During this period, the annual mean temperature was 8 °C, July being the warmest month (17 °C average) and January the coldest (0.5 °C average). The average annual precipitation was approximately 933 mm with no pronounced seasonality. The dominant land use is agriculture (63 %) and the dominant soil type is loamy sand (51 %) (NERI, 2000).

There are 101 drinking water pumping wells registered in the municipality (Hjørring Municipality, 2009) (Fig. 1). The wastewater treatment plant in Sindal, located in subbasin 16 of the SWAT model delineation, is the only significant point source in the Uggerby River Catchment. Based on the data available for the period 2007-2010, the average daily wastewater discharge to the stream is 2769 m³, including a few minor sources. Like many catchments in Denmark, the Uggerby River is to a large extent groundwater-fed. Direct abstraction from surface water is prohibited and groundwater abstraction is only allowed with a permit license.

2.2 SWAT-MODFLOW model

We used the SWAT-MODFLOW model set-up from Liu et al. (2019) as the basis for our study. It represents a SWAT model for the Uggerby River Catchment, fully coupled with a MODFLOW-NWT model for the entire Hjørring Municipality. Although the MODFLOW model encompassed the entire municipality, only the portion covered by the Uggerby River Catchment was coupled with the SWAT model, and the original functionality of MODFLOW was retained beyond the Uggerby River Catchment.

In the SWAT set-up, the Uggerby River Catchment was divided into 19 subbasins and discretized into 2620 individual Hydrological Response Units (HRUs) (Fig. 1). The daily streamflows of two hydrologically connected monitoring stations, located at the outlet of subbasin 13

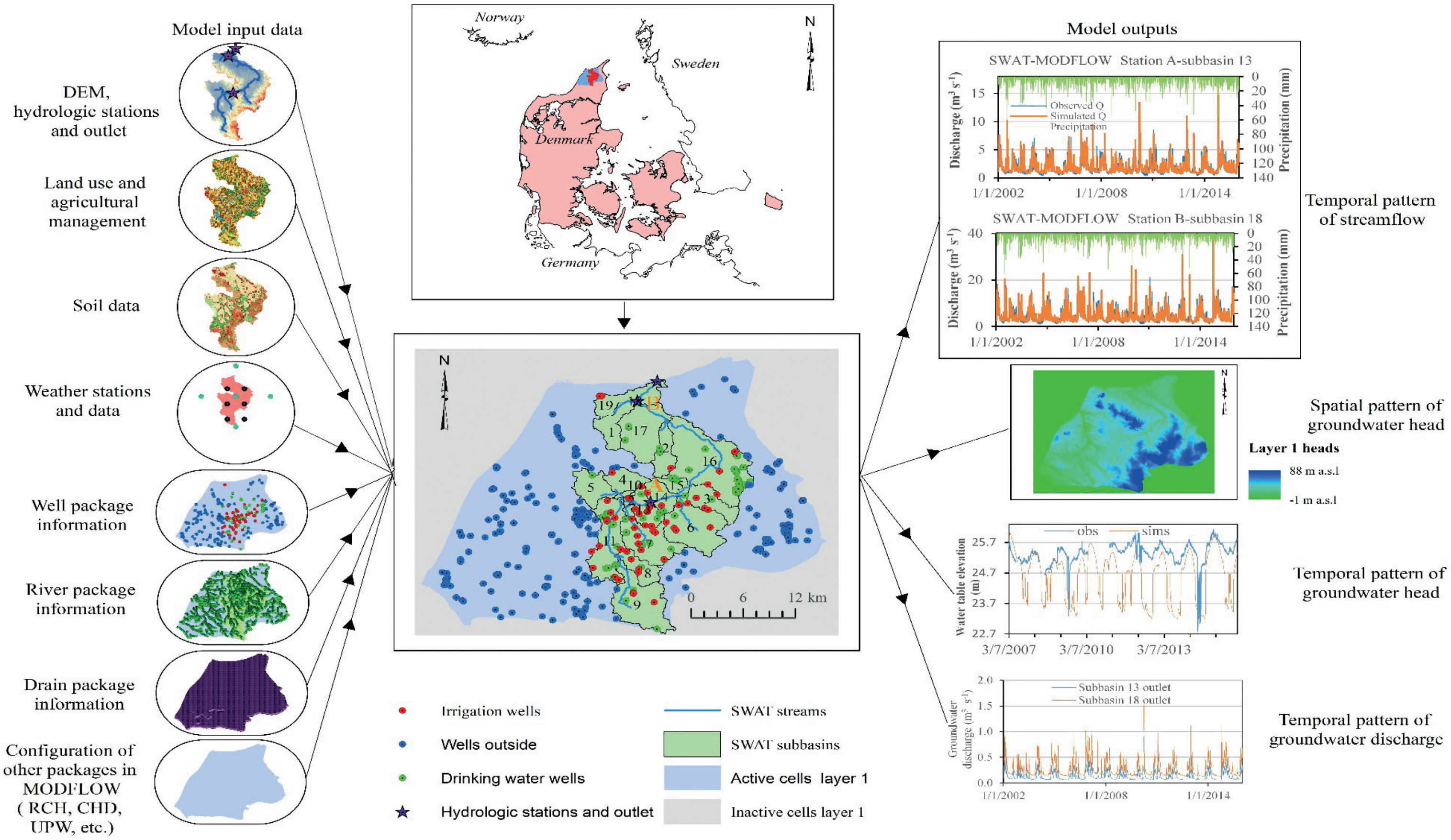


Figure 1. Input and output data of the SWAT-MODFLOW model set-up for the Uggerby River Catchment. Location of the catchment is also shown. (The figure will be rotated to be shown clearly).

Table 1. Average annual abstraction (2002-2015) for each scenario in the areas from which the outlets of subbasin 7, 13, and 18 receive water and the corresponding annual stream flow change from the baseline scenario simulated in SWAT-MODFLOW set-up.

Scenarios		No drinking water wells	Baseline scenario	Extreme abstraction in subbasin 7
Annual abstraction (106 m^3 yr^{-1})	Subbasin 7	0	0.38	7.71 (0.38+7.33)
	Subbasins 4-5, 7-13	0	1.28	8.61 (1.28+7.33)
	The entire catchment excl. subbasin 19	0	3.96	11.29 (3.96+7.33)
Average annual stream flow decrease (-) or increase (+) (106 m^3 yr^{-1})	Subbasin 7 outlet	0.28 (3.1 %)	9.1 (baseline)	-3.04 (-33.4 %)
	Subbasin 13 outlet	0.97 (1.7 %)	54.34 (baseline)	-5.16 (9.5 %)
	Subbasin 18 outlet	1.25 (1 %)	131.7 (baseline)	-5.78 (- 4.4%)

Notes: Subbasin 7 outlet receives water from subbasin 7; Subbasin 13 outlet receives streamflow from subbasins 4-5, 7-13; Subbasin 18 outlet receives streamflow from the entire catchment excluding subbasin 19.

(station A) and subbasin 18 (station B), were used for calibration (period: 2002-2008) and validation (period: 2009-2015) of the SWAT model. Generally, the model demonstrated satisfactory performance on the temporal pattern of streamflow simulation (Liu et al., 2019). Further details on the SWAT set-up can be found in (Liu et al., 2019).

The original MODFLOW model set-up for the entire Hjørring Municipality was configured as a steady-state MODFLOW-NWT model that serves as a basis for water resources management by the Hjørring municipality. Aquifers were conceptually represented by 5 hydro-stratigraphic layers, the uppermost layer being unconfined and the other four confined. Each layer was discretized into grids having a cell-size of 100 m × 100 m. Both the river package (RIV) and the drain package (DRN) were employed in the model to simulate groundwater-surface water exchange. The model was calibrated using 1,063 head observations during the period 1996-2010 at 1, 006 wells distributed at the first, third, and fifth layer by a combination of manual calibration and auto-calibration using the PEST software (http://www.pesthomepage.org/). For facilitating SWAT-MODFLOW coupling and its calibration, the specific aquifer hydraulic conductivities were reclassified and grouped into five groups, and the MODFLOW model was converted from steady state into transient state by assigning storage coefficients (specific storage, specific yield) to each MODFLOW grid cell.

SWAT and MODFLOW were combined using the coupling framework by Bailey et al. (2016), but with further developments to enable the application of the Drain package and an auto-irrigation routine. Groundwater outflow simulated by the Drain package was fed to SWAT subbasin channels, and SWAT auto-irrigation depths dictated groundwater pumping using MODFLOW's Well package (Liu et al., 2019). The coupled SWAT-MODFLOW set-up was then calibrated through a PEST-based approach by calibrating SWAT and MODFLOW parameters simultaneously with both stream flow and groundwater levels as the objective observations. The calibrated SWAT-MODFLOW set-up demonstrated a good performance in hydrological simulation and provided more realistic outputs when assessing the impacts of groundwater abstraction for drinking water and irrigation on stream flow than the stand-alone SWAT (see (Liu et al., 2019) for further calibration and validation details).

2.3 Groundwater abstraction scenarios

In order to evaluate the impacts of groundwater abstraction on streamflow and biota in streams of different sizes, three scenarios were set up and analyzed: 1) Baseline scenario, where all the wells in the calibrated SWAT-MODFLOW were maintained, reflecting the current state. 2) No drinking water wells scenario, where all the drinking water wells in the Uggerby River Catchment were terminated. The wastewater point source was also terminated as we are simulating absence of people in the catchment; 3) Extreme abstraction scenario, where the pumping rates of all the drinking water wells in an upstream subbasin (subbasin 7) with an independent reach receiving no water from other subbasins (Fig. 1) were increased by a factor of 20 (Table 1). In the extreme abstraction scenario, we assumed that the extra water was due to the establishment of a new bottled water company and the bottled water was transported outside the catchment instead of being used locally and therefore not returned to the stream. In all the scenarios, the irrigation wells and their pumping rates remained unchanged.

2.4 The flow-biota empirical models

The flow-biota empirical models refer to the empirical relationships between flow regime variables (e.g. Q90, the flow below the 90th percentile of the flow-duration curve) and the ecological quality ratio (EQR, ranging from 0 to 1 with 0 being the worst condition and 1 being the reference condition) of DFFVa (fish index), DVPI (macrophytes index), and DVFI (macroinvertebrate index) according to (Gräber et al., 2015).

Table 2. Calculation of sinuosity classes based on class borders.

Class	Description	Class borders
1	Straight/channelized	Sin < 1.05
2	Slightly sinuous	1.05 < Sin < 1.25
3	Sinuous	1.25 < Sin < 1.50
4	Meandering	Sin > 1.50

Notes: Sin is the sinuosity index, calculated from the stream length divided by linear distance. The Sin was calculated for all the reaches within each subbasin. The stream length within each subbasin was available from main channel input file (.rte) of SWAT (Arnold et al., 2013). The linear distance of the stream within each subbasin was measured using QGIS.

For DFFVa, the model with three flow regime variables was developed based on a dataset of 61 sites and with an R^2 of 0.53 ($p < 0.001$):

$$\mathrm{DFFVa}_{\mathrm{EQR}} = 0.811{*}\mathrm{BFI} + 0.058{*}\mathrm{Sin} + 0.050{*}\mathrm{Fre}_{25} - 0.319 - 0.0413{*}\mathrm{Fre}_{75} \qquad (1)$$

where BFI is the baseflow index (baseflow volume divided by total flow volume), Sin is the class of sinuosity (Table 2), Fre_{25} is the average annual frequency of events with flows above the 25th percentile from the flow duration curve, and Fre_{75} is the average annual frequency of events with flows below the 75th percentile from the flow duration curve.

For DVPI, the model with three flow regime variables was developed based on a dataset of 91 sites and with an R^2 of 0.34 ($p < 0.001$):

$$\mathrm{DVPI}_{\mathrm{EQR}} = 0.546 + 0.020{*}\mathrm{Fre}_{25} - 0.019{*}\mathrm{Dur}_{3} - 0.025{*}\mathrm{Fre}_{75} \qquad (2)$$

where Dur_3 is the average annual duration (days) of flows 3 times the median flow. Fre_{25} and Fre_{75} are the same as in equation (1).

For DVFI, the model with two flow regime variables was developed based on a dataset from 122 stream sites in Denmark and with an R^2 of 0.44 ($p < 0.001$):

$$\mathrm{DVFI}_{\mathrm{EQR}} = 0.217 + 0.103{*}\mathrm{Sin} + 0.020{*}Q_{90}{*}\mathrm{Fre}_{1} \qquad (3)$$

where Q_{90} is the flow below the 90th percentile of the flow-duration curve, divided (standardized) by median flow (Q_{50}), and Fre_1 is the average annual frequency of events with flows above the median flow. Sin is the same as in equation (1).

Scripts for deriving the flow regime variables and biota indices (EQR values) were created and run through SAS 9.4 (www.sas.com/) with the SWAT-MODFLOW streamflow output file output.rch as the imported data.

