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Improved Targeting Technique and Parsimonious Optimization as Synergistic Combination for Nitrate Hot Spots Identification and Best Management Practices Implementation in a watershed of the Midwestern USA

DISSERTATION

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Doctor rerum naturalium (Dr. rer. nat.)

by

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Declaration of conformity

I hereby confirm that this copy conforms to the original dissertation on the topic:

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Abstract

The contamination of rivers with nitrate from agricultural diffuse sources is not just a risk for ecosystems and their services, but also a health risk for water users. The Great Lakes (USA and Canada) are suffering from eutrophication problems. The Midwest is one of the richest farming land and one of the most productive areas on the planet. Thus, agriculture is one of the biggest drivers of local economies, accounting for billions of dollars of exports and thousands of jobs. The Midwest encompasses the Corn Belt region, a specialised system in corn production. Many of its agricultural basins drain into the Great Lakes. Corn requires a heavy amount of fertilizer to keep the best-yielding varieties. Some of the soils also require artificial drainage due to their low permeability, and to enable agriculture. The Cedar Creek watershed (CCW) in northeastern Indiana in the Corn Belt region is used as a case study area in this dissertation. Intensive agriculture in the CCW is characterised mainly by corn and soybean production. Tile drains are used, ejecting nitrate directly into the water. To find hotspots of nitrate is, then, crucial to avoid water quality deterioration.

Identification of critical source areas of nitrate (CSAs) impairing waters is challenging. There are, mainly, two methodologies to identify hotspots of nitrate for the implementation of Best Management Practices (BMP): the targeting technique and the optimization approach. The targeting technique tends to identify hotspots based on loads of nitrate, omitting geomorphological watershed characteristics, costs for BMP implementation, and their spatial interactions. On the other hand, the parsimonious strategy does contemplate the trade-off of the economic and environmental contribution but requires sophisticated computational resources and it is more data-intense.

This research presents a new framework based on the synergistic combination of both methodologies for the identification of CSAs in agricultural watersheds. Changes in watershed response due to alternative BMP applications were assessed using the model Soil and Water Assessment Tool (SWAT). Outputs in SWAT (nitrate export rates and nitrate concentration at the subbasin level) were used to evaluate the changes in water quality for the CCW. The newly developed targeting technique (HosNIT) considers SWAT

outputs and intrinsic watershed parameters such as stream order, crop distance to the draining stream, and downstream nitrate enrichment/dilution effects within the river network. HosNIT establishes a workflow, based on a threshold system for the parameters considered, in order to spatially identify priority areas from where nitrate is reaching water. The more precise hotspots of nitrate are identified, the more improved the allocation of limited resources for conservation practices will be.

HosNIT allows for a more spatially accurate CSAs identification, which enables a parsimonious optimization for BMP implementation. This parsimonious strategy will test BMP's performance based on the environmental contribution and cost at the hotspots determined by HosNIT.

The optimised solution for the CCW comes from the environmental contribution (decrease percentage of nitrate concentration at outlets) per dollar spent. For this case study means a year average of 3.7% of nitrate reduction with the optimised selection of scenarios for the studied period.

Zusammenfassung

Die Verunreinigung von Flüssen mit Nitrat aus diffusen landwirtschaftlichen Quellen ist nicht nur eine Gefahr für die Ökosysteme und ihre Leistungen, sondern auch ein Gesundheitsrisiko für die Wassernutzer. Die Großen Seen (USA und Kanada) leiden unter Eutrophierungsproblemen. Der Mittlere Westen ist eines der reichsten Agrargebiete und eines der produktivsten Gebiete der Erde. Daher ist die Landwirtschaft eine der wichtigsten Triebfedern der lokalen Wirtschaft, die für Exporte in Milliardenhöhe und Tausende von Arbeitsplätzen verantwortlich ist. Der Mittlere Westen umfasst die Region Corn Belt, ein auf den Maisanbau spezialisiertes System. Viele seiner landwirtschaftlichen Einzugsgebiete entwässern in die Großen Seen. Mais benötigt viel Dünger, um die ertragreichsten Sorten zu erhalten. Einige der Böden müssen außerdem aufgrund ihrer geringen Durchlässigkeit künstlich entwässert werden, um die Landwirtschaft zu ermöglichen. Das Wassereinzugsgebiet des Cedar Creek (CCW) im Nordosten Indianas im Maisgürtel wird in dieser Dissertation als Fallstudiengebiet verwendet. Die intensive Landwirtschaft im CCW ist hauptsächlich durch den Anbau von Mais und Sojabohnen gekennzeichnet. Es werden Flächendrainagen verwendet, die Nitrat direkt in das Wasser ausstoßen. Um eine Verschlechterung der Wasserqualität zu vermeiden, ist es daher von entscheidender Bedeutung, Nitrat-Hotspots zu finden.

Die Identifizierung von kritischen Nitratquellen (CSA), die die Gewässer beeinträchtigen, ist eine Herausforderung. Es gibt im Wesentlichen zwei Methoden zur Ermittlung von Nitrat-Hotspots für die Umsetzung der besten Bewirtschaftungspraktiken (BMP): die Targeting-Technik und der Optimierungsansatz. Bei der Targeting-Technik werden die Hotspots in der Regel anhand der Nitratbelastung ermittelt, wobei die geomorphologischen Merkmale des Einzugsgebiets, die Kosten für die Umsetzung von BMP und deren räumliche Wechselwirkungen außer Acht gelassen werden. Andererseits berücksichtigt die parsimonische Strategie den Kompromiss zwischen wirtschaftlichem und ökologischem Beitrag, erfordert jedoch anspruchsvolle Rechenressourcen und ist datenintensiver.

Diese Forschungsarbeit stellt einen neuen Rahmen vor, der auf der synergetischen Kombination beider Methoden zur Identifizierung von CSAs in landwirtschaftlichen Wassereinzugsgebieten basiert. Veränderungen in der Reaktion von Wassereinzugsgebieten aufgrund alternativer BMP-Anwendungen wurden mit dem Modell Soil and Water Assessment Tool (SWAT) bewertet. Die Ergebnisse von SWAT (Nitratexportraten und Nitratkonzentration auf der Ebene der Teileinzugsgebiete) wurden verwendet, um die Veränderungen der Wasserqualität für die CCW zu bewerten. Die neu entwickelte Zielsetzungstechnik (HosNIT) berücksichtigt die SWAT-Ergebnisse und intrinsische Wassereinzugsgebietsparameter wie die Ordnung der Flüsse, den Abstand der Kulturen zum abfließenden Bach und die flussabwärts gelegenen Nitratanreicherungs-/Verdünnungseffekte innerhalb des Flussnetzes. HosNIT legt einen Arbeitsablauf fest, der auf einem Schwellenwertsystem für die berücksichtigten Parameter basiert, um räumlich prioritäre Gebiete zu identifizieren, von denen aus Nitrat ins Wasser gelangt. Je genauer Nitrat-Hotspots identifiziert werden, desto besser können die begrenzten Ressourcen für Schutzmaßnahmen zugewiesen werden.

HosNIT ermöglicht eine räumlich genauere Identifizierung von CSAs, was eine sparsame Optimierung für die Umsetzung von BMP ermöglicht. Mit dieser vereinfachten Strategie wird die Leistung der BMP auf der Grundlage des Umweltbeitrags und der Kosten an den von HosNIT ermittelten Hotspots getestet.

Die optimierte Lösung für die CCW ergibt sich aus dem Umweltbeitrag (prozentuale Verringerung der Nitratkonzentration an den Auslässen) pro ausgegebenem Dollar. Für diese Fallstudie bedeutet die optimierte Auswahl der Szenarien für den untersuchten Zeitraum eine durchschnittliche jährliche Nitratreduzierung von 3,7 %.

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Nomenclature

ALF	**Alf**alfa
AA	**A**nhydrous-**A**mmonia
APP	**A**mmonium-**P**olyphosphate
ARS	**A**gricultural **R**esearch **S**ervice
BMPs	**B**est **M**anagement **P**ractices
Bu	**B**ushel
CCDT	**C**over **C**rop **D**ecision **T**ool
CCW	**C**edar **C**reek **W**atershed
CWPS	**M**onocrop Soybean
CEAP	**C**onservation **E**ffects **A**ssessment **P**roject
CDL	**C**ropland **D**ata **L**ayer
CFD	**C**rop **F**requency **D**ata
CSAs	**C**ritical **S**ource **A**reas
CSIL	**M**onocrop corn
DDRAIN	**D**istance to **S**ub-Surface **D**rain
DEM	**D**igital **E**levation **M**odel
DIS_STREAM	**A**verage **D**istance to **S**tream
DLU	**D**efault **L**and **U**se
EEA	**E**uropean **E**nvironment **A**gency
EQIP	**E**nvironmental **Q**uality **I**ncentive **P**rogram
FLOCNST	**A**verage **D**aily **W**ater **L**oading
GDRAIN	**D**rainage **L**ag **T**ime
Ha	**H**ectare
HYGRP	**H**ydrologic characteristics of the soil
HRU	**H**ydrologic **R**esponse **U**nit
IDEM	**I**ndiana **D**epartment of **E**nvironmental **M**anagement
Kg	**K**ilograms
Ksat	**S**aturated **H**ydraulic **C**onductivity of Soil

LL	**L**iquid **L**imit
m	**M**eters
m^3	**C**ubic **M**eter
MCL	**M**aximum **C**ontaminant **L**evel
mg/l	**m**illigrams/**l**itre
mm	**m**illimeters
MMT	**M**illion **M**etric **T**ons
N	**N**itrogen
NSE	**N**ash **S**utcliffe **E**fficiency
NASS	**N**ational **A**gricultural **S**tatistics **S**ervice
NCDC	**N**ational **C**limate **D**ata **C**enter
NHD	**N**ational **H**ydrography **D**ataset
NO_3-	**N**itrate
NRCS	**N**atural **R**esource **C**onservation **S**ervice
P	**P**hosphorous
PBIAS	**P**ercent **B**ias
R^2	**C**oefficient of determination
RE	**R**adius for tile
Rh	**H**ydraulic **R**adius
SJRW	**S**aint **J**oseph **R**iver **W**atershed
SJRWI	**S**aint **J**oseph **R**iver **W**atershed **I**nitiative program
SOYB	**S**oybean
STATSGO	**S**tate **S**oil **G**eographic
SSURGO	**S**oil **S**urvey **G**eographic **D**atabase
SWAT	**S**oil and **W**ater **A**ssessment **T**ool
USDA	**U**nited **S**tates **D**epartment of **A**griculture
USGS	**U**nited **S**tates **G**eological **S**urvey
WMO	**W**orld **M**eteorological **O**rganization
WWHT	**W**inter **Wheat**

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1 Introduction

1.1 Background and motivation

Population growth and the need for continuous production of food lead to the farming of high-yielding crop varieties. This maximization of food produced by agricultural ecosystems in the context of intensive agriculture has led to high fertilizer farming inputs, and to the degradation of ecosystems due to the diminishing of water quality. The contamination of water due to nitrate from diffuse pollution is, in most cases, caused by human activities.

Especially, nitrate in water is involved in groundwater pollution from agricultural diffuse sources and contributes to the eutrophication of coastal waters in many parts of the world. Also, nitrate contamination of drinking water is especially harmful for babies (baby blue syndrome), and it is a concern in drinking-water supply sources for urban areas.

The Corn Belt region in the Midwest area of the USA, is an intensive food producer and exporter of grain crops. A worldwide famous corn region, whose soil requires fertilizer inputs of nitrate and, in some parts, artificial drainage to enable agriculture in low permeable, but fertile, soils. This artificial drainage that removes the excess of water also ejects nitrate directly into the water.

Conservation practices (or BMP) make an effort to control the nitrate export rate to aquifers. Despite of the many efforts from conservation programs, farmers and the national administration, the Great Lakes and the Gulf of Mexico are facing hypoxia and eutrophication problems in their waters because of agricultural diffuse sources. Resources have been, sometimes, allocated at places where not the greatest pollutant reduction is achieved. Diffuse pollution originates from the idea of the difficulty of spatially identifying the source of the pollutants. This specific trait makes diffuse pollution one of the major pressures on water quality.

This research aims to allocate BMPs where they would be more environmental and economic efficient in order to face the nitrate problem contamination of groundwater.

1.2 Structure of the dissertation

The dissertation is a monograph structured into seven chapters:

Chapter 1 provides a general introduction of the dissertation and background and the motivation for addressing this research topic.

Chapter 2 introduces the research background; a series of subchapters that tackles the problem of nitrate in the Corn Belt region from diffuse sources (agriculture) and the importance of the land use input in the performance of the SWAT hydrological model. The last subchapter focuses on the two different Plans (methods) in order to target CSAs of nitrate for later BMPs implementation.

Chapter 3 presents the objective of the dissertation and the specific hypotheses, which are tested.

Chapter 4 describes the geographical, hydrological, and land-use characteristics of the study region, the Cedar Creek Watershed of northeast Indiana in the US. It provides an overview of the region.

Chapter 5 gives a description of the research methods used in this study, broken down into six subchapters. First, the SWAT model is introduced with the two different land use scenarios tested. Second, the Targeting technique (HosNIT) is developed as the importance to combine the nitrate export parameter with intrinsic watersheds characteristics such as: the distance to stream and the stream network morphology (stream order) for spatial identification of CSAs. In subchapter three, the BMPs to implement from an adaptive targeting perspective are described with their combination and scenario analysis in subchapter four. Subchapter five presents the new methodology: Combination of Plan-based methods (HosNIT) & Process-based methods (Parsimonious optimization) for CSA identification and BMP implementation. The first part introduces the HosNIT methodology as part of a developed Targeting technique for hotspot identification, and the second addresses the BMP implementation in already identified CSAs through a Parsimonious optimization approach. In this section, the synergy of the targeting technique with parsimonious optimization is explained for the finer identification of hotspots of nitrate. The Parsimonious optimization will consider two functions: the environmental contribution (nitrate concentration reduction in surface waters) and the costs of conservation practices. The last subchapter tests the sensitivity of HosNIT through fertilizer reduction rates and SWAT simulations.

Chapter 6 has five subchapters related to the results and their discussion. The first subchapter shows results on the SWAT model calibration, the second addresses and depicts the spatio-temporal variation of hotspots with HosNIT due to different crop rotation scenarios. It follows with the BMP implementation where functions for the optimization are analysed through SWAT simulations. Finally, the optimized solution for the watershed is presented in subchapter 4 and hypotheses developed in Chapter 3 are verified from the results.

Chapter 7 consists of a synthesis of the study with a summary of the major findings and an outlook, closing with a last subchapter of a critical evaluation and potential further improvements in the methodology.

The list of references and the supplementary material are added at the end of the monograph.

2 Research background

2.1 Corn Belt region (USA) and its nitrate problem impairing waters

In the 1970s, Kohl et al (1971) brought already to discuss the relation of nitrate fertilisation with the increase of nitrate concentration in water bodies in the Corn Belt region in the Midwestern United States.

Many studies have aimed at identifying critical CSAs of nitrate in agricultural watersheds in recent decades (Kurunc et al., 2011; Andersen et al., 2016, Teshager et al., 2017, Serra et al., 2019, Shukla and Saxena, 2020). After the Green Revolution, increasing application of nitrogen-based fertilisers became common in intensive agriculture, which led to higher yields worldwide. The amount of applied nitrogen fertilisers increased from 5 MMT (million metric tons) in 1950 to 90 MMT in 2000, with predictions of 120 MMT in 2030 (Vance, 2001). At the same time, increasing concentrations of nitrate in waterbodies have caused numerous environmental problems for ecosystems and also affected human health via drink water (i.e. blue baby syndrome (Majumdar, 2003)). The Corn Belt region is well-known for the problem with nitrate pollution from non-point sources. The transition to specialised farming systems has been very apparent in the states of Ohio, Indiana, Illinois, Iowa, Wisconsin, and Minnesota (Sulc and Tracy, 2007).