3 Results

3.1 The impacts of groundwater abstractions on streamflow

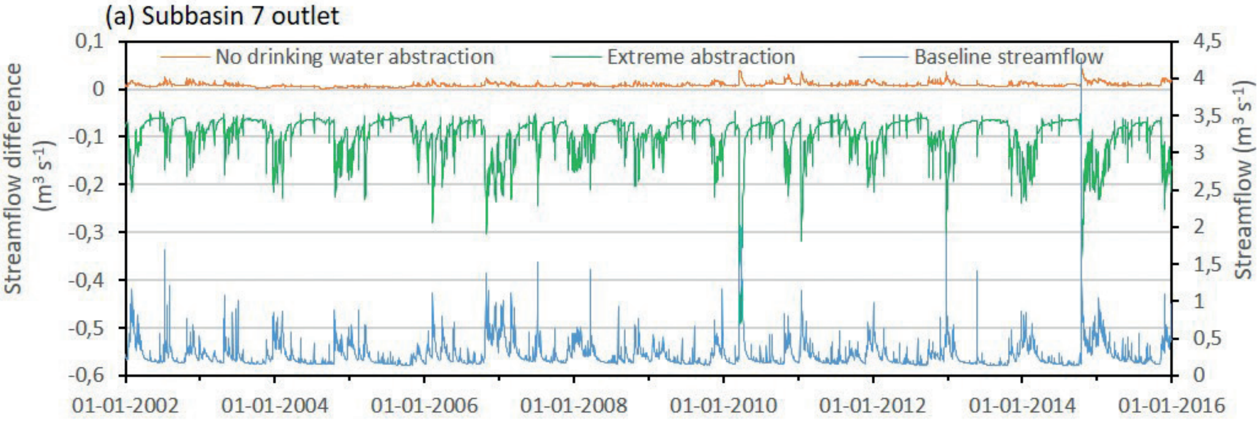
Simulated average daily flow at the outlets of subbasin 7, 13, and 18 during the study period (2002-2015) was 0.29, 1.72, and 4.17 $m^3\ s^{-1}$, respectively, representing a small, medium-sized, and relatively large stream in Denmark.

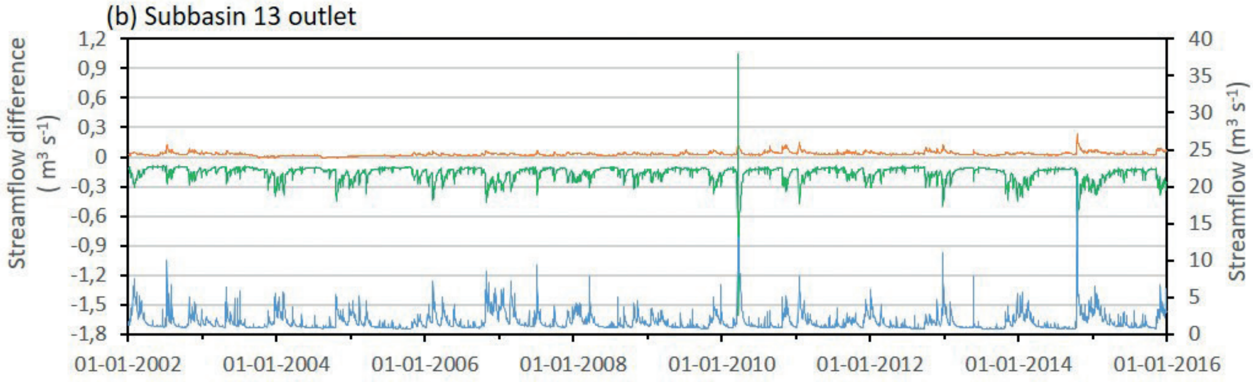
The temporal patterns of streamflow in the three stream segments in the different scenarios were compared (Fig. 2). The streamflow difference between the scenario with no drinking water abstraction and the baseline scenario was almost always greater than or equal to 0, indicating a daily streamflow decrease caused by the current groundwater abstraction. The absolute difference was generally largest for subbasin 18, and the average differences were 0.009 $m^3\ s^{-1}$ (subbasin 7), 0.031 $m^3\ s^{-1}$ (subbasin 13), and 0.039 $m^3\ s^{-1}$ (subbasin 18). The streamflow difference between the extreme abstraction scenario and the baseline scenario was almost always negative except for one day at the subbasin 13 outlet and two days at the subbasin 18 outlet, indicating a daily streamflow decrease due to an extreme abstraction situation. Again, the decrease was almost always largest at the subbasin 18 outlet and average values of decrease at the three subbasin outlets were 0.096 $m^3\ s^{-1}$ (subbasin 7), 0.164 $m^3\ s^{-1}$ (subbasin 13), and 0.183 $m^3\ s^{-1}$ (subbasin 18). Average annual stream flow change from baseline scenario was also largest at the subbasin 18 outlet out of the three outlets for both the no drinking water wells scenario and the extreme abstraction scenario, but the stream flow change percentage at the subbasin 18 outlet was smallest compared with the baseline streamflow (Table 1).

3.2 The impacts of groundwater abstractions on groundwater discharge to streams

According to the water balance output of the SWAT-MODFLOW set-up, groundwater discharge constitutes 75% of the streamflow in the baseline scenario, highlighting the benefit of assessing groundwater discharge change in groundwater abstraction scenarios.

The average daily groundwater discharge in all subbasins in the scenario with no drinking water abstraction was higher than in the baseline scenario with different extents, demonstrating the subbasin-level spatially varying impacts of the current level of drinking water abstraction on the groundwater discharge to streams (Fig. 3a, 3b). The average difference in the groundwater contribution to the streamflow was 327 $m^3\ day^{-1}$ for the entire catchment, while the maximum difference was 1684 $m^3\ day^{-1}$ in subbasin 16 and the minimum differ-





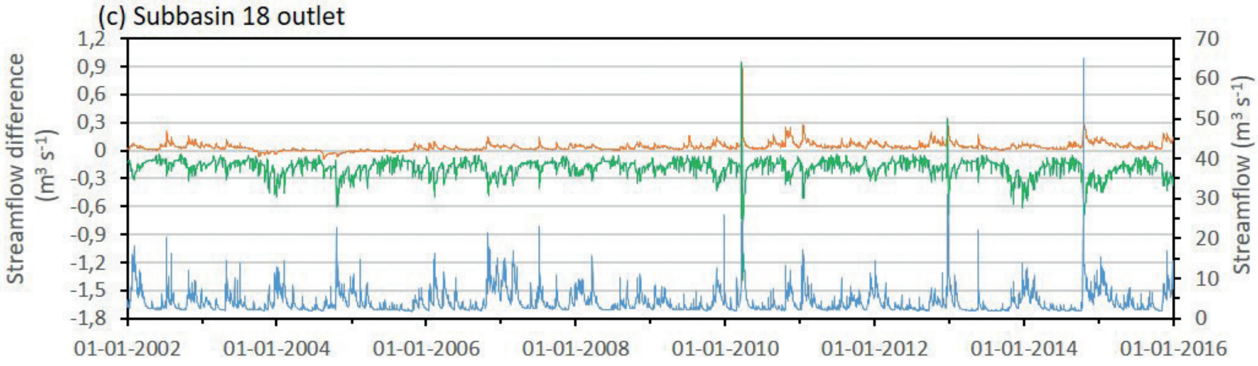


Figure 2. Simulated daily streamflow in the baseline scenario and differences in daily streamflow between the baseline scenario and the model scenarios (no drinking water abstraction, extreme abstraction; in the latter the pumping rates of the drinking water wells at subbasin 7 were increased by 20) for the outlets of subbasin 7, subbasin 13 (station A), and subbasin 18 (station B) during the entire study period (2002-2015) based on SWAT-MODFLOW.

ence was approximately 0 m^3 day^{-1} in subbasin 18 (Fig. 3b). Similarly, the average daily groundwater discharge in all subbasins in the baseline scenario was higher than in the extreme abstraction scenario, and again the differences varied among the individual subbasins of the catchment (Fig. 3a, 3c). The average difference was 842 m^3 day^{-1} for the entire catchment, with a maximum difference of 8328 m^3 day^{-1} in subbasin 7 and a minimum difference of 1 m^3 day^{-1} in subbasin 18 (Fig. 3c).

3.3 The impacts of groundwater abstractions on flow regime variables

Six flow regime variables constitute the basis for the predictability in the three flow-biota empirical models. Four of them (Fre_1, Fre_{25}, BFI, Q_{90}) have positive effects on the biotic indices as they increase, while the other two (Fre_{75}, Dur_3) have negative effects on biotic indices, as indicated by the positive and negative operational signs (Fig. 4).

Compared with the scenario with no drinking water abstraction, BFI under the baseline scenario decreased by 0.4 % at subbasin 7 outlet and 0.3 % at subbasin 13 out-

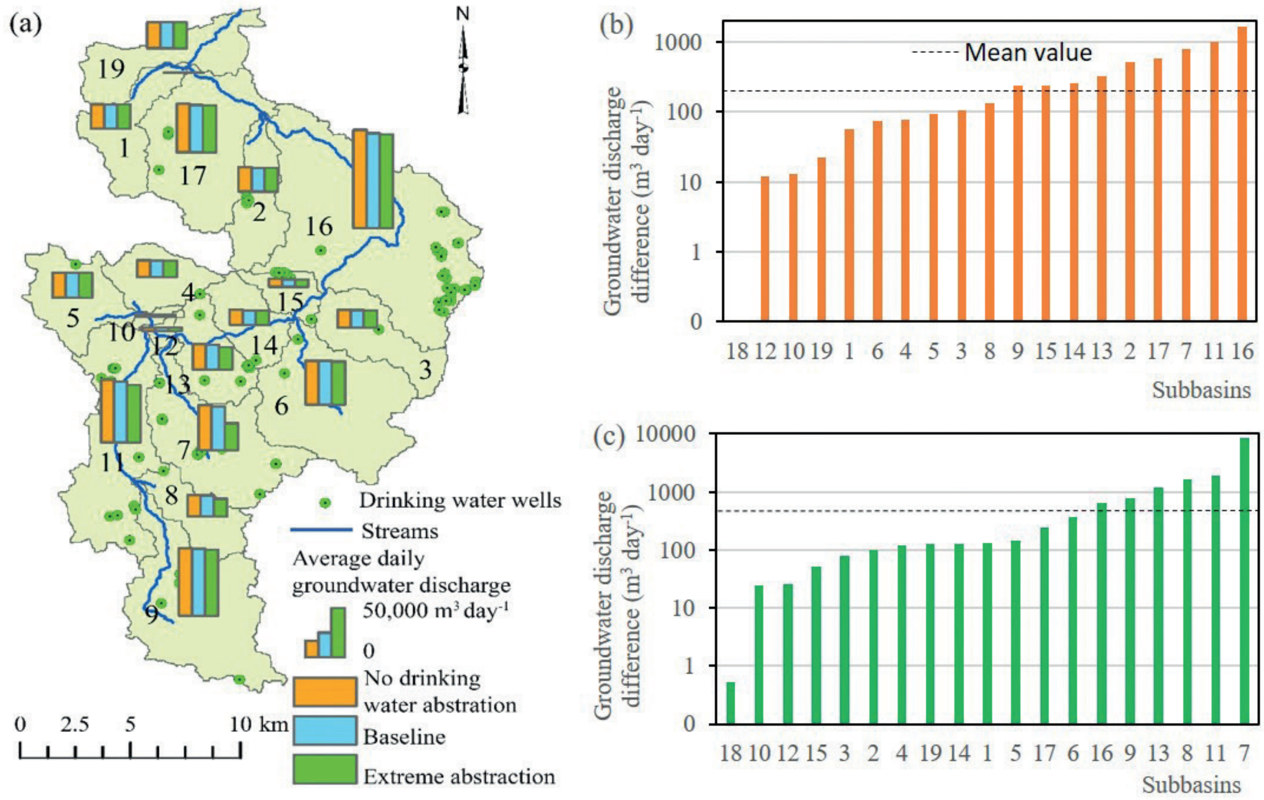


Figure 3. Average daily groundwater discharge (m3 day-1) in each subbasin from the aquifer to the stream network during the period 2002-2015 in different groundwater abstraction scenarios (no drinking water abstraction, baseline, extreme abstraction) simulated by the calibrated SWAT-MODFLOW model. (a): Groundwater discharge difference between the no drinking abstraction scenario and the baseline scenario in each subbasin; (b): groundwater discharge difference between the baseline scenario and the extreme abstraction scenario.