Agricultural nutrient exports to river bodies contribute to hypoxia in the Gulf of Mexico and eutrophication in the Great Lakes (Smith et al., 2008). Nutrient exports from agricultural ecosystems are also a concern in Europe. Because of nitrate inputs, many water-related ecosystem services in watersheds are impaired, affecting notably municipal drinking water provision, river habitats, recreational swimming and beach use, and fishing (EUROSTAT, 2012). Eutrophication problems in coastal waters are characterised by the proliferation of algal blooms that are aesthetically unappealing and reduce water clarity. The algal blooms frequently involve toxic cyanobacteria, which pose a threat to public health, and the decomposition of algae under anaerobic conditions may produce toxic gases (EUROSTAT, 2012).

To face this crisis, ambitious efforts are being undertaken in order to be able to reduce 40% in nutrient losses from agriculture by states in the Mississippi River and Great Lakes drainage basins (McLellan *et al.*, 2018).

Since the 1990s, numerous agri-environmental indicators were developed to assess the adverse effects of cropping and farming systems on the environment, such as water pollution, soil erosion, and emission of greenhouse gases (Bockstaller et al., 2008). In the US, water quality is, nowadays, deteriorated through the Corn Belt region, and it is a key environmental indicator of sustainability in agricultural landscapes (Tyndall and Roesch, 2014).

The United States Environmental Protection Agency (US EPA) has set a maximum contaminant level (MCL) for nitrate to 10 (nitrate, expressed as nitrogen, N) mg N/l (milligrams/litre) and for nitrites at 1 ppm (1 mg/L) in water as enforceable standard (U.S. Department of Health and Human Services, 2013). In addition, in Europe waters are impaired from diffuse sources of nitrate and authorities are making efforts to improve the situation. According to the Nitrates and Drinking Water Directives of the European Environment Agency (EEA), nitrate concentrations and loads in rivers of the European Union countries should be below the 11.3 mg/l (as N) limit (equivalent to 50 mg NO_3^--/l). However, current concentrations are often higher and lead to eutrophication in many of Europe’s coastal waters (EUROSTAT, 2012).

The trend in the late–20th-century presents a cautionary tale for nutrient management policy in a changing climate with an accelerated hydrologic cycle (Donner and Scavia, 2007). Future climate change will further impact water quality in both direct and indirect ways by influencing the hydrological cycle and processes of nutrient transportation and transformation (Wang, Flanagan, *et al.*, 2018) which might make CSAs identification even more challenging. Conservation programs are seen as crucial for restoring, but also for protecting the good ecological status of freshwater bodies (Udias *et al.*, 2016).

2.2 Best Management Practices for water quality improvement

BMPs are physical or cultural controls working individually or as a group, appropriate to the source, location, and area climate for the pollutant to be controlled (US EPA, 2011). Agricultural conservation practices, often called best management practices or BMPs, are widely used as effective measures for preventing or minimising pollution from nonpoint sources within agricultural watersheds (Motsinger *et al.*, 2016). Despite the United States Department of Agriculture (USDA) efforts to fund conservation activities, agriculture-related water quality problems persist across the US. and, nationwide, the effectiveness of BMPs implementation strategies at watershed-scale are still not well understood (Teshager *et al.*, 2017).

There are two types of BMPs, cultural and structural.

Cultural BMPs are characterised by in-field practices. BMPs such as no-till and nutrient management minimise and prevent erosion or nutrient transport at the field level. Structural BMPs are land-based installations designed to capture, buffer, or treat sediment or nutrients before reaching the water. They normally involve different kinds of structures (natural or artificial) placed within field-edges and often feature perennial vegetation and/or landform engineering generally considered, most of the time, permanent. Some examples of structural BMPs for the Corn Belt region are vegetative filter strips, terraces, constructed/restored wetlands, and riparian buffers (Tyndall and Roesch, 2014). Edge-of-field and beyond-field practices are structural practices that require upfront investment but can deliver environmental benefits for 30 years or more if placed, designed, and managed correctly (McLellan *et al.*, 2018). Interaction of BMPs can further impact the amount and types of diffuse source pollutants transported to the watershed outlet (Veith *et al.*, 2004).

In this study, related to nitrate in water quality, just cultural BMPs were implemented: reduced tillage, winter catch crops and transformation of monocropping practices into rotations.

Diversification of crop rotations is considered an option to increase the resilience of European crop production under climate change (Kollas *et al.*, 2015). Some areas in the CCW are still under soybean/corn monocropping practices. Cover cropping in the off-season months offers a potential solution for reducing NO_3^-, because it can increase the amount of time the land is covered with growing vegetation. Growing cover crops remove water and N from the soil profile through transpiration and N uptake (Strock *et al.*, 2004). The use of cereal rye helps to avoid the nitrate leaching due to its potential as a scavenger of residual soil N following corn.

On the other hand, reduced tillage is one of the most studied BMPs in reducing pollutants. Tillage removes larger pores when disturbing the soil in order to make planting easy or mix in fertiliser into the soil. Reducing tillage will reduce these disruptions but not eliminate them (Motsinger *et al.*, 2016).

In Extension materials about the implementation of BMPs and before farmers choose one or several BMPs, it is important to consider a balance between three factors: 1) the bio-physical effectiveness of the BMP in performing its task at the selected level; 2) the compatibility of the practice according to equipment and time/labour availability, etc.; and 3) the economic feasibility of the BMP relative to farmer willingness to pay and/or alternative management options (Tyndall and Roesch, 2014).

Several federal and state sources provide funding, depending on which BMP is implemented. Most funding will be available through the USDA-Natural Resource Conservation Service (NRCS) Environmental Quality Incentive Program (EQIP) (Gregory and Meier, 2008).

2.3 The importance of crop rotations as input for good performance of hydrological models

Hydrological models can eliminate the complexity and expensive nature of laboratory and field observations on implementing BMPs in improving water quality. However, they must be calibrated and validated using experimental field data (Maski *et al.*, 2007). The spatial land use information is one of the key input parameters for regional agro-ecosystem modelling. The SWAT model is one of the few models suitable for calculating yield and environmental impacts with crop rotation information as input. Furthermore, to assess crop-specific management in a spatio-temporal context accurately, parcel-related crop rotation information is additionally needed (Waldhoff *et al.*, 2017). Crop rotations are an important factor in the design and implementation of sustainable agricultural systems (Schönhart *et al.*, 2009). They are an important property of agricultural systems and should be accounted for in integrated land-use impact assessments. Different crop rotations can have different environmental footprints depending on the crop types and rotation frequencies (Jiang *et al.*, 2021). These crop rotations are essential for bio-physical process models and economic land use optimisation models, which are increasingly used to jointly assess economic and environmental impacts (Schönhart *et al.*, 2009). For these tools and methodologies, data quality plays an important role in generating accurate outputs and results. Using realistic crop rotations can be essential for capturing the proper model (Witing and Volk, 2013). Therefore, the correct identifications of practices and crop rotations in the fields are relevant for proper model performance. However, insufficient data on crop rotations often challenge their implementation (Schönhart *et al.*, 2009). Ullrich and Volk (2009) showed that the SWAT model is very sensitive to applied crop rotations – with the implementation of catch crops first in their sensitivity ranking.

In the Corn Belt region approximately 20% of the corn (*Zea mays* L.) is grown in continuous monoculture, while most of the remaining 80% is grown in 2-yr rotation with soybean [*Glycine max* (L.) Merr.](Sulc and Tracy, 2007). Cover cropping with rye reduced drainage discharge relative to winter fallow, although the magnitude of the effect varied with annual precipitation (Strock *et al.*, 2004). These intermediate crops are grown for the purpose of catching and recycling nutrients, in particular nitrogen, preventing rainfall from percolating through the soil and leaching nutrients out of the rooting zone (Kollas *et al.*, 2015). Extensive use of simple, short-term crop rotations and continuous, annual cropping systems has generally been economically successful, resulting in dramatic growth of output for US farmers (Sulc and Tracy, 2007).

These specific crop patterns and their location in a watershed will affect water quality, e.g. by influencing nitrogen content in water. It is absolutely necessary to have spatial information on the actually applied crop rotations available to conduct regional agro-ecosystem modeling (Waldhoff *et al.*, 2017).

2.4 Conventional methods for the identification of Critical Source Areas (CSAs) for nitrate and implementation of Best Management Practices (BMPs): Plan and Process based

Both point and non-point sources contribute pollution of Great Lakes surface waters (Giri *et al.*, 2012). (Gitau *et al.*, 2007) suggests that there is a need to evaluate potential BMP solutions prior to implementation in order to preclude solutions that are unlikely to offer adequate pollutant reduction benefits. CSAs are diffuse sources whose spatial location represents difficulties in their identification, leading many times to the non-effective allocation of economic resources from regional and national programs. Comparative evaluation of non-point sources control through selective BMP application is more feasibly accomplished through plan− or performance−based methods (Veith *et al.*, 2004). The trade-off between the decrease data intensity and skill requirements of targeting (plan), and benefits of achieving selective BMP placement through optimization (performance) should be considered (Veith *et al.*, 2004).

2.4.1 Plan based: Targeting approach for BMPs placement

Plan-based methods assign BMPs based on the previous spatial identification of critical areas in a watershed. State and federal programs implement water and soil conservation measures where they are needed most due to the previous identification of CSAs at the watershed scale. Even with the potential advantages, many of these programs do not actively target CSAs (White *et al.*, 2009).

Targeting is a plan−based method. It focuses on critical areas that are anticipated to heavily contribute to diffuse pollution (Veith *et al.*, 2004). Still, interactions among BMPs on pollutant reduction are rarely considered (Chiang *et al.*, 2014). Targeting CSAs in the watershed is a well-known procedure for implementing BMPs to control non-point source pollution and to improve environmental quality (Giri *et al.*, 2012). According to Her *et al.* (2017) the spatial variation of pollutant loads is normally used as the basis of targeting strategies because it is easy and simple to be identified while their temporal variations are few times considered. Areas producing substantial pollutant loads are often regarded as optimal locations for the implementation of conservation practices”.

Compared to the optimization method, and in order to obtain the same pollutant reduction, larger areas are needed for BMP implementation with the targeting technique (Chiang *et al.*, 2014). The identification of hotspots of nitrate leaching is important in mitigating environmental effect of nitrate. Once identified, the hotspots can be further analyzed in detail for evaluating appropriate alternative management techniques to reduce impact of nitrate on groundwater (Kurunc *et al.*, 2011). While using the targeting approach in published studies, indicators for CSAs are often focusing at nitrate loads and/or spatial distributed hotspots of the rates of nitrate being leached (Jha *et al.*, 2010, Panagopoulos *et al.*, 2011; Chiang *et al.*, 2014; Mehdi *et al.*, 2015). Also in some studies are considered the Concentration Impact Index, Load Impact Index, Load per Subbasin Area Index, and Load per Unit Area Index as indicator for the detection of CSAs (Giri *et al.*, 2012; Srinivasan, 2008).

2.4.2 Performance based: Optimisation approach for BMPs placement

When establishing a targeting strategy, the spatial interactions among BMPs which consider environmental and cost traits, are not typically analysed. Optimization problems involving conflicting objectives introduce trade-off solutions rather than a single optimal solution (Bekele and Nicklow, 2005). Based on the targeting criteria, the single BMP scenario for the specific watershed may be (or not) the most cost-effective scenario. The optimization procedure can achieve the same water quality goals as intended by the targeting strategy, and in a more cost−effective way (Veith *et al.*, 2004). On the other hand, disadvantages are the much longer computation times than plan based methods (Chiang *et al.*, 2014).

The identification of efficient BMP strategies is a spatial multi-criterion optimization problem when different management practices are to be considered together at the watershed scale (Udias *et al.*, 2016). The optimization approach provides flexibility in implementation because of the number of near-optimal solutions suggested, offering different alternatives to stakeholders. At the same time, optimization plans will accomplish the same pollutant load criterion in a less expensive way (Veith *et al.*, 2004). The conservation strategy must find a balance between costs and the environmental level objective. The trade-off solutions for gross margin and the environmental contribution are important to policy makers since they provide information about the cost-efficiency of alternative agricultural landscapes (Bekele and Nicklow, 2005).

3 Objective and Hypotheses

3.1 Objective: New concept for improvement of water quality (nitrate) in agricultural watersheds: Critical Source Area identification (HosNIT) + BMP implementation (Parsimonious optimization)

An important challenge to address is the water quality issue faced by agricultural interests in the Corn Belt region (Tyndall and Roesch, 2014). Nutrient losses from agro-ecosystems are caused by a complex interplay between climate, topography, soil properties and agricultural management practices (Andersen *et al.*, 2016). Non-point sources of nutrient pollution are one primary reason for the degradation of water quality in the Great Lakes, which impacts millions of residents in the states and provinces that border them (Wang, Flanagan, *et al.*, 2018). Identification of critical sources of nitrate is more challenging in agricultural watersheds due to diffuse pollution from fields. There are certain critical areas within a watershed that are disproportionally contributing with large amounts of pollutants (Chiang *et al.*, 2014). Meanwhile, resources for the improvement of water quality are limited. This highlights the importance of being sure that scarce resources are targeting locations where they will be most effective (McLellan *et al.*, 2018). Prioritisation of stream management is a crucial goal to protect water quality downstream and to obtain an overall water quality improvement across the stream network. BMPs selected through a targeting strategy might not be the most cost-effective conservation practice for the watershed. In contrast, the optimisation approach, evaluates numerous BMP scenarios while considering their interactions and assessing the cost-effectiveness of the different scenarios (Chiang *et al.*, 2014). In this research, an approach has been developed, combining both plans without considering a large amount of data and avoiding time-consuming computer processes, incorporating into the targeting approach a cost/benefit analysis (Parsimonious optimisation).

It requires an in-depth understanding of the hydrology and related nutrient flow at the watershed scale in order to effectively implement BMPs to select the "right conservation practice” and the “right place” along the flow path—this is and analytical process that, still, has to be well incorporated into conservation planning (McLellan *et al.*, 2018). Given this background the purpose of this research is to develop a decision-making framework that can be adequately extended to other watersheds for (1) assessing the role of basin-wide, agricultural landscapes in reducing nitrate diffuse pollution and (2) to extract the synergy of targeting (HosNIT) and optimization (parsimonious optimization) approaches' combination for a new methodology in BMPs implementation.

The reference for parsimonious optimisation is given by the idea behind of the process-based methods where functions such as environmental contribution *vs* costs on BMP implementation are assessed, rather than providing a near-optimal number of solutions, what is not the scope of this study.

Moreover, two different land-use scenarios will be implemented in order to quantify the importance of the use of reliable data (crop rotations) in detecting hotspots of nitrate release into water resources.

3.2 Hypotheses

The Cedar Creek Watershed (CCW) in Indiana is used as a case study area in this dissertation and underlying research was conducted in this watershed.

1- The hypothesis of this research is that important reductions of nitrate in the stream network can be achieved at an optimized cost by applying spatial targeting approaches (plan-based) to identify optimal conservation practice combinations. Adding watershed characteristics (such as network morphology, drainage distances and headwater contribution to downstream waters), to nitrate loads as regular parameter in conventional methods for the spatial detection of CSAs, will obtain a more precise and finer identification of them. This finer targeting technique in this study is mentioned as HosNIT. Sharpening the targeting technique with geomorphological traits of watersheds will improve the spatial location of areas which contribute at most to impairing waters with nitrate pollution.

As the study area of this work is dominated by agricultural land, the reduction of nitrate concentration in aquifers and rivers should focus on reducing diffuse nitrate losses from agriculture. Looking at alternative management options (i.e., conservation practices) will help to avoid the impairing of waters.

2- Through the combination of the targeting technique methodology (HosNIT) and an optimisation approach (parsimonious optimisation), a synergy will be created from both plans, where the best for both methodologies will be used to a better extent. Parsimonious optimization on critical nitrate areas leads to the effective reduction of nitrate in water without sophisticated computational resources, and considering costs on BMP implementation and environmental contribution.