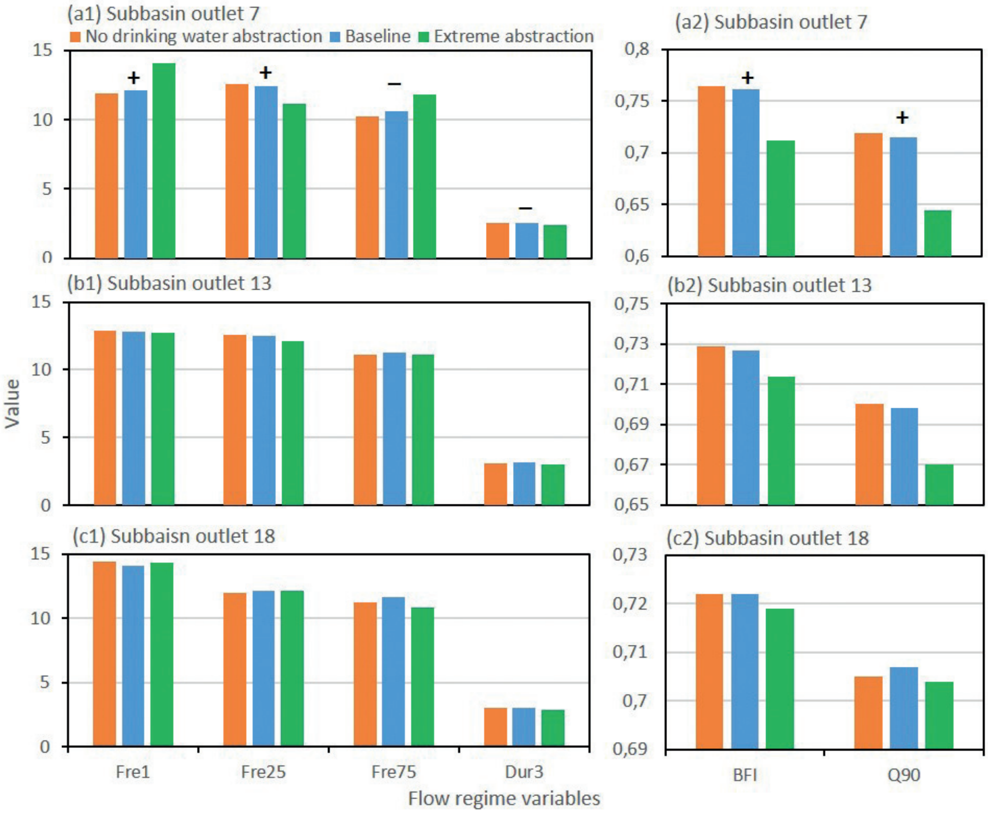


Figure 4. Comparison of the flow regime variables for the streamflow at subbasin outlet 7, 13, and 18, respectively, during 2002-2015 between the three different scenarios (no drinking water abstraction, baseline, and extreme abstraction). "+" and "-"mean that the variable has a positive or negative effect on stream ecology quality state.

let, but no change was found at subbasin outlet 18. Similarly, compared with the baseline scenario, BFI in the extreme abstraction scenario decreased by 6.4 %, 1.8 %, and 0.4 % at the outlets of subbasins 7, 13, 18, respectively. For the other flow regime variables, value differences between the scenario with no drinking water wells and baseline scenario was minimum. In contrast, the differences between the extreme abstraction scenario and the baseline scenario were more apparent, being largest for subbasin 7. Compared with the baseline scenario, at the subbasin 7 outlet, three of the four flow regime variables (Fre_{25}, BFI, Q_{90}) that play positive role on the biotic indices decreased by 10.5 %, 6.4 % and 10 %, and the remaining one (Fre_1) increased by 11.3 %. One of the two flow regime variables (Fre_{75}) that has a negative effect on the biotic indices increased by 11.3 % and the other one (Dur_3) decreased by 5.1 %.

3.4 The impacts of groundwater abstraction on stream biota

The biotic indices at the three subbasin outlets under the three different groundwater abstraction scenarios were compared (Fig. 5). No apparent difference of DVFI values were observed at the three subbasin outlets. When comparing the baseline scenario with the scenario with no drinking water abstraction, the fish index DFFVa decreased by 4.5 %, 2.3 % and 2.8 %, and the macrophytes index DVPI by 3.2 %, 1.7 % and 2.1 % at the outlets of subbasin 7, 13 and 18, respectively, under the baseline scenario. Compared with the baseline scenario, the DFFVa decreased by 23.5 % and 3.8 %, and the DVPI by 11.2 % and 0.4 %, at the outlets of subbasin 7 and 13, respectively, in the extreme abstraction scenario, while the DFFVa and DVPI at subbasin 18 outlet increased by 5.9 % and 4.9 %.

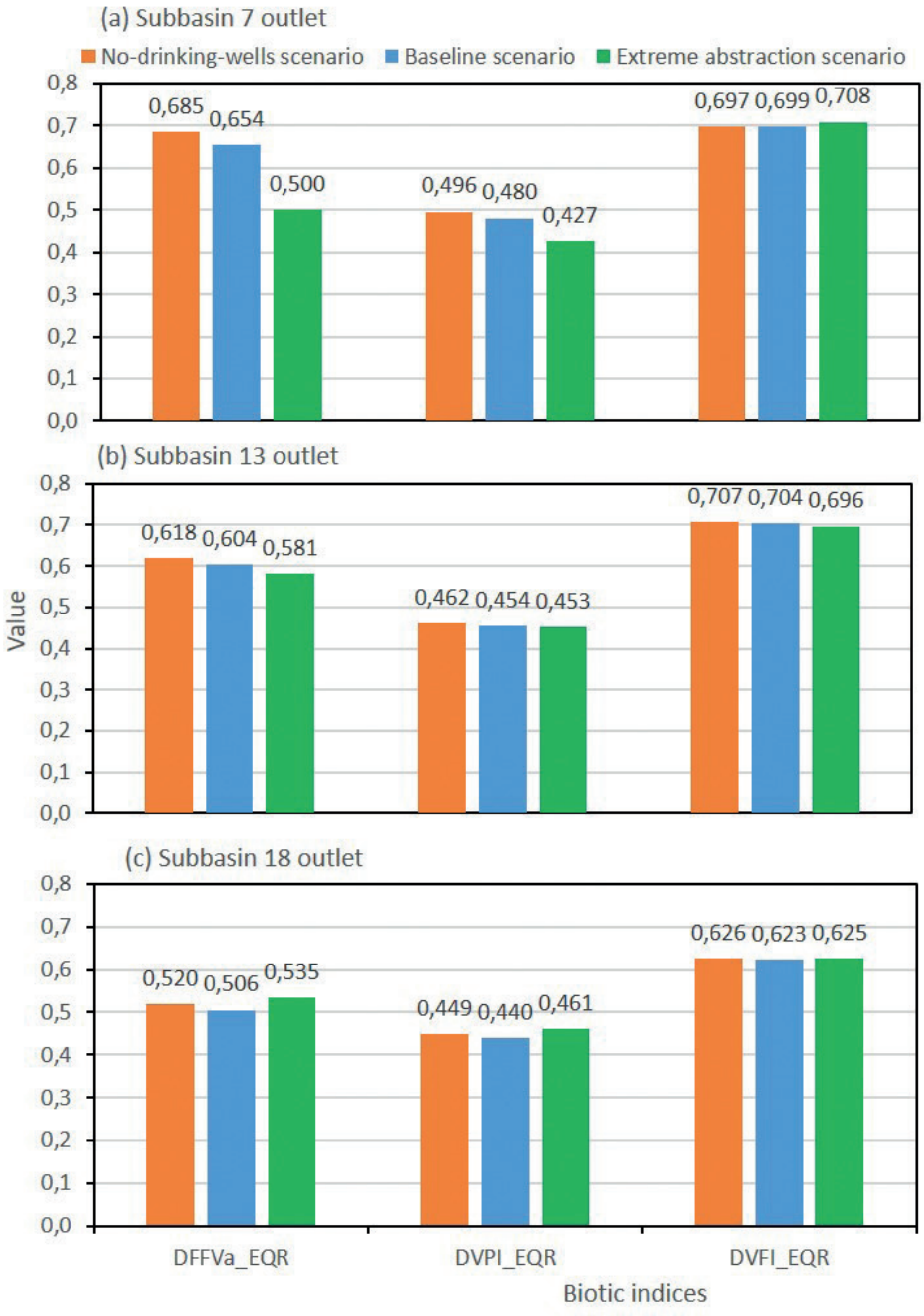


Figure 5. Comparison of the biotic indices (DFFVa: fish index; DVPI: macrophyte index; and DVFI: macroinvertebrate index) at subbasin outlet 7, 13, and 18, respectively, during 2002-2015 between the three different scenarios (no drinking water abstraction, baseline, and extreme abstraction).

4 Discussion

4.1 The impact of groundwater abstractions on hydrology, flow regime and stream biota

The current groundwater abstraction in the Uggerby River Catchment has generally caused minor decreases in groundwater discharge and streamflow throughout the catchment. Consequently, the flow regime variables and the biotic indices for stream ecology quality have only shown modest changes. In contrast, the assumed extreme abstraction in subbasin 7, in which the abstraction rates increased 20-fold compared with the current abstraction, caused larger streamflow decrease at all three subbasin outlets, but only for subbasin 7 there was considerable impacts on the flow regime variables and the biotic indices despite the larger streamflow decreases in the outlets of subbasin 13 and 18. Besides subbasin 7, the outlets of subbasin 13 and subbasin 18 also receive water from other subbasins, so in subbasins 13 and 18 the impact of extreme abstraction in subbasin 7 is buffered by the water contribution from the other subbasins in the catchment. This may reflect differences in the response by streams of different sizes, but it also highlights the importance of resolving these differences in a model set-up to advance today's water management and render groundwater abstraction permit confirmation according to such basin heterogeneities.

The DFFVa is positively related to BFI and negatively related to Fre_{75}, reflecting a positive effect on the fish community of a stable discharge regime with rare occurrence of low flows (Poff and Zimmerman, 2010). Furthermore DFFVa is positively related to $Fre_{25,}$ suggesting that slight disturbances due to weak peak flows may improve the quality of the fish community. The relationship of DVPI to the two coefficients Fre_{25} and Dur_3 confirms the hypothesis of a higher quality of the macrophyte community at intermediate disturbances and a lower quality at strong peak flows, as was also found by Riis et al. (2008) for Danish streams and rivers. Furthermore, the negative correlation with Fre_{75} may indicate that, due to the lack of disturbance at a high frequency of low flows, competitive species dominate the macrophyte community, resulting in lower diversity and hence lower DVPI. It has been reported that lotic macroinvertebrate species are lost and substituted by ubiquitous and lentic species when extreme low flow or stagnant conditions occur (Graeber et al., 2013; Hille et al., 2014). A Q_{90} value close to 0 means that the low flows are much more extreme (lower) than that if the Q_{90} is close to 1. Due to the positive correlation between Q_{90} and DVFI, DVFI will be higher when the low flows are less extreme (Gräber et al., 2015). Fre_1 is the frequency of peak flows above the median flow. Such weak peak flows can positively affect lotic macroinvertebrate communities due to the removal of fine sediment (Dunbar et al., 2010; Pan et al., 2013) and the potentially increased habitat diversity (Poff et al., 2010).

Among the three biotic indices, the DEFVa (fish index) was the most affected by groundwater abstractions. Groundwater abstractions affect streamflow mainly through reducing the baseflow, thereby lowering the BFI, which is highly dependent on the baseflow. All the flow-biota empirical models are based on multiple linear regressions. According to the coefficients related to each flow regime variable, the BFI, of which the coefficient is 0.811 and much larger than the coefficients of the other flow regime variables, has the strongest influence on ecological state, making the DEFVa the most vulnerable index to groundwater abstractions. The impacts of groundwater abstraction on the other variables are more uncertain (can be either positive or negative) as their values are based on percentiles of the flow-duration curve. This may also explain why the biotic indices for the subbasin 18 outlet in the extreme groundwater abstraction scenario did not decrease but rather showed a small increase. According to the definitions, BFI, Fre_{75}, and Q_{90} are highly related to low flow on which groundwater abstractions have direct influence. In the flow-biota empirical relationship equation (1) and equation (2), the values of Fre_{75} and BFI can have direct influence on ecology quality, and the impact of groundwater abstraction on streamflow ecology is thereby reflected in the fish and macrophyte indices (Fig. 5). In equation (3), the coefficient of Q_{90} for the effect on the macroinvertebrate index is only 0.02, which is the lowest among all the flow regime variables, and its effect is weakened due to its bundling with Fre1, which may increase with enhanced groundwater abstraction (Fig. 5). Hence, no obvious groundwater abstraction effects on macroinvertebrates were recorded when using this equation (Fig. 5).

4.2 Advantages of the approach

SWAT-MODFLOW is a useful tool for managing water resources in groundwater-affected catchments, especially when assessing the impacts of groundwater abstraction on streamflow (Liu et al., 2019; Molina-Navarro et al., 2019). A number of advantages of SWAT-MODFLOW over SWAT have been reported in earlier studies. The results from this study illustrate another advantage. In the extreme abstraction scenario, the abstraction from wells in subbasin 7 not only decreased the groundwater discharge to the stream network but also in the discharge to all other subbasins, allowing us to conclude that the streamflow changes in subbasin 13 and 18 were larger than in subbasin 7. In the SWAT-MODFLOW model, realistic interaction of groundwater between subbasins can be simulated, and abstraction can therefore impact the groundwater hydrology in surrounding areas. However, in the widely used catchment model SWAT the subbasin aquifers are closed and independent of each other, meaning that pumping within one subbasin does not affect the groundwater hydrology in other subbasins within the watershed.

The flow-biota empirical models applied in this study are easy to employ and applicable in many lowland, temperate stream systems. Firstly, they are formulated as equations based on multiple easily understandable linear regressions, and the ecological quality ratio is a comprehensive coefficient that considers both species diversity and the quantity of each taxonomic identity. Secondly, the determination coefficients of the models are fairly good (Gräber et al., 2015). Thirdly, they were developed based on samples and stream locations from numerous sites spread across Denmark and include three key taxonomical groups (fish, macrophytes, and macroinvertebrates). In contrast, most of previous flow alteration-ecology response studies report relationships for only specific stream segments, catchments or regions (Crossman et al., 2011; Belmar et al., 2013; Stein et al., 2017; Stein et al., 2018). They do not include formulated equations (Kennen et al., 2009; Stromberg et al., 2010; Meador and Carlisle, 2012; Buchanan et al., 2013; Domisch et al., 2017) and are often focused on only one taxonomic identity (Kennen et al., 2009; Stromberg et al., 2010; Falke et al., 2011; Domisch et al., 2017; Perkin et al., 2017; Ruhi et al., 2018).

The combination of SWAT-MODFLOW and the flow-biota empirical models enables scenario studies for quantitative assessment of the impacts of groundwater abstraction on ecological quality, not only for stream segments with observed streamflow but also for segments without observations. With simulated long-term streamflow data and the flow-biota empirical models, the ecological quality indices and their alteration due to groundwater abstraction at all the subbasin outlets can be derived. This study provides a methodology for doing so.