4 Study area: Cedar Creek Watershed, Indiana, US

The CCW is located in northeastern of Indiana (41°04'48" to 41°56'24" N and 84°52'12" to 85°19'48"W), USA, within the St. Joseph River Watershed (SJRW) which is situated in northeastern Indiana, northwestern Ohio and southeastern Michigan, with a drainage area of 2,821 km². The SJRW is one of 14 benchmark watersheds in the USDA Agricultural Research Service (ARS) Conservation Effects Assessment Project (CEAP) watershed assessment studies. The CEAP watershed assessment studies are a combined effort of USDA NRCS and ARS to quantify the environmental benefits of conservation practices supported by the USDA (Heathman *et al.*, 2009). The SJRW is primarily rural with little urban land outside of one large metropolitan area (Fort Wayne) and a few small municipalities. The CCW is its largest tributary and covers an area of approximately 707 km². It belongs to the United States Geological Survey (USGS) hydrologic unit region 04 Great Lakes. The CCW connects Allen, Dekalb and Nobel Counties.

Figure 1 shows the average per month for the period 2005 - 2020 for total precipitation (mm) and temperature in °C.

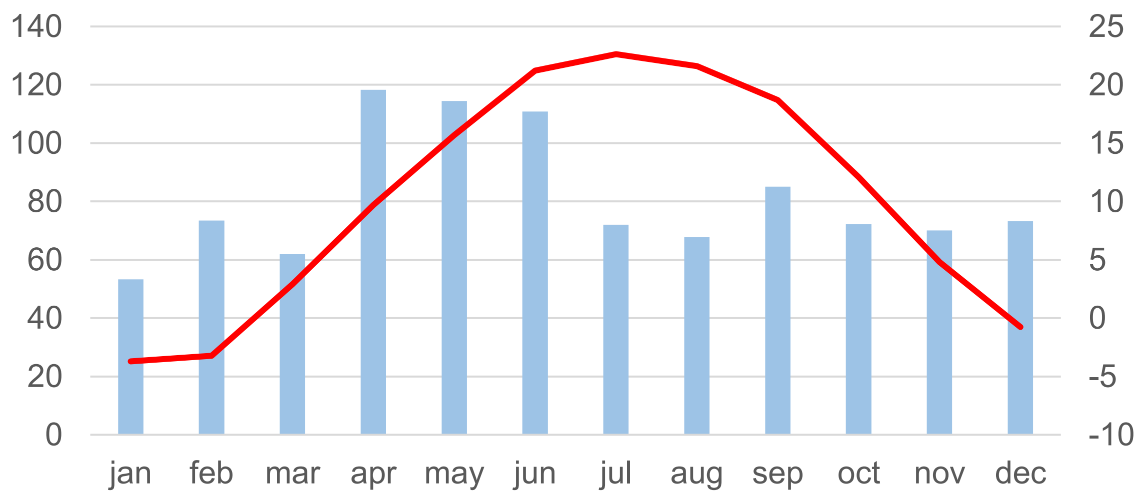


Figure 1. Monthly average for total precipitation and temperature for the period 2005 - 2020 in the Cedar Creek Watershed (CCW).

Regarding climatic data, the average annual precipitation is 966 mm. The average temperature during crop growth seasons ranges from 10 to 23ºC (Heathman *et al.*, 2009).

The region is characterized by flat, hot and humid summers; and diverse rainfall (Spalding and Exner, 1993). Slopes of the terrain vary between 2% to 9.5%. The outlet (in red) is located in the southeastern part of CCW (Figure 2).

In general, the soils of the Corn Belt states of Iowa, Missouri, Illinois, Indiana, and Ohio are some of the most productive (and intensively cropped) around the globe. Soils in the watershed originate from compacted glacial till and fluvial materials and they are predominately mollisols and alfisols (Smith *et al.*, 2008). According to the USDA Soil Classification, alfisols are leached basic or slightly acid soils with a clay-enriched B horizon, typical of deciduous forests; and mollisols are soils with a dark, humus-rich surface layer containing high concentrations of calcium and magnesium, typical of prairies. Predominant soil textures are silt loam, silty clay loam, and clay loam. In Figure 2(b) the soils classes refer to different Map Unit Identifiers in the STATSGO classification: IN004, IN005, IN007, IN016, IN019, IN025, IN028. Each Map Unit has numeric specific values about: available water content, clay content, organic matter content, permeability rate, drainage quality, liquid limit, slope of surface, hydric soil indicator, soil erodibility f-factor, annual flood frequency and total thickness of all sampled soil layers.

The humid climate combined with the slow permeability of some of the soils and the pothole topography require the extensive use of subsurface tile drainage in order to enable agricultural management. This subsurface tile-drainage systems increase crop productivity and reduce the risk of low yields from root zone water stress during wet years (Strock *et al.*, 2004), but nitrate finds direct pathways to end up in stream and rivers. Like other watersheds in northeast Indiana and northwest Ohio, the SJRW is dominated by agricultural land use, including both cultivated row crops and pastureland for livestock grazing (Degraves, 2005), being the CCW predominantly agricultural, with approximately 72% of the land dedicated to crop cultivation, followed by 14% forests, 10% developed urban areas and the rest 4% wetlands. The predominant crops cultivated within the watershed are corn and soybean (Hoque *et al.*, 2012).

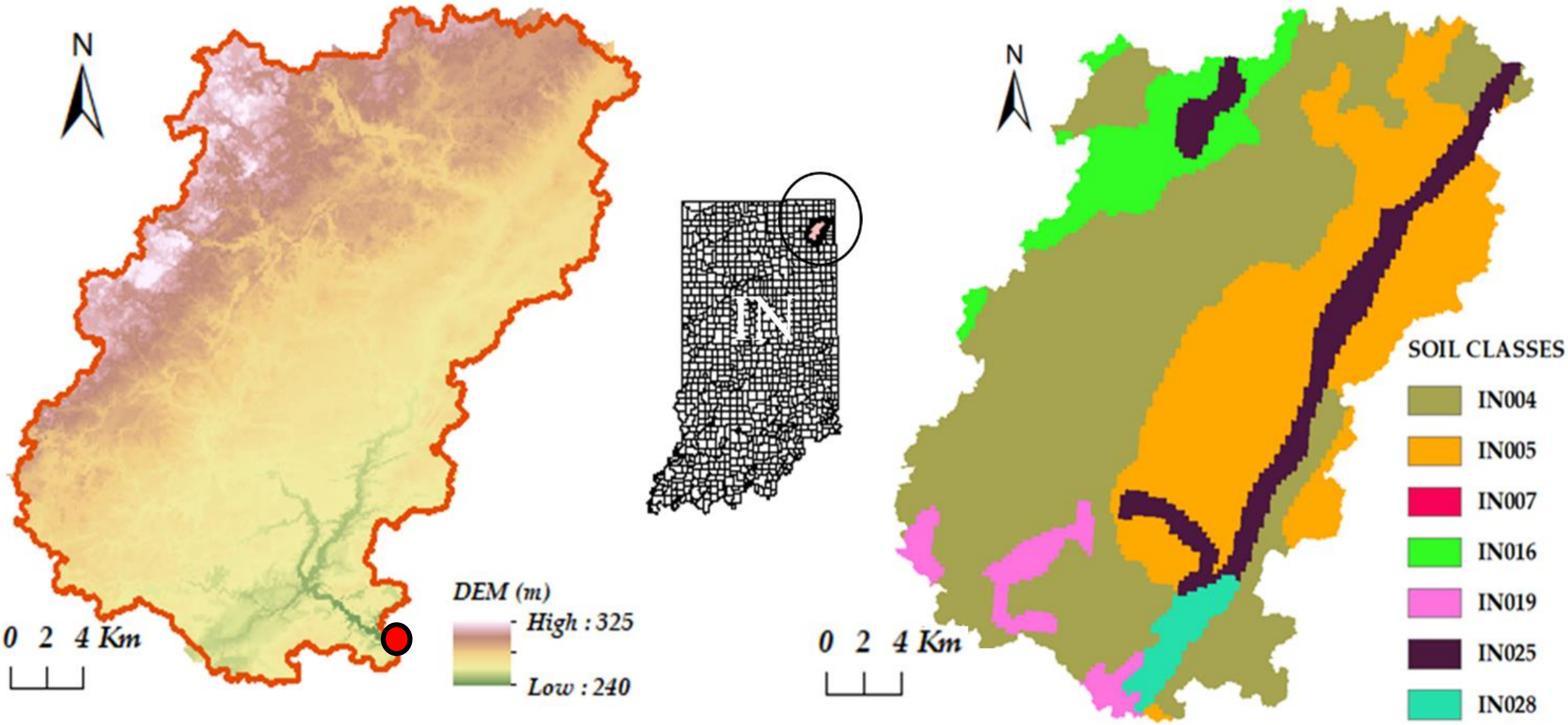


Figure 2. (a) CCW Digital Elevation Model at 30 m resolution and location in Indiana, (b) STATSGO soil classes in Cedar Creek Watershed (CCW).

5 Research methods

5.1 SWAT model

5.1.1 General concept and model inputs

Performance−based methods are supported by simulation models, which assess variations in the watershed response due to alternative BMP applications (Veith *et al.*, 2004). SWAT was developed to evaluate the effects of alternative management decisions on water resources and nonpoint-source pollution in large river basins (Arnold *et al.*, 2012b). According to Arnold *et al.* (2012 (a)) the water balance is the driving force behind all the processes in SWAT. This movement influences the transport of sediments, nutrients, pesticides, and pathogens, and also, the plant growth. SWAT is a physically based, conceptual, continuous-time river basin model with spatially distributed parameters operating on a daily time step (Ullrich and Volk, 2009) (except basin parameters that have only one value for the whole basin). The watershed is divided into subwatersheds which are divided into Hydrologic Response Units (HRUs), which are unique combinations of land use, slope and soil within the subbasin. It consists of a land phase and a water or routing phase to simulate the water fluxes in the watershed. One of the key advantages of SWAT is that it can be used to represent a broader suite of BMPs relative to similar watershed- or river basin-scale models (Teshager et al., 2017). There is a need for more detailed process-based models that realistically simulate (in an integrated way) impacts of agricultural management on water quality in river basins (Malagó *et al.*, 2019). The SWAT model (version 664) is used to account for the nitrate export and the different nitrate concentrations at the outlets of each subbasin that is then used by HosNIT to identify the CSAs.

Input files used for the SWAT model setup included climate data (precipitation, minimum and maximum temperatures) from the National Climate Data Center (NCDC). The remaining required meteorological data (wind speed, relative humidity, and solar radiation) were estimated using the SWAT weather generator program. The potential evapotranspiration is calculated through the Penman-Monteith equation. Climatic stations are located in Angola, Columbia and Garrett (Figure 3 in blue). The Digital Elevation Model (DEM) was obtained from USGS at the 30-m resolution, land-use data from the National Agricultural Statistics Service (NASS) of the USDA and soil data from the State Soil Geographic (STATSGO) database, 250 m. STATSGO data were selected given their native grid structure provided by the SWAT soils database and relatively fewer soil classes than other soil databases (e.g., SSURGO—Soil Survey Geographic Database) (Pignotti *et al.*, 2017). Several land-use classifications with less than 0.05% of the area within the watershed were reclassified to general agriculture (SWAT land use database classification), also applies for the following: all developed areas to urban, different types of forest to its major category, deciduous forest, as well as with the wetlands, to woody wetlands. Following Arnold *et al.* (2012a), the Bermuda grass parameters input for Hay and Pasture are valid for latitudes less than 35 to 37°. Fescue parameters should be used for watersheds with higher latitudes when modeling Hay and Pasture. Fallow/Idle cropland was reclassified to barren. The ArcSWAT interface was used for the first parameterisation and delineation of the watershed and its subbasins. For the river network delineation, a shapefile from the USGS- National Hydrography Dataset (NHD) was "burnt" to the DEM in order to get closer to natural conditions, the HRU definition for soils, land use and slope was set to 0%. No areas were excluded. Watershed delineation produced 70 subbasins consisting of 3,183 HRUs and 3,440 for the two Land Use scenarios analysed. Three point sources (inlets: 40p, 41p and 16p (Figure 3 in orange) were taken into account for the average daily water loading (FLOCNST) in cubic meters (m^3) per day for Indiana, calculated from Dieter and Maupin (2017), the domestic water use of the three major cities in the CCW: Auburn, Garrett and Waterloo, together with the inhabitants of each town.

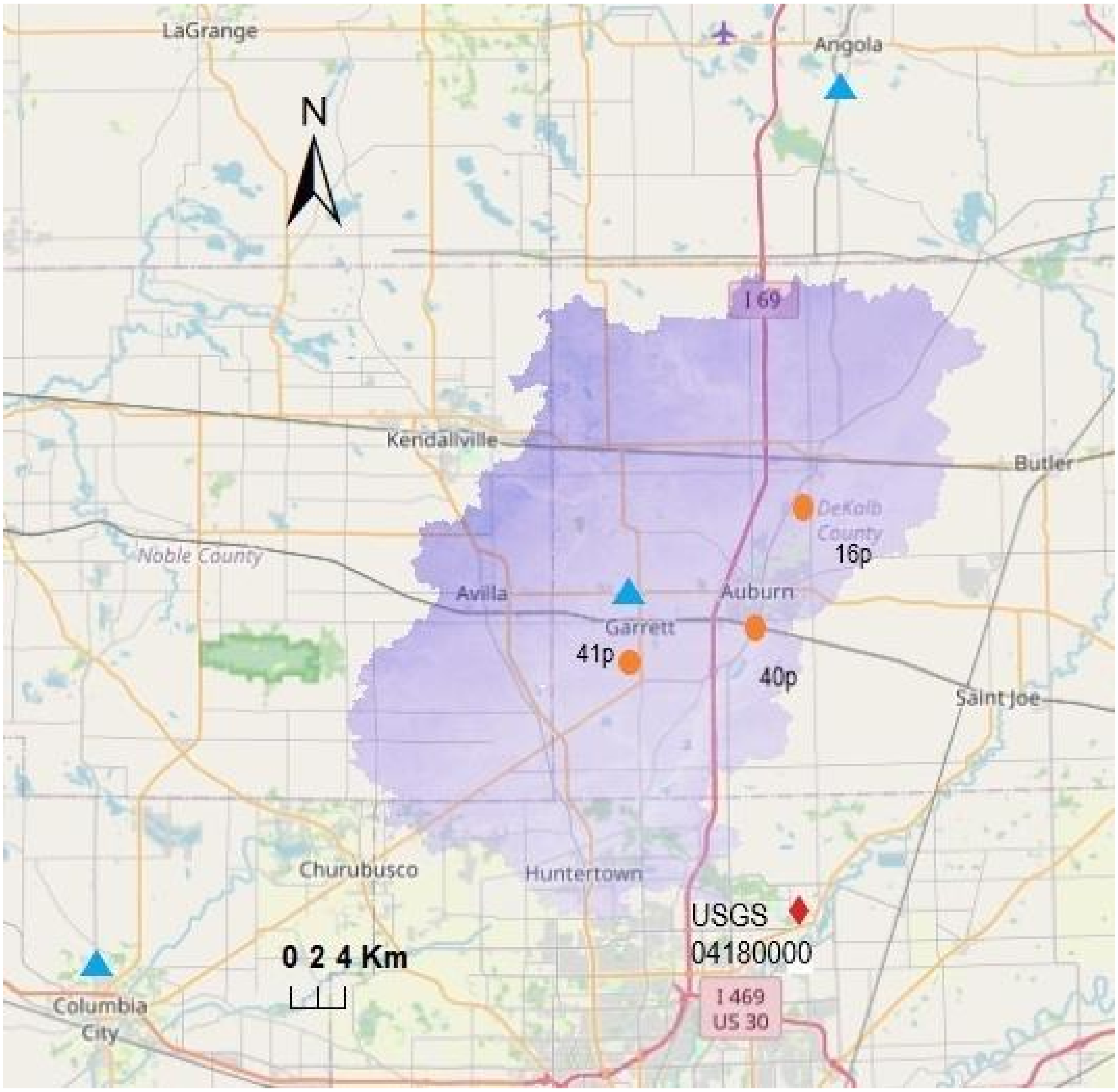


Figure 3. Location of the climatic stations (in blue), Inlets (in orange) and USGS041800000 stream gauge station (in red) in Cedar Creek Watershed (CCW).