4.3 Limitations and future research

The patterns of daily streamflow differences among scenarios were generally as expected, but, surprisingly, the streamflow difference between the extreme abstraction scenario and the baseline scenario was positive at the outlets of subbasin 13 and 18 on 23 March, 2010, and at the subbasin 18 outlet on 24 December, 2012, being 1.05, 0.95 and 0.34 m^3 s^{-1}, respectively (Fig. 2). This cannot readily be explained. However, in tests of how these ”outliers” affected our general results and conclusions, in which these two dates were omitted from the calculation of biotic indices, we found that the impacts on the flow regime variables and biotic indices were insignificant.

The flow-biota empirical models were developed based on the stream sites where the biological data and long-term hydrological data are available. Generally, these hydrological stations in Danish stream segments are established in the middle and downstream receiving waters, i.e. not smaller headwater streams, and the equations therefore mainly represent relatively large streams. This implies that the equations may not adequately represent the small headwater streams that presumably are particularly sensitive to changes in groundwater discharge. If empirical biotic models for small streams become available, then the overall predictions of the coupled model complex would become even more reliable.

Case studies provide a critical bridge between the science of flow-ecology and real-world implementation of best management practices (Stein et al., 2017). Our study is an example of how to quantitatively assess the effects of groundwater abstractions on stream biota through scenario simulations, which could have potential implications for groundwater abstraction management decisions. Broader application of the approach to other catchments could help foster science-informed groundwater management in Denmark or other countries (or other countries (if flow-biota empirical models in those countries are developed).

5 Conclusions

We jointly applied the SWAT-MODFLOW model and the flow-biota empirical model to a Danish groundwater-dominated catchment, the Uggerby River Catchment, to quantitatively assess the effects of groundwater abstractions on flow regime and stream biota.

Effects were analyzed at three subbasin outlets representing stream segments of different sizes. The current groundwater abstraction level had slight impacts on the flow regime and stream biota for all three stream seg-ments. The extreme abstraction scenario had significant impacts on the small stream but only slight impacts on the larger streams. Among the three biotic indices, the fish index was most severely affected by groundwater abstractions, followed by the macrophyte index, while no apparent impact of groundwater abstractions was found on the macroinvertebrate index.

We conclude that the novel approach of combining the SWAT-MODFLOW model with comprehensive flow-bi-ota empirical models to quantitatively assess the effects of groundwater abstraction on stream biota is useful for developing water planning and regulation in Denmark and elsewhere. However, there is a need for developing more sufficient biotic models that also represent small headwater streams, which due to low flows can be sig-nificantly impacted by nearby groundwater abstraction.

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MANUSCRIPT 3

QUANTIFYING THE EFFECTS OF CLIMATE CHANGE ON HYDROLOGICAL REGIME AND STREAM BIOTA IN A LOWLAND CATCHMENT: A MODELLING APPROACH COMBINING SWAT-MODFLOW WITH FLOW-BIOTA EMPIRICAL MODELS

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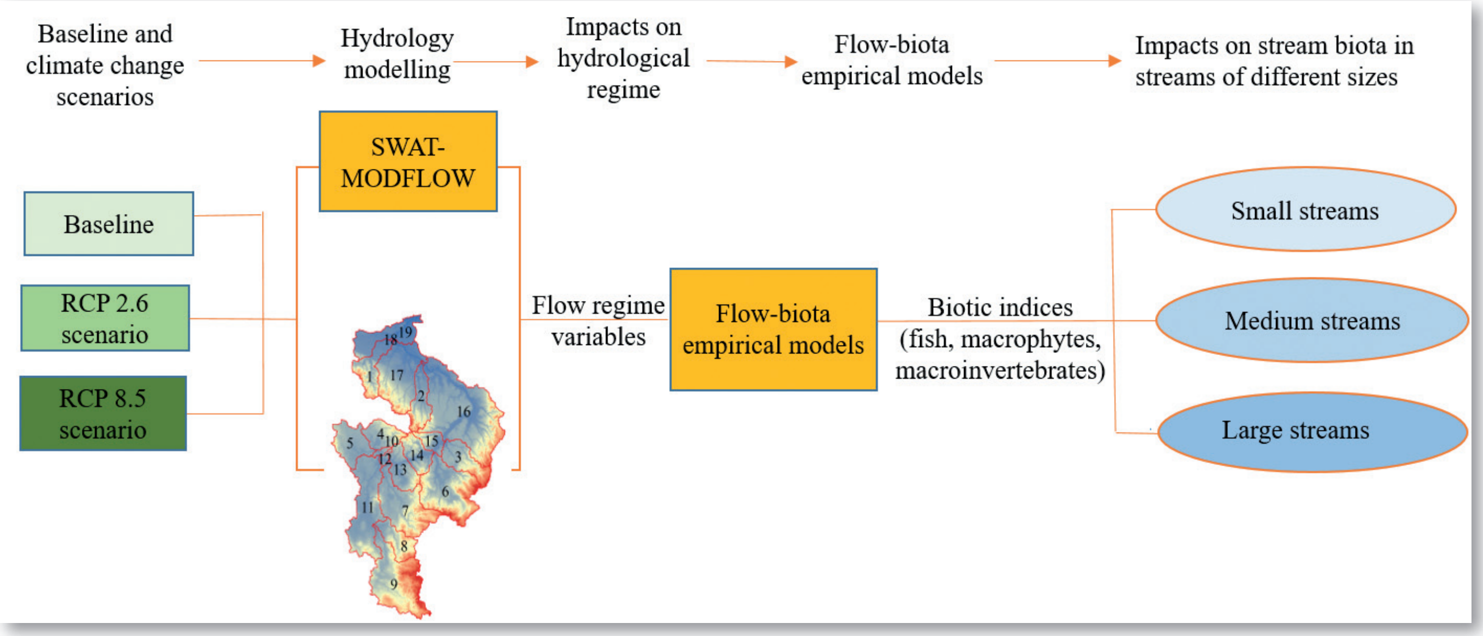

Graphical abstract

QUANTIFYING THE EFFECTS OF CLIMATE CHANGE ON HYDROLOGICAL REGIME AND STREAM BIOTA IN A LOWLAND CATCHMENT: A MODELLING APPROACH COMBINING SWAT-MODFLOW WITH FLOW-BIOTA EMPIRICAL MODELS

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Abstract

Climate change affects stream ecosystems not only by increasing water temperatures but also by alter-ing the flow regime. To quantitatively assess the impacts of climate change on hydrological regime characteristics and stream biota, we linked the SWAT-MODFLOW model with flow-biota empirical models including indices for three key biological taxonomic identities (fish, macroinvertebrates, and macrophytes) and applied them to a Danish lowland, groundwater-dominated catchment. Effects were tested with two climate change scenarios of different greenhouse gas emissions (RCP2.6 and RCP8.5) and analyzed for all subbasin outlets grouped into streams of three sizes. The overall stream-flow and groundwater discharge in the catchment decreased slightly in the RCP2.6 scenario while it increased in the RCP8.5 scenario. The differently sized streams underwent different alterations in flow regime and thereby also demonstrated different biotic responses to climate change as represented by the fish and macrophyte indices. Large and some small streams suffered most from climate change, as the fish and macrophyte quality indices decreased up to -14.4 % and -11.2 %, respectively, whereas these indices increased by up to 14.4 % and 6.0 % respectively, in medium and some small streams. The climate change effects were, as expected, larger in the RCP8.5 scenario than in the RCP2.6 scenario. Our study is the first to quantitatively assess the impacts of streamflow alterations induced by climate change on stream biota beyond specific species, which would assist in water planning and regulations in response of the challenges posed by climate change.

Key words: SWAT-MODFLOW, climate change, flow regime, biotic indices, fish, macrophytes, macroinvertebrates.

1 Introduction

Global circulation models (GCMs) project an increase in globally annual average surface air temperatures of 1.5-7.8 °C by 2100 under scenarios of different greenhouse gas emissions relative to the period 1850-1900 (Pachauri et al., 2014). Alterations in global seasonal and inter-annual precipi-tation patterns are also expected, as well as increases in the intensity, duration and frequency of extreme climate events, and this could lead to substantial flow regime changes, massive floods and prolonged droughts (Filipe et al., 2012). Such alterations will be particularly com-plex in streams with significant groundwater contribu-tion as climate change will lead to marked changes in the groundwater recharge (Döll, 2009).

Increasing temperatures in inland waters are expected to occur globally due to changes in meteorological factors (e.g. solar radiation and heat fluxes), and this may result in a reduction or even extinction of biota (Eaton and Scheller, 1996) and it may enhance eutrophication too (Trolle et al., 2015; Trolle et al., 2019) .So far, nearly all broad-scaled studies of climate change effects on freshwater ecosystems have focused on the effects of temperature shifts (Wenger et al., 2011). However, climate change affects stream ecosystems not only by increasing the water temperatures but also by altering the flow regime due to changes in precipitation and poten-tial/actual evapotranspiration (Döll and Zhang, 2010; Thodsen, 2007).

The flow regime, describing the characteristics of a river's flow quantity, timing and variability, organizes and dictates the environmental physical structure, biodiver-sity and integrity of river ecosystems (Poff et al., 1997). Alterations in flow regime may lead to a series of nega-tive impacts on stream ecosystems, such as lower bio-diversity and ecological quality, local species extinction and invasion of exotic species (Bunn and Arthington, 2002). Numerous studies have investigated the effects of climate change on the flow regime at various spatial and temporal scales (Kim et al., 2011; Mittal et al., 2016; Pradhanang et al., 2013; Yang et al., 2017) and they have shown strong regional differences (Cui et al., 2018) with some areas (e.g. mid-latitude land areas of the North-ern Hemisphere) facing increases in runoff, while other areas will experience decreases (Goudie, 2006; Pachauri et al., 2014). A global-scale analysis of ecologically rele-vant river flow alterations conducted by Döll and Zhang (2010) showed that the impacts of climate change on the flow regime may be even larger than those of dams and water withdrawal by the mid-21st century.

While discharge decreases are generally considered det-rimental to stream ecosystems, the effects of discharge increases triggered by climate change are less clear (Döll and Zhang, 2010). Potentially, discharge increases may decrease habitat availability (Gibson et al., 2005), change species composition (Döll and Zhang, 2010) and damage of new habitats by extreme flooding (Stefanidis et al., 2016). However, increased flow induced by climate change may also have positive effects on the aquatic biota by counteracting the negative effect of the presently decreased streamflow and rising temperatures (Cui et al., 2018; Wenger et al., 2011). Therefore, quantitative assessment of the impacts of flow alteration induced by climate change on stream ecosystems is needed.

Denmark is a lowland country surrounded by oceans and highly dependent on groundwater resources. The groundwater contribution to average streamflow is around 76 % in continental Denmark (Olesen, 2009). At national level, the temperature in Denmark has increased by approximately 1.5 °C and the annual precipitation has increased by about 100 mm since 1870. Moreover, the frequency of heavy precipitation events (>100 mm in a few hours) appears to higher now than in the last century (Olesen et al., 2014). (Olesen et al., 2014). Based on climate model studies, this tendency is expected to continue during this century (Pachauri et al., 2014).

In this study, to quantitatively assess the effects of climate change on hydrology, flow regime and stream biota, we combined the newly developed coupled surface-subsurface hydrological model SWAT-MODFLOW (Bailey et al., 2016), which performs well for groundwater-dominated atchments (Liu et al., 2019b; Molina-Navarro et al., 2019), with novel nationwide flow-biota empirical models developed for Denmark by Gräber et al. (2015) formulated as equations based on relationships between flow regimes and three biotical indices (fish, macroinvertebates and macrophytes). We used a Danish groundwater-dominated catchment, the Uggerby River Catchment, as a case study to assess to what extent the flow regime and key biota in stream segments of different sizes may be altered by future climate change under two scenarios of different greenhouse gas emissions. To the best of our knowledge, ours is the first study to quantitatively assess the impacts of flow regime alterations induced by climate change on stream biota with three key taxonomic identities.

2 Methods

2.1 Study area

The Uggerby River Catchment is located in the northernmost part of Jutland, Denmark (latitude 57.28 - 57.58 N, longitude 9.95 - 10.33 E). The main channel of Uggerby River originates from the southern part of Hjørring and ends at the coast of the North Sea (Fig.1). The catchment has an area of 357 km^2 and is administratively covered by the Municipality of Hjørring having a total area of 930 km^2. Two hydrologically connected monitoring stations, which are respectively located at the upstream and downstream of the Uggerby River Catchment (Fig. 1) and have long-term observations of daily runoff, provide a good basis for hydrological model evaluations. The catchment is dominated by intensive agricultural land use (approximately 63 %). Like many catchments in Denmark, the Uggerby River is to a large extent groundwater-fed (approximately 75 %). There are 101 drinking water wells and 57 irrigation wells registered within the Uggerby River Catchment (Hjørring Municipality, 2009). Generally, the irrigation wells are placed on pasture and agricultural land, and irrigation occurs from April to October, with an average annual irrigation amount varying from 80 to 200 mm. For the period 1996-2005, the mean annual temperature was 8 °C, and the mean annual precipitation was approximately 900 mm with no major seasonal differences.