Tile drains were simulated for fields managed with corn, winter wheat, alfalfa or generic agriculture with slope ranges between 0 to 5% (Rice, 2005) and soils defined in STATSGO as "somewhat poorly drained", "poorly drained" or "very poorly drained.

Based on SWAT documentation (Pignotti *et al.*, 2017), SWAT Baseflow Filter Program (Arnold *et al.*, 1995; 1999) and previous studies in CCW and Indiana (Pignotti *et al.*, 2017; Franzmeier *et al.*, 2001; Cibin *et al.*, 2016), several initial parameters were adjusted

(Table 1). GDRAIN (Drainage lag time) and DIS_STREAM (average distance to stream) were both calculated as follows.

DIS_STREAM is a parameter in the .hru file with a default value of 35 meters (m). The nearest distance to a reach was calculated by programming for each pixel (30 m x 30 m) within the CCW to improve the accuracy of the DIS_STREAM estimates. Since DIS_STREAM is required at the HRU level, average distances of every subbasin were obtained and applied to the HRUs which encompass them. So, DIS_STREAM is the average distance of all the pixels to the stream within the subbasin where the HRU belongs.

GDRAIN is measured in hours and refers to the water travel time from the surface through the tiles to the reach. This parameter is required for HRUs where tiles are present. Calculations were made in two parts: first, the time from the surface to the tile, based on the hydraulic conductivity (mm/h) at different depths until the tile´s depth and second, the time t of the water travelling through the tile.

$$t = d/v \tag{1}$$

where d, distance the average distance of all pixels to the reach under tile drainage and within a subbasin, and v, velocity given by Manning´s equation (Fischenich, 2000):

$$v = \left(Rh^{\frac{2}{3}} \times \sqrt{S}\right)/n \tag{2}$$

where the Manning's roughness coefficient, n is set to 0.013 for closed conduits, the slope, S, to 3% (average for the CCW) and the hydraulic radius, Rh set to its maximum, being the radius, the SWAT parameter RE.

Table 1. Initial parameters adjusted for CCW of the SWAT mode and their references

Parameter	**Definition**	**Value**
HVSTI (soybean)	Harvest index for optimal growing conditions	0.4 (Cibin *et al.,* 2016)
T_BASE (soybean)(ºC)	Minimum (base) temperature for plant growth	8 (Cibin *et al.,* 2016)
CPYLD(soybean)(kg P/kg yiel	Normal fraction of phosphorus in yield	0.0067 (Cibin *et al.,* 2016)
BIO_E (corn)((kg/ha)/(MJ/m2))	Radiation-use efficiency or biomass-energy ratio	36 (Cibin *et al.,* 2016)
RCN(mgN/l)	Concentration of nitrogen in rainfall	1.6 (Arnold *et al.,* 2012)
rammo_sub(mg/l)	Atmospheric deposition of ammonium for watershec	0.45 (Arnold *et al.,* 2012)
rcn_sub (mg/l)	Atmospheric deposition of nitrate for watershed	1.6 (Arnold *et al.,* 2012)
dry_dep_nh4(kg/ha/yr)	Atmospheric dry deposition of ammonium for water:	0.5 (Arnold *et al.,* 2012)
dry_dep_no3(kg/ha/yr)	Atmospheric dry deposition of nitrates for watershed	0.5 (Arnold *et al.,* 2012)
ALPHA_BF(days)	Baseflow alpha factor	0.048 (Arnold *et al.,* 1999) (Arnold *et al.,* 2012)
ALPHA_BF_D(days)	Baseflow alpha factor for deep aquifer	0.01 (Arnold *et al.,* 1999) (Arnold *et al.,* 2012)
DDRAIN (mm)	Depth from surface to tile drains	1000 (Soils: IN25&IN19), 730 (Soil: IN5) (Franzmeier *et al.* , 2001)
TDRAIN (h)	Time to drain to field capacity	24 (Pignotti *et al.* , 2017)
GDRAIN (h)	Drainage lag time	Calculated
DEP_IMP (mm)	Depth from surface to impervious layer	HRUs under Tiles: 1500. Rest of HRUs: 0
ITDRN (flag)	Drainage routine	1
RE (mm)	Effective drain radius	20 (Pignotti *et al.,* 2017)
SDRAIN (mm)	Distance between tile drains	20000 (Pignotti *et al.,* 2017)
DRAIN_CO (mm/day)	Drainage coefficient	10 (Pignotti *et al.,* 2017)
LATKSATF	Multiplication factor for lateral conductivity	1.2 (Pignotti *et al.,* 2017)
PC (mm/h)	Pump capacity	0 (Pignotti *et al.,* 2017)
ICN	Daily curve number calculation method	2 (Arnold *et al.,* 2012)
DIS_STREAM(m)	Average distance to stream	Calculated

There is few information on actual crop rotations (beyond single farms), and published data on optimal crop rotations comes from expert opinions (Schönhart *et al.*, 2009); therefore, there is a need for generalisation. For the land-use input data in the SWAT model for the CCW, it is a common practice to assume a general corn-soybean rotation for the research in the area (Larose *et al.*, 2007; Heathman *et al.*, 2012; Hoque *et al.*, 2012). This is the Default Land Use (DLU) scenario. Other crops in the area, such as winter wheat and alfalfa, are not really incorporated in the simulation of rotations and their management is rarely considered. The Land Use of 2016 is used as reference. The NASS-USDA produces the Cropland Data Layer (CDL) product, which is a georeferenced raster with a crop-specific, land cover map. CDL program inputs include USDA-collected ground truth and other ancillary data with medium-resolution satellite imagery, such as the National Land Cover Data set (Boryan *et al.*, 2011). The Crop Frequency Layer Data from NASS-USDA identifies crop-specific planting frequency, based on land cover information at a resolution of 30 m x 30 m. The 2016 Crop Frequency Layer identifies crop-specific planting frequency based on land cover information derived from 2008 through 2016 CDL's. There are currently four individual crop frequency data layers representing four significant crops in the United States: corn, soybean, cotton and winter wheat. The data used is for 2008-2016 and for the most common crops in the region: corn, soybean, and wheat. Each crop layer from CDL spatially expresses the number of years, within the period selected, the crop appears at the pixel scale of 30 m x 30 m. Literature has shown that the SWAT model is very sensitive to applied crop rotations and, in some cases, even to minor variations of management practices (Ullrich and Volk, 2009). With CDL data sets and crop/agricultural statistics at the county level, through GIS and R programming tools, it was differed from the assumption of a general corn-soybean rotation, to an adaptation of winter wheat (WWHT), alfalfa (ALF) and monocropping practices.

For a pixel to be classified as a monocrop practice in this study, it has to appear at least 7 years at the same pixel-location. Monocropping practices for corn and soybean in the CCW for the period of study which are not reflected in the DLU are observed. The Cedar Creek Watershed Management Plan (Rice, 2005) includes crop rotations where winter wheat fits as a winter crop between corn and soybean and, to a lesser extent, alfalfa is incorporated fitting winter wheat. The Land Use obtained is called Crop Frequency Data scenario (CFD). It is observed in Figure 4, pixels in DLU (left-(a) and pixels which in DLU were an assumed rotation of corn and soybean that have been changed to other identified practice (right-(b)) for creating CFD land use scenario.