2.2 SWAT-MODFLOW model

SWAT (Soil and water assessment tool) is a semi-distributed, physically-based, continuous-time eco-hydrological model used for simulating hydrology and water quality at different catchment scales and predicting the environmental impact from anthropogenic activities and climate change (Gassman et al., 2007; Neitsch et al., 2011). The model is computationally efficient for long-term simulation due to its semi-distributed and lumped approach, but groundwater dynamics is highly simplified. MODFLOW (Harbaugh 2005) is a fully-distributed, physically-based, three-dimensional groundwater model that has been widely used for groundwater resources management worldwide. However, model application is limited to groundwater-related issues and its performance is highly dependent on the quality of the input data on recharge rates and groundwater-surface water interactions. To overcome the disadvantages of both SWAT and MODFLOW, Bailey et al. (2016) coupled SWAT and MODFLOW-NWT (a Newton-Raphson formulation for MODFLOW-2005 (Niswonger et al., 2011)) into the SWAT-MODFLOW model. In the SWAT-MODFLOW framework, SWAT simulates surface processes and MODFLOW simulates subsurface processes. SWAT-calculated deep percolation at HRU-scale (Hydrological Response Units) is passed to MODFLOW cells as recharge, and MODFLOW-calculated surface-groundwater exchange fluxes are passed to the stream channels of SWAT. Good hydrological simulation performance of SWAT-MODFLOW in catchments and watersheds of varying sizes where groundwater discharge

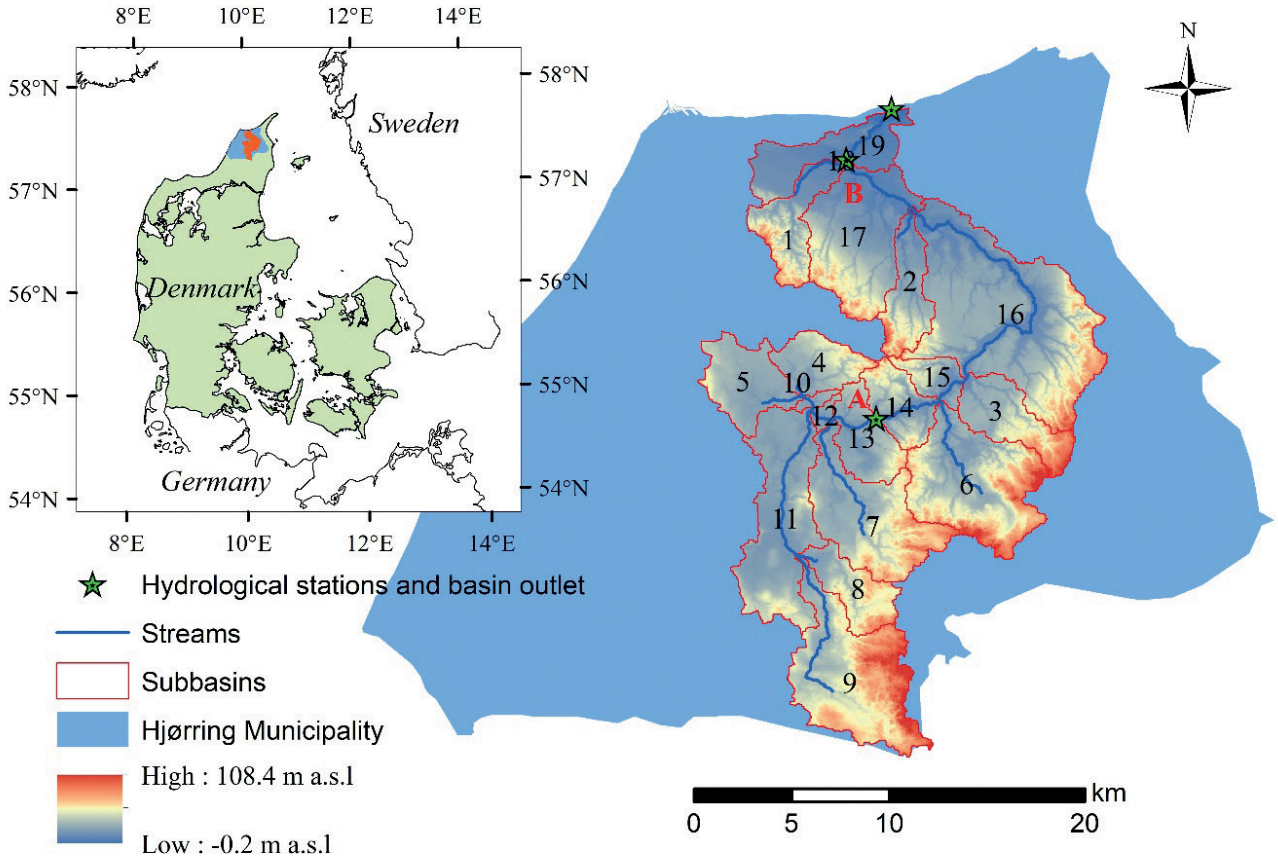

Figure 1. Location of Uggerby River Catchment and Hjørring Municipality and their delineation in SWAT and MODFLOW, respectively.

contributes significantly to the streamflow has been proved in several studies (Bailey et al., 2016; Aliyari et al., 2019; Liu et al., 2019b; Molina-Navarro et al., 2019; Wei and Bailey, 2019).

The SWAT-MODFLOW model for the Uggerby River Catchment was developed by linking a calibrated SWAT model for the Uggerby River Catchment with a calibrated MODFLOW-NWT model for the entire municipality of Hjørring. The coupled model has previously undergone rigorous calibration (period: 2002-2008) and validation (period: 2009-2015) based on a PEST-based approach against observations of both streamflow and the groundwater table. Details on the model development, calibration and validation procedures can be found in (Liu et al., 2019b). In this study, we utilised the calibrated and validated SWAT-MODFLOW model for running a baseline simulation (period: 1996-2005 with 7 years ahead as a warm-up period) and future climatic scenarios. The model's performance on streamflow simulation during the baseline period was evaluated through visual inspection and statistical performance measures, including the Nash-Sutcliffe efficiency coefficient (N_{SE}), the percent bias (P_{BIAS}) and the coefficient of determination (R^2).

2.3 Flow-biota empirical models

The flow-biota empirical models refer to the empirical relationships between flow regime variables and three biotic indices (DFFVa (fish index), DVPI (macrophyte index) and DVFI (macroinvertebrate index)) based on a number of Danish stream sites developed by Gräber et al. (2015).

$$\mathrm{DFFVa}_{\mathrm{EQR}} = 0.811{*}\mathrm{BFI} + 0.058{*}\mathrm{Sin} + 0.050{*}\mathrm{Fre}_{25} - 0.319 - 0.0413{*}\mathrm{Fre}_{75} \quad (1)$$

$$\mathrm{DVPI}_{\mathrm{EQR}} = 0.546 + 0.020{*}\mathrm{Fre}_{25} - 0.019{*}\mathrm{Dur}_{3} - 0.0_{25}{*}\mathrm{Fre}_{75} \quad (2)$$

$$\mathrm{DVFI}_{\mathrm{EQR}} = 0.217 + 0.103{*}\mathrm{Sin} + 0.020{*}Q_{90}{*}\mathrm{Fre}_{1} \quad (3)$$

where EQR is the ecological quality ratio (ranging from 0 to 1 with 0 as the worst condition and 1 the reference condition), BFI is the baseflow index (baseflow volume divided by total flow volume), Sin is the class of stream sinuosity (calculated from the stream length divided by linear distance), Fre_{25} is the annual frequency of events with flows above the 25th percentile from the flow duration curve, and Fre_{75} is the annual frequency of events with flows below the 75th percentile from the flow duration curve. Dur_3 is the duration (days) of flows 3 times the median flow. Q_{90} is the flow below the 90th percentile of the flow-duration curve divided (standardised) by median flow (Q_{50}), and Fre_1 is the annual frequency of events with flows above the median flow. More details about the models can be found in (Gräber et al., 2015; Liu et al., 2019a).

Two code files to derive, respectively, the flow regime variables and biotic indices for each subbasin outlet were created and run through SAS 9.4 (www.sas.com/) with the SWAT-MODFLOW streamflow output file output.rch as the imported data (Liu et al., 2019a).

2.4 Climate change scenarios

Denmark is located in northern Europe. The country has an area of about 42,933 km² and is surrounded by the North Sea. According to the Köppen-Geiger Classification, the climate of the entire country is oceanic (warm temperate, fully humid, (Karlsson et al., 2016)). The Danish Meteorological Institute (DMI) has estimated the expected climate change in Denmark towards the end of this century based on IPCC (Intergovernmental Panel on Climate Change), BACC (BALTEX Assessment of Climate Change for the Baltic Sea Basin), European studies and the Danish CRES (Centre for Regional Change in the Earth System) project where a number of climate simulations were performed with several regional and global climate models (Olesen et al., 2014). The results generally predicted a warmer climate with overall higher precipitation and more extreme weather events. The temperature trend in Denmark largely follows the trend in the average global annual mean temperature, both in terms of observations since the 1870s and projections of future temperatures up to 2100 (Olesen et al., 2014). Particularly, milder winters are expected, implying that the plants' growing season is extended, and summers get warmer, creating more and longer heat waves. Denmark can expect more rain, especially in winter, and probably longer drought periods and more extreme rainfall during summer.

From an ensemble of 23 global climate models DMI has predicted a mean future temperature and precipitation change towards the end of this century (2080-2100) in Denmark at seasonal level. They used the period 1986-2005 as reference and two greenhouse gas emission scenarios (RCP 2.6 and RCP 8.5), which represents the lowest and highest scenarios assessed by IPCC (Table 1).

With the climate change data in Table 1, we performed an evaluation of climate change impacts on streamflow and biota through a baseline simulation and two climate change prediction scenarios. The baseline represents the state during the reference period (1996-2005). Scenario 1 – the RCP2.6 scenario, a climate change prediction scenario with stringent greenhouse gas emissions mitigation that aims to keep global warming below 2 °C above pre-industrial temperatures (Pachauri et al., 2014). Scenario 2 – the RCP8.5 scenario, a climate change prediction scenario with very high greenhouse gas emissions. As the changes of the other meteorological factors, for instance, humidity, wind speed and solar radiation,

Table 1. Projected changes (seasonally averages) in temperature and precipitation in 2081-2100 relative to the reference period (1986-2005) in entire Denmark at the seasonal level in the form of mean values predicted by DMI using an ensemble of 23 global climate models (Olesen et al., 2014).

Seasons	Temperature increase (°C)		Precipitation change (%)	
	RCP2.6	RCP8.5	RCP2.6	RCP8.5
Winter (Dec-Feb)	1.2	3.7	3.1	18
Spring (Mar-May)	1.2	3.2	3.7	10.7
Summer (June-Aug)	1.2	4	-0.5	-16.6
Autumn (Sep-Dec)	1.3	4	0.8	10.2

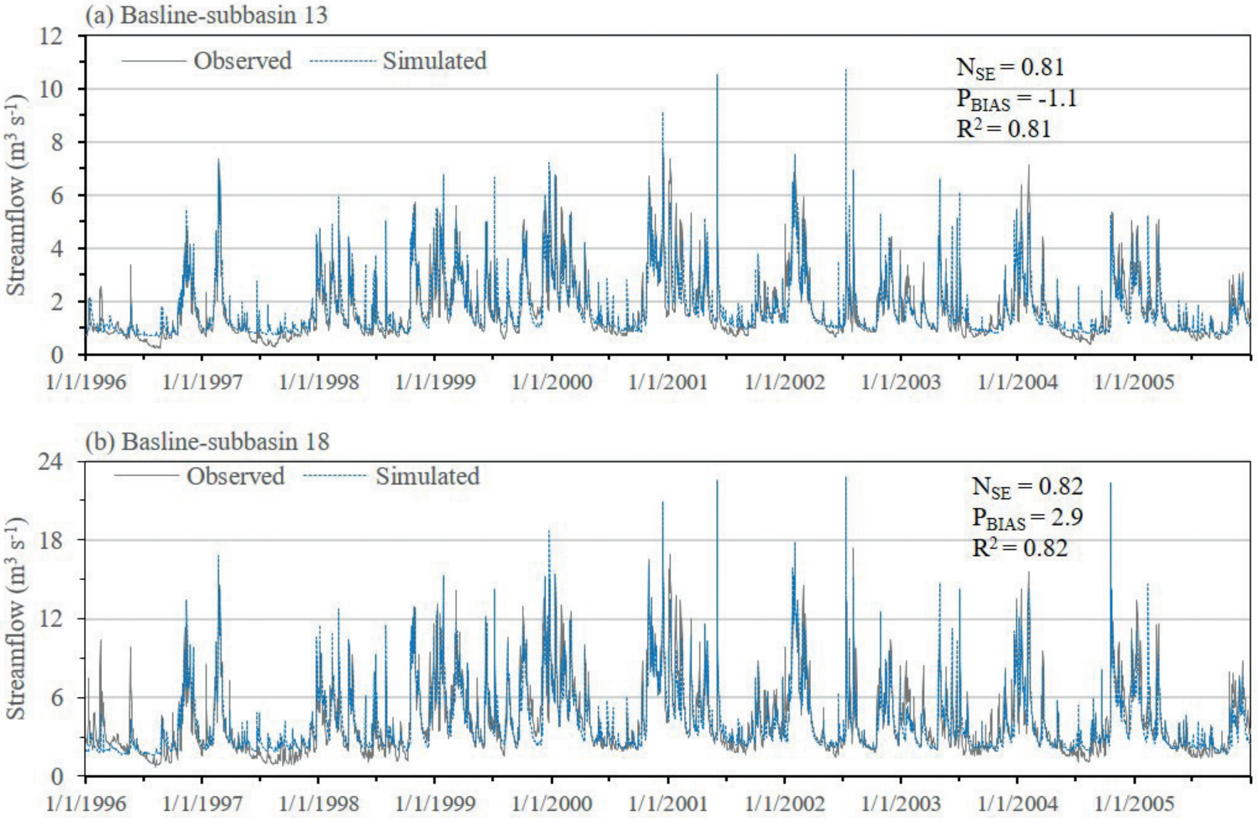

Figure 2. SWAT-MODFLOW daily streamflow simulations and their performance statistics values at the two hydrological stations (subbasin 13 and subbasin 18 outlet) during the baseline period 1996-2005.

have not been quantitatively estimated by DMI due to their unpredictability and high uncertainty, in this study we assume they remain unchanged compared with the reference period, and we discuss the potential implications of this assumption.

3 Results

3.1 Baseline simulation performance

The calibrated and validated SWAT-MODFLOW represented the streamflow hydrographs during the baseline period well (Fig. 2). Compared with the recommended evaluation criteria by (Moriasi et al., 2015), the N_{SE} and P_{BIAS} values suggested "very good" performance on streamflow simulation of the SWAT-MODFLOW model during the baseline period (P_{BIAS}), and R^2 values suggested "good" performance (Fig. 2).

3.2 Climate change impacts on hydrological components, streamflow and groundwater discharge

Compared with the baseline, the average annual precipitation increased by 14 and 41 mm yr^{-1} and average annual actual evapotranspiration increased by 18 and 42 mm yr^{-1} in the RCP2.6 and the RCP8.5 scenarios, respectively (Table 1). The water yield (total flow) decreased by 1 mm yr^{-1} (0.26 %) in the RCP2.6 scenario, while it increased by 9 mm yr^{-1} (2.4 %) in the RCP8.5 scenario. According to the water balance, the average annual increase of water storage in soil or aquifers (ΔS) decreased

Table 2. Average annual values of the main components of the hydrological cycle in the Uggerby River Catchment in the baseline simulation and the two climate change scenarios (RCP2.6 and RCP8.5) simulated by SWAT-MODFLOW.

Components	Baseline	RCP2.6	RCP8.5
Precipitation (mm yr^{-1})	899	913	940
Surface runoff (mm yr^{-1})	29	27	27
Lateral soil runoff (mm yr^{-1})	62	64	68
Drain flow (MODFLOW, mm yr^{-1})	265	264	271
Groundwater flow (mm yr^{-1})	22	22	22
Total water yield (mm yr^{-1})	378	377	387
Total aquifer recharge (mm yr^{-1})	323	317	321
Actual evapotranspiration (mm yr^{-1})	495	513	537
Average annual irrigation amount in the irrigated HRUs (mm yr^{-1})	155	158	203

by 3 and 10 mm yr^{-1} in the RCP2.6 and RCP8.5 scenarios, respectively. The average annual groundwater discharge (including drain flow and groundwater flow) within the entire catchment decreased by 1 mm yr^{-1} in the RCP2.6 scenario, while it increased by 6 mm yr^{-1} in the RCP8.5 scenario (Table 2). Average annual irrigation in the irrigated HRUs (mm yr^{-1}) increased by 3 (2 %) and 58 mm yr^{-1} (31 %) in the RCP 2.6 and RCP8.5 scenarios, respectively (Table 2).

The average annual streamflow levels at every subbasin outlet in the baseline simulation and the two climate change scenarios were compared (Fig. 3). The average annual streamflow at all subbasin outlets excluding subbasin 6 outlet (0.002 m^3 s^{-1} higher) in the RCP2.6 scenario was less than or equal to those in the baseline simulation; the differences being minor, though, with a maximum of -0.009 m^3 s^{-1} (subbasin 19 outlet) (Fig. 1). However, for all subbasin outlets the average annual streamflow are larger in the RCP8.5 scenario than in the baseline simulation, the maximum increase being 0.101 m^3 s^{-1} (subbasin 19) and the minimum difference 0.002 m^3 s^{-1} (subbasin 1).

We chose the subbasin 13 and 18 outlets where the two hydrological stations were located (Fig. 1) as examples to represent the climate change impacts on daily streamflow patterns (Fig. 4) and average monthly streamflow patterns (Fig. 5). In the RCP2.6 scenario, the daily streamflow changes at the subbasin 13 outlet ranged between -1.6 and 3.72 m^3 s^{-1} (Fig. 4a) and between -4.82 and 4.35 m^3 s^{-1} at the subbasin 18 outlet (Fig. 4b). In the RCP8.5 scenario, the daily streamflow changes at the subbasin 13 outlet varied between -3.52 and 7.44 m^3 s^{-1} (Fig. 4a) and between -11.76 and 9.9 m^3 s^{-1} at the subbasin 18 outlet (Fig. 4b). The fluctuation amplitude of daily streamflow change from the baseline is thus predicted to be larger in the RCP8.5 scenario than in the RCP2.6 scenario. The average annual frequency of large daily streamflow change events from the baseline (> 30 %) was 7.9 days in the RCP2.6 scenario and 25.6 days in the RCP8.5 scenario, and the peak streamflow increase events mainly occurred during winter and spring and the peak streamflow decrease primarily during summer and autumn (Fig. 4). In both scenarios, the average monthly streamflow increased during winter and spring with a January peak, while it decreased during summer and autumn, peaking in July (Fig. 5).

The changes in the average daily groundwater discharge from the baseline in different subbasins varied and the trends differed between the two scenarios, demonstrating subbasin-level spatially varying impacts of climate change on the groundwater discharge to streams (Fig. 6). In the RCP2.6 scenario, more subbasins showed a decrease in the average daily groundwater discharge rather than an increase, the trend being opposite in the RCP8.5 scenario. The range of the average daily groundwater discharge changes from the baseline simulation at subbasin-level in the RCP8.5 scenario (-474 to 1404 m^3 s^{-1}, Fig. 6c) is, of course, larger than in the RCP2.6 scenario (- 430 to 75 m^3 s^{-1}, Fig. 6b).

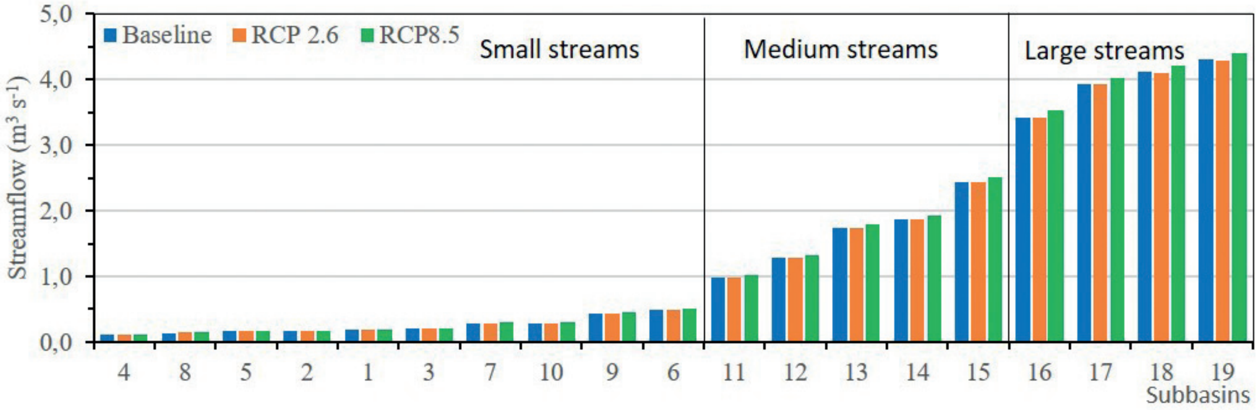

Figure 3. Average annual streamflow at all subbasin outlets in the baseline and the two climate change scenarios together with stream size classification based on the average annual streamflow (small streams: < 0.5 m^3 s^{-1}; medium streams: 0.5-3 m^3 s^{-1}; large streams: > 3 m^3 s^{-1}).

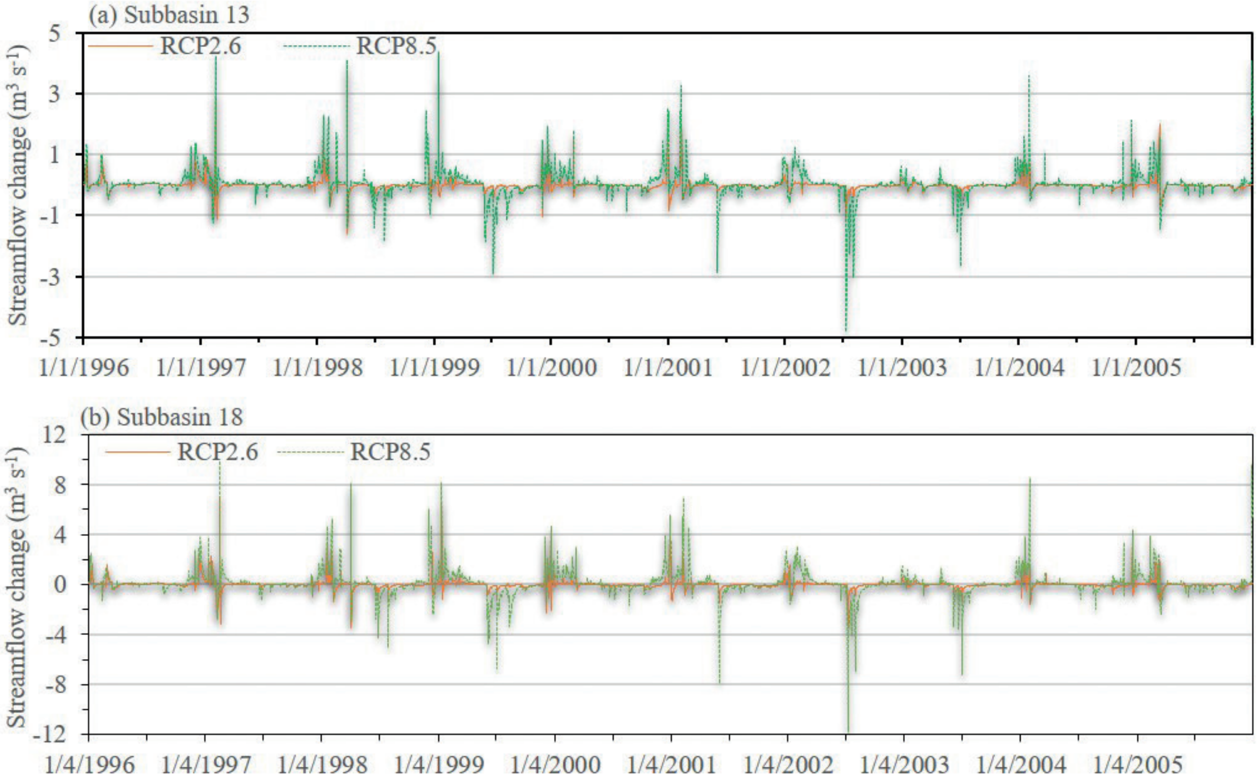

Figure 4. Hydrograph of daily streamflow differences between the climate change scenarios and the baseline simulation at the two hydrological stations (subbasin 13 and subbasin 18 outlets).

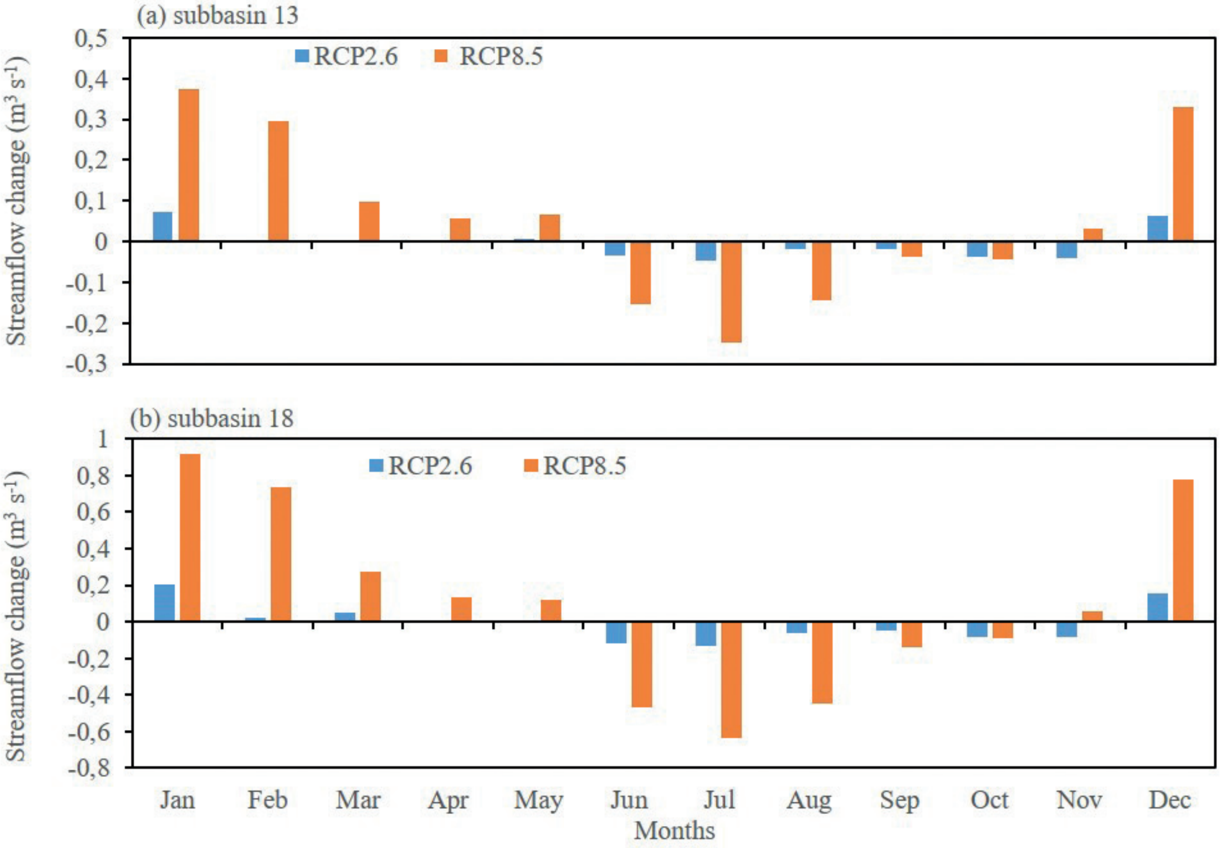

Figure 5. Average monthly streamflow changes in the climate change scenarios from the baseline simulation at the two hydrological stations (subbasin 13 and subbasin 18 outlets).

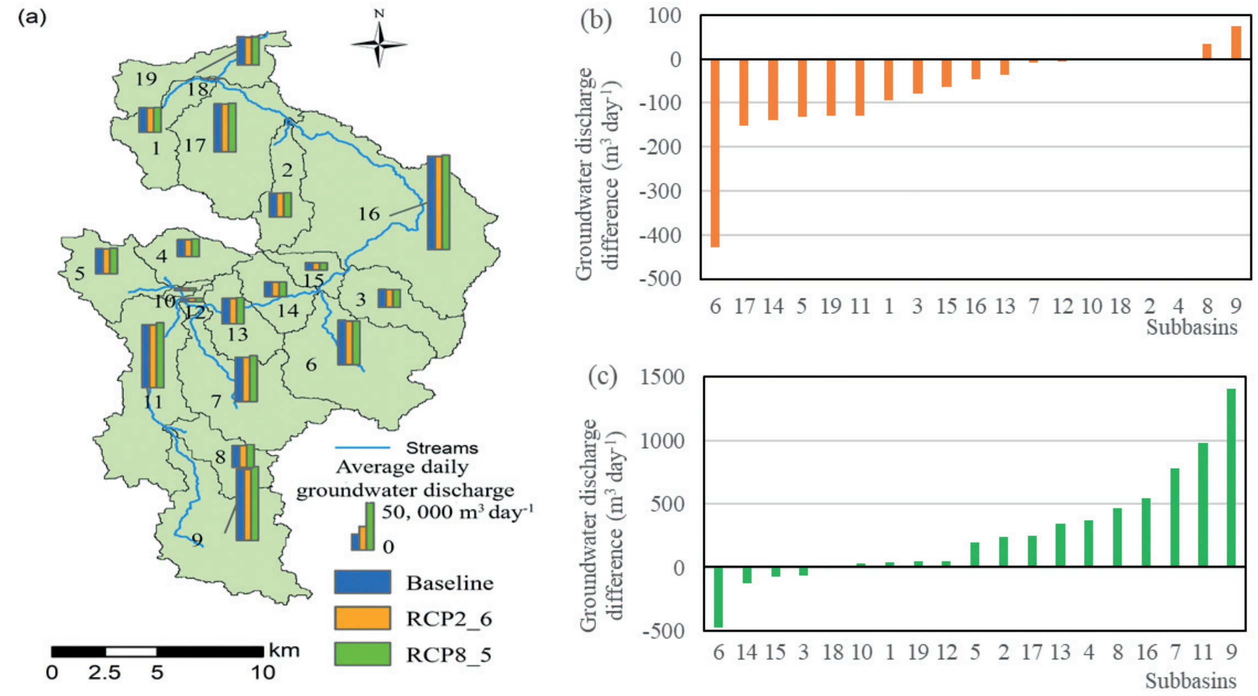

Figure 6. Average daily groundwater discharge (m3 day-1) in each subbasin from the aquifer to the stream network during the baseline period and under the two climate change scenarios as simulated by the calibrated SWAT-MODFLOW model (a); groundwater discharge difference between the RCP2.6 scenario and the baseline simulation in each subbasin (b); groundwater discharge difference between the RCP8.5 scenario and the baseline simulation in each subbasin (c).

3.3 Climate change impacts on flow regime variables

To better represent the climate change impacts on the flow regime and the biota, we classified the streams of all the subbasins into three groups based on their average annual streamflow. They are small streams: < 0.5 $m^3\ s^{-1}$, medium streams: 0.5-3 $m^3\ s^{-1}$ and relatively large streams: > 3 $m^3\ s^{-1}$ (Fig. 3).

Four flow regime variables (BFI, Fre_1, Fre_{25} and Q_{90}) positively affected biotic indices while the other two variables (Dur_3 and Fre_{75}) had negative effects according to the flow-biota empirical equations. Compared with the baseline simulation, BFI slightly increased in all subbasins in both scenarios (Fig. 7). Fre_{25} decreased in all large streams in both scenarios and generally decreased in medium and small streams in the RCP8.5 scenario, while it fluctuated around the baseline in the medium and small streams in the RCP2.6 scenario. Fre_1

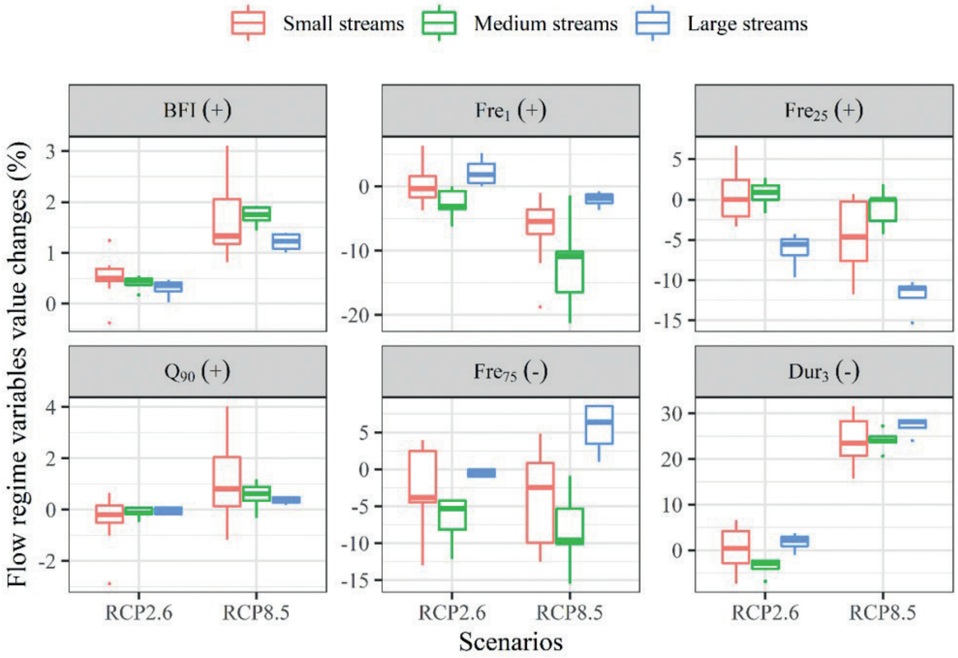

Figure 7. Changes in flow regime variable values from the baseline in the two climate change scenarios (RCP2.6, RCP8.5) in the three differently sized streams (small, medium and large). "+" and "-" indicate, respectively, a positive and a negative effect on stream biotic indices as predicted by the flow-biota empirical models.

decreased in all streams in the RCP8.5 scenario and in the medium streams in the RCP2.6 scenario, whereas it increased in the medium streams and fluctuated around the baseline in the small streams in the RCP2.6 scenario. Q_{90} generally increased slightly in all streams in the RCP8.5 scenario and fluctuated around the baseline in the RCP2.6 scenario. Dur3 generally showed an increase above 20 % in all streams, reaching as much as 32 % in the RCP8.5 scenario, while the changes were much smaller and fluctuated around zero in the RCP2.6 scenario. Fre_{75} increased in all large streams in the RCP8.5 scenario, while decreasing in medium streams in both scenarios and in large streams in the RCP2.6 scenario as well. In the small streams, it fluctuated around the baseline with wide ranges in both scenarios.

3.4 Climate change impacts on biota

For small streams, relative to the baseline simulation, all three biotic indices exhibited both increases and decreases, and the changes differed markedly in both scenarios (Fig. 8). For the medium streams, the fish index ($DFFVa_{EQR}$) increased (>2.5 %) in all subbasins in both scenarios; the macrophyte index ($DVPI_{EQR}$) increased in all subbasins in the RCP2.6 scenario, while in the RCP8.5 scenario both increases and decreases occurred. The macroinvertebrate index ($DVFI_{EQR}$) decreased in all subbasins in both scenarios. For the relatively large streams, both the fish index and the macrophyte index decreased in all subbasins in both scenarios, while the macroinvertebrate index increased in all subbasins in the RCP2.6 scenario but decreased in all subbasins in the RCP8.5 scenario. Comparing the two climate change scenarios, the changes in biotic indices from the baseline, particularly the decreases, were generally larger in the RCP8.5 scenario than in the RCP2.6 scenario (Fig. 8).

4 Discussion

4.1 Climate change impacts on hydrological components, streamflow and groundwater discharge

In this study, the predicted climate change in both scenarios led to an increase of the average annual precipitation, resulting in a change in total flow and a decrease of the average annual water storage increase (ΔS) in soil and aquifers, though most of the increase of precipitation was offset by an increase of evapotranspiration due to elevated temperatures. The predicted climate change will raise the irrigation demand for agriculture and pastures, with an average annual increment of 2 % in the RCP2.6 scenario and of 31 % in the RCP8.5 scenario. In both scenarios, the spatial patterns of the groundwater discharge to the streams were also affected by the climate change due to spatially-varying changes in groundwater recharge, water table elevation, and stream stage. The streamflow changes induced by the climate change demonstrated seasonal characteristics in both scenarios in the form of an increase in the average monthly streamflow during winter and spring and a decrease during summer and autumn (Fig. 5).

Moreover, the two climate change scenarios had different effects on hydrology – the overall streamflow and groundwater discharge in the study area decreased slightly in the RCP2.6 scenario while it increased in the RCP8.5 scenario where the differences from the baseline simulation were larger than in the RCP2.6 scenario.

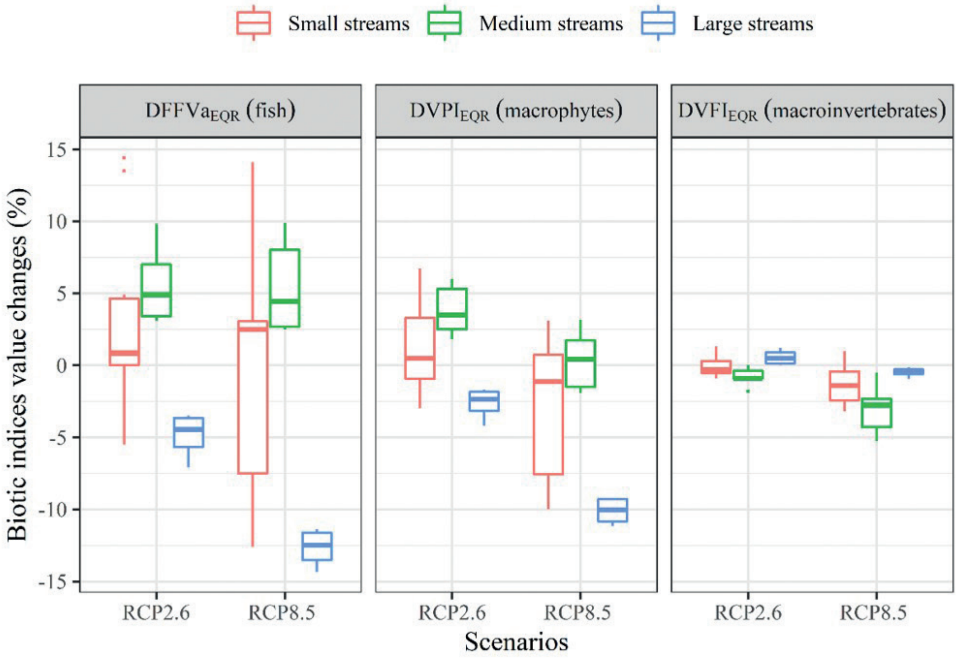

Figure 8. Changes in biotic index values from the baseline in the two climate change scenarios (RCP2.6, RCP8.5) in the three differently sized streams (small, medium, and large).

4.2 Climate change impacts on flow regime variables and biotic indices

In the RCP8.5 scenario, five flow regime variables demonstrated the same change trends from the baseline in terms of different sizes of streams: the values of BFI, Q_{90} and Dur_3 generally increased, while the values of Fre_1 and Fre_{25} decreased, indicating a higher baseflow proportion (BFI) and less extreme low flows (Q_{90}), a longer duration of the peak flow (Dur_3), a reduced weak peak flow events frequency (Fre_{25}) and a lower frequency of high flow (above median flow) events (Fre_1). Fre_{75} (low flow events frequency) increased in the large streams, decreased in the medium streams and fluctuated around the baseline in the small streams. DFFVa is positively related to BFI and Fre_{25} but negatively related to Fre_{75}, reflecting the quality of fish community benefits from a stable discharge regime with low frequency of low flow events and slight disturbances due to weak peak flows (Gräber et al., 2015; Liu et al., 2019a). While BFI increased in all the streams, DFFVa declined in the large streams and in some small streams, which reflects a decrease of Fre_{25} and an increase of Fre_{75}, while the increase of DFFVa occurring in the medium streams and in some small streams was due to an increase of BFI and the decrease of Fre_{75}. That DVPI is positively related to Fre_{25} and negatively related to Dur_3 and Fre_{75} suggests a higher quality of the macrophyte community at intermediate disturbances and a lower quality at strong peak flows or a high frequency of low flow events (Gräber et al., 2015; Liu et al., 2019a). With Dur_3 increasing in all streams, the decline of DFFVa in the large streams and in some small and medium streams was attributed to the decrease of Fre_{25} and the increase of Fre_{75} and Dur_3, while the increase of DFFVa occurring in some medium and some small streams was mainly due to the decrease of Fre_{75}. The positive relationship between DVFI to the two coefficients Q_{90} and Fre1 indicates that the quality of microinvertebrates community DVFI will be higher when the low flows are less extreme and with a higher frequency of flows above the median flow (Gräber et al., 2015; Liu et al., 2019a). With the increase of Q_{90}, the general decline of DVPI in all subbasins was due to the decrease of Fre_1.

In the RCP2.6 scenario, the change trends in flow regime variable values from the baseline demonstrated more differences in terms of different sizes of streams in the RCP8.5 scenario; BFI increasing in all streams as in RCP8.5 scenario, though. Except for BFI, all the other flow regime variables fluctuated strongly around the baseline in the small streams with a wide range of either positive or negative changes in biotic indices changes (Fig. 6). For the medium streams, Fre_1, Fre_{75} and Dur_3 decreased, while Fre_{25} generally increased, indicating a lower frequency of high flow (above median flow) events (Fre_1), a lower frequency of low flow events (Fre_{75}), a shorter duration of peak flow (Dur_3) and a higher frequency of weak peak flow (Fre_{25}). The decrease of Fre_{75} and the increase of BFI and Fre_{25} led to an increase of DFFVa. The decrease of Fre_{75} and Dur_3 and the increase of Fre_{25} produced the increase of DVPI. The decrease of Fre_1 caused the decline of DVFI. For the large streams, Fre_1 and Dur_3 generally increased, while Fre_{25} and Fre_{75} overall decreased. The decrease of Fre_{25} led to the decline of DFFVa, though with a slight increase of BFI and a slight decrease of Fre_{75}. The decrease of Fre_{25} and the increase of Dur_3 created the decline of DVPI, though with the decrease of Fre_{75}. The increase of Fre_1 produced the slight increase of DVFI.

The DFFVa and DVPI were clearly more responsive to the climate change scenarios than DVFI (Fig. 8). The main reason for this is a weakened effect of the two flow regime variables Q_{90} and Fre_1 due to intertwining, yielding a combined impact on DVFI of only 0.02, which is almost the lowest among all the flow regime variables, as shown in the flow-biota empirical relationship equations. The other reason is that the changes in the flow regime variables (BFI, Fre_{25}, Fre_{75} and Dur_3) affecting DFFVa and DVPI were generally larger than of those (Q_{90} and Fre_1) affecting DVFI (Fig. 7).

In both scenarios, DFFVa and DVPI in the large and some small streams showed the largest decrease from the baseline among all the streams (up to - 14.4 % and - 11.2 %, respectively), and these streams are thus most affected due to a higher low flow events frequency (Fre_{75}), a lower weak peak flow events frequency (Fre_{25}) and longer peak flow duration (Dur_3) relative to the baseline. However, DFFVa and DVPI values in the medium and some small streams increased from the baseline in both scenarios (up to 14.4 % and 6.0 %, respectively), indicating that the biota in these streams may benefit from climate change because of a higher baseflow proportion of total flow (BFI), a higher frequency of weak peak flow events (Fre_{25}), shorter peak flow duration (Dur_3) and maybe also a lower frequency of low flow events (Fre_{75}) relative to the baseline.

4.3 Comparison with other studies of the ecological responses to flow regime alterations induced by climate change

Former studies (Kim et al., 2011; Mittal et al., 2016; Pradhanang et al., 2013; Yang et al., 2017) investigating the effects of climate change revealed large regional differences in flow regime alterations – some areas will experience an overall increase in runoff, while others will exhibit a decrease (Goudie, 2006; Pachauri et al., 2014). Besides regional differences, we also found that the overall increase or decrease of runoff depends on the climate change scenario; thus, total flow in the study area decreased by 0.26 % in the RCP2.6 scenario but increased by 2.4 % in the RCP8.5 scenario.

In an analysis of recent observations, Filipe et al. (2012) concluded that the biota communities change composition and homogenize when facing climate changes, but also pointed to the limitation that accurate forecasts of biotic changes induced by climate change are difficult to disentangle from disturbances caused by natural variability, particularly regarding hydrology. In our study, we overcame this limitation to some extent by using the hydrological model SWAT-MODFLOW in the climate change scenario analysis in order to distinguish the streamflow change induced by climate change from that of natural variability and then applied flow-biota empirical models to obtain accurate forecasts of changes in biotic indices due to the streamflow change. Filipe et al. (2012) also suggested that studies of ecological responses to climate change should focus on taxa beyond fish and macroinvertebrates. We quantitatively assessed the impacts of climate change-induced flow regime alterations on stream biota using three key taxonomic identities: fish, macroinvertebates and macrophytes.

A number of studies have discussed the potential impacts of flow regime shifts triggered by climate change on stream ecosystems. Increased streamflow may benefit macroinvertebrates by reducing the sediment concentration, improving the functions of riparian ecosystems (Shen et al., 2011) and increasing the connectivity between the floodplain and main channel, which may lead to increased breeding success of fish and other mobile organisms and allow them access to shallow habitats (Arthington et al., 2010; Cui et al., 2018). Wenger et al. (2011) concluded that flow regime alterations induced by climate change may benefit rainbow trout, *Oncorhynchus mykiss*, as they showed a strong positive response to winter high flows, based on empirical statistical models built from fish surveys at 9,890 sites. Concerning deterioration effects, a decrease of streamflow may lead to a higher frequency of low flow events or prolonged droughts, potentially resulting in temporal die off or complete elimination of some biota and thereby lower species diversity (Bunn and Arthington, 2002). The significant increase of magnitude of streamflow variation will supposedly increase the mortality of benthic invertebrates (Palmer et al., 1992; Townsend et al., 1997) and decrease substrate stability due to high flow velocities and shear stresses (Poff et al., 1997), and thereby damage the river habitat (Stefanidis et al., 2016). In addition, more frequent floods can decrease water quality by transporting more sediment into streams and may wash away some important food sources (e.g. small organisms and organic matter) for aquatic animals (Poff et al., 1997; Cui et al., 2018). Through summarizing the related literatures, Cui et al. (2018) concluded that flow regime shifts induced by climate change could have both positive and negative influences on river ecosystems depending on the degree of flow regime alteration as well as the hydromorphological characteristics of rivers. In correspondence with their conclusion, we found that the predicted flow regime shifts caused by climate change generally improves the ecological state in some small and medium streams but reduces it in the large and in some small streams.

4.4 Uncertainties

The main source of uncertainty regarding our study results arises from the climate change data used. As input data in our study, we used the expected future temperature and precipitation change in entire Denmark at the seasonal level in the form of mean values predicted by DMI using an ensemble of 23 global climate models. As a detailed climate change is hardly accurately predictable, we deem that daily or monthly forecast climate change data are not necessarily more reliable than seasonal forecast data. However, the global climate models themselves contain large uncertainties (Knutti and Sedláček, 2012), though the projection of future climate changes based on an ensemble of climate models is more robust than estimates based on a single model (Olesen et al., 2014; Karlsson et al., 2016; Molina-Navarro et al., 2018). In addition, using the climate projections for Denmark as a whole may create an additional uncertainty in a catchment-scale study.

Uncertainty might also arise from the flow-biota empirical models. Even though these were developed based on hydrological and biological observations from a number of stream sites with varying characteristics (e.g. temperature, stream size and nutrient concentration), the characteristics of the streams of this study in the different scenarios may possibly exceed the application scope of the empirical models. With further development of the flow-biota empirical models based on a larger number of streams and including more factors affecting ecology status quality than flow regime variables, for instance temperature and nutrient concentrations, the overall predictions of the coupled model complex may become more reliable.

5 Conclusions

We combined the SWAT-MODFLOW model with flow-biota empirical models and applied them to a Danish groundwater-dominated catchment to quantitatively assess the impacts of climate change under two scenarios of different greenhouse gas emissions on hydrology and stream biota. Effects were analysed at all subbasin outlets classified into streams of three sizes (small, medium and large).

In both scenarios, the predicted climate change caused obvious changes in hydrology – an increase of the average annual precipitation, evapotranspiration and irrigation demand, a decrease of the average annual water storage increase (ΔS) in soil and aquifers and spatially-varying changes in streamflow and groundwater discharge rates. The differently sized streams experienced different alterations in flow regime variables and thus exhibited different biotic responses to the predicted climate change. The fish and macrophyte quality indices were most responsive in the large and some small streams, decreasing up to - 14.4 % and -11.2 %, respectively, whereas in the medium and some small streams the two indices benefitted from climate change, showing an increase of up to 14.4 % and 6.0 %, respectively. The overall streamflow and groundwater discharge in the study area decreased slightly in the RCP2.6 scenario but increased in the RCP8.5 scenario. In the RCP8.5 scenario, the climate change caused larger changes of biotic indices from the baseline than in the RCP2.6 scenario.

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Appendix A

Comparison of biotic indices at all subbasin outlets between the baseline and the two climate change scenarios (RCP2.6, RCP8.5).

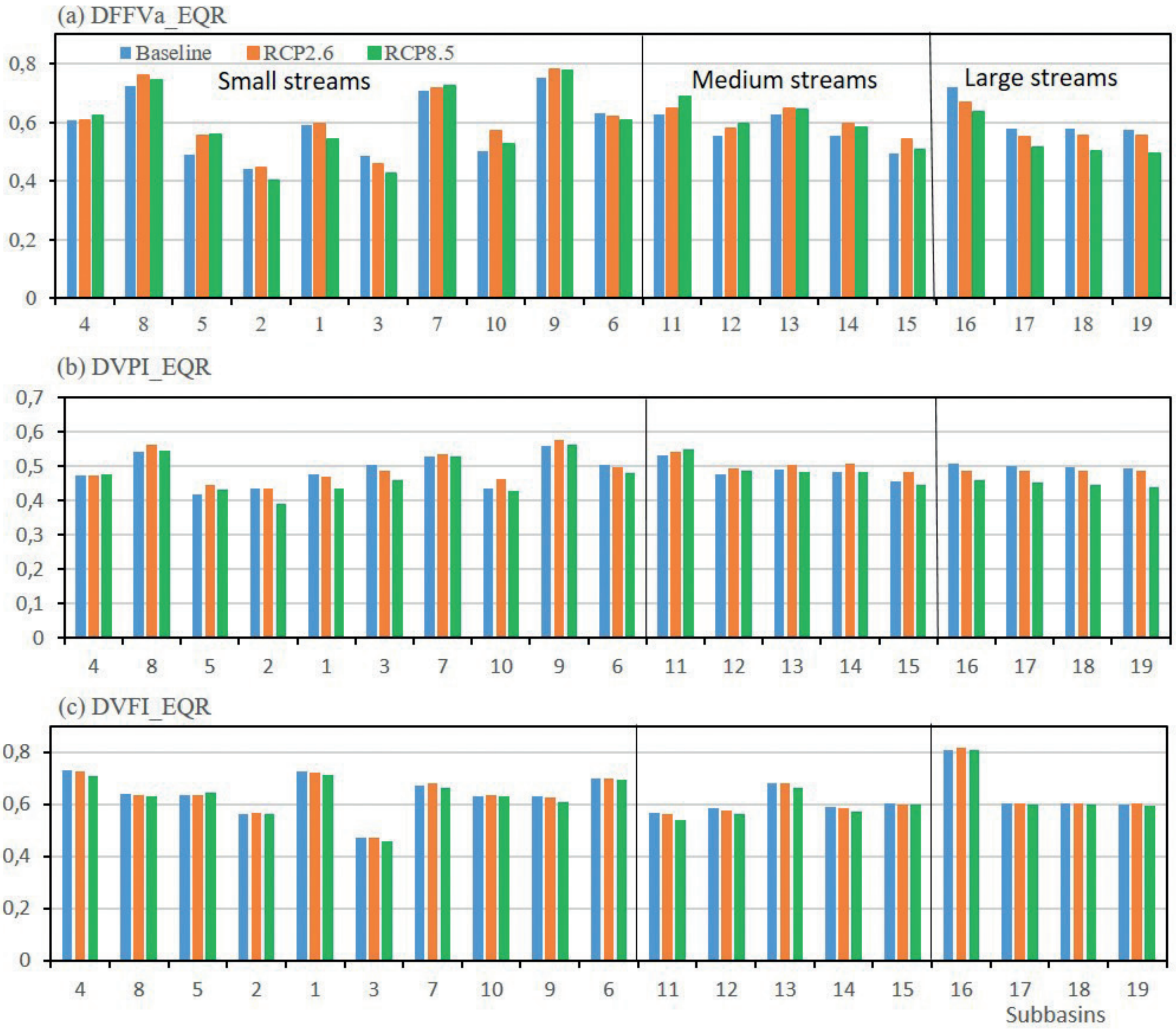

Fig. A1. Comparison of the biotic indices (DFFVa: fish index; DVPI: macrophytes index; and DVFI: macroinvertebrate index) at all subbasin outlets between the baseline and the two climate change scenarios (RCP2.6, RCP8.5).

MODELLING INTERACTIONS BETWEEN GROUNDWATER AND SURFACE WATER AT CATCHMENT-SCALE INFLUENCED BY GROUNDWATER ABSTRACTIONS AND CLIMATE CHANGE