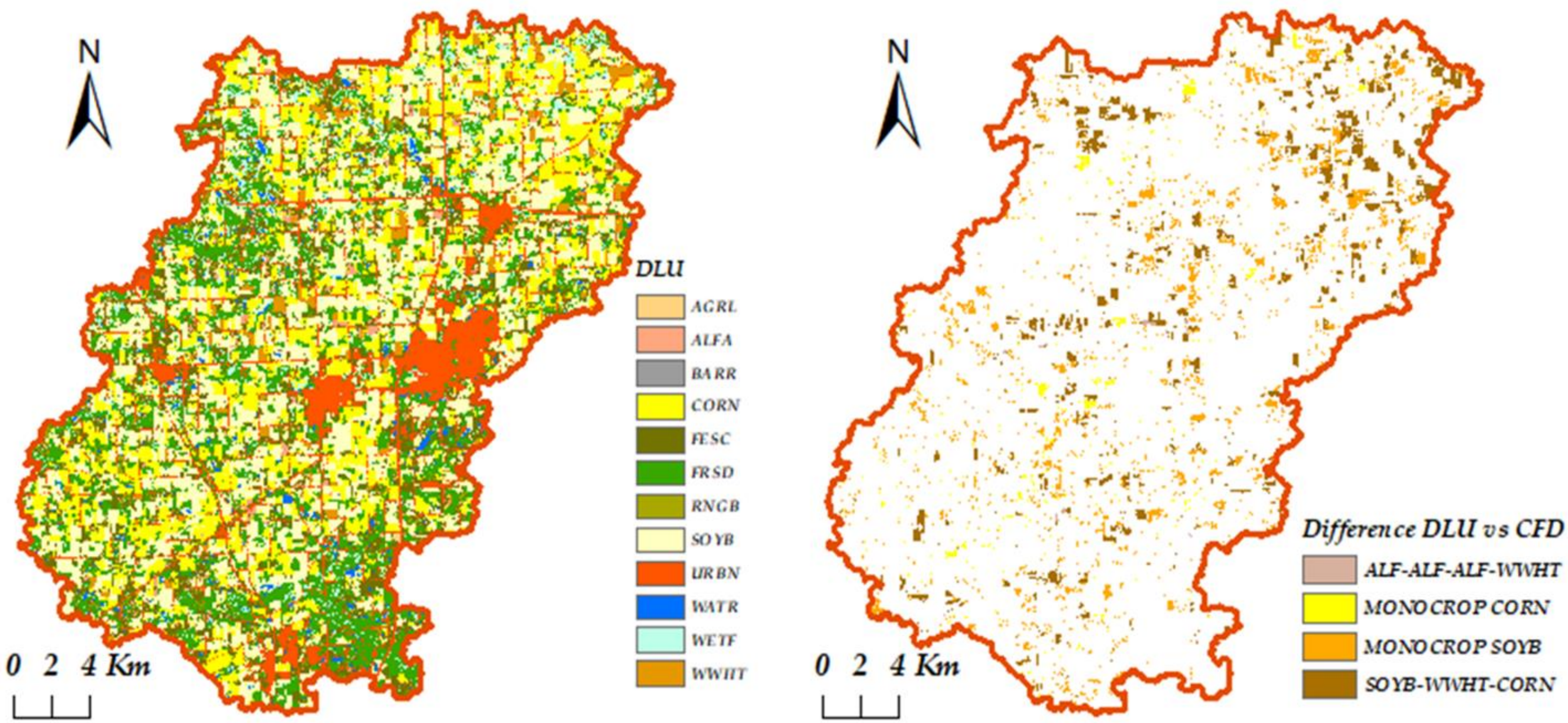


Figure 4. (a) DLU map LU, (b) Pixels where changes in crop practices were made for CFD.

5.1.2 Calibration and validation

Data used for calibration includes wet, average, and dry years. Calibration was carried out for discharge and nitrate loads (at the same time) with daily simulations between 2005 and 2016. For model warm-up, years from 2005 to 2007 were used, for calibration 2008 to 2012, and 2013 to 2016 were used for validation. Daily discharge data at the watershed outlet was obtained from the USGS Water Data Server for Station Number 04180000 (Figure 3 in red), Cedar Creek near Cedarville, Indiana; and by-weekly (with some periods with lacking data) nitrate concentration data at the outlet obtained from the Indiana Department of Environmental Management (IDEM) and from St. Joseph River Watershed Initiative (SJRWI) program.

The parameters changed during the calibration process and their ranges are summarised in Table 2 (parameters are changed relative to their initial value within the given ranges for all other parameters the parameter value has been replaced within the given ranges). Within the given ranges 1,000 parameter sets where obtained by applying an automated Latin-Hypercube-Sampling with the FME package in R (Soetaert and Petzoldt, 2010). Following Kamamia *et al.* (2019) for each parameter set on simulation was carried out and the simulation efficiency based on coefficient of determination (R^2) and the Nash-Sutcliffe-efficiency (Nash and Sutcliffe, 1970) for simulated discharge and N loads were calculated. The parameter sets where selected based on the Latin-Hypercube-Sampling method which ensures that the multidimensional parameter space is equally searched. This means with this method you get good results with relatively low number of runs. Then, increasing the number of runs will not lead to improvement of the simulation quality. Model uncertainty regarding crop management practices such as planting date, tillage date, fertilizer rate and date of application make it challenging to have a day-to-day comparison of simulated nutrient loads with the observed values (Femeena *et al.*, 2018). Simulation quality was calculated by using the common tests. The by far most widely statistics tests reported for calibration and validation is used: R^2 and Nash Sutcliffe Efficiency (NSE) (Arnold *et al.*, 2012b). Percent bias (PBIAS) was also calculated. A modified NSE evaluation based on (Cibin *et al.*, 2011) was used for loads in order to evaluate the SWAT performance with a ±5 day window for constructing the uncertainty band.

Table 2. Calibrated parameters for the 30-m baseline model

Parameter	Definition	Units	Range	Calibrated_DLU	Calibrated_CFD
SURLAG	Surface runoff lag coefficient	day	0.5 to 2	0.9389	0.9389
SFTMP	Snowfall temperature	◦C	-5 to 0	-1.8905	-1.8905
SMTMP	Snow melt base temperature	◦C	0 to 2	1.4931	1.4931
TIMP	Snow pack temperature lag factor	-	0.01 to 1	0.5054	0.5054
SMFMX	Maximum melt factor	mmH2O/◦C	1 to 10	5.2873	5.2873
SMFMN	Minimum melt factor	mmH2O/◦C	1 to 10	6.6626	6.6626
ESCO	Soil evaporation compensation factor	-	0.01 to 1	0.5399	0.5399
CMN	Rate factor for humus mineralization of active organic nutrients	-	0.0001 to 0.001	0.0009	0.0009
N_UPDIS	Nitrogen uptake distribution	-	10 to 30	18.0002	18.0002
NPERCO	Nitrogen percolation coefficient	-	0 to 1	0.7806	0.7806
RSDCO	Residue decomposition coefficient	-	0.01 to 0.1	0.0472	0.0472
CDN	Denitrification exponential rate coefficient	-	0 to 2	0.1836	0.1836
SDNCO	Denitrification threshold water content.	-	0.95 to 1.01	1.0044	1.0044
SHALLST_N	Initial concentration of nitrate in shallow aquifer	mg N/L or ppm	0 to 5	0.5147	0.5147
HLIFE_NGW	Half-life of nitrate in the shallow aquifer	days	0 to 10	5.5653	5.5653
CH_N1	Manning’s “n” value for the tributary channels	-	0.01 to 0.3	0.1472	0.1472
CH_K1	Effective hydraulic conductivity in tributary channel alluvium	mm/hr	0 to 100	79.1603	79.1603
SOL_AWC()	Available water capacity of the soil layer	mm H2O/mm soil	-0.2 to 0.2	0.0531	0.0531
SOL_K()	Saturated hydraulic conductivity	mm/hr	-0.2 to 0.2	0.1893	0.1893
CN2()	Initial SCS runoff curve number for moisture condition II	-	-0.2 to -0.1	-0.1686	-0.1686
R2ADJ	Curve number retention parameter adjustment for low gradient	-	0.6 to 0.9	0.6042	0.6042
GW_DELAY	Groundwater delay time	days	0 to 100	0.4831	0.4831
GWQMN	Threshold depth of water in the shallow aquifer for return flow	mm H2O	0.0 to 1000	226.8268	226.8268
GW_REVAP	Groundwater "revap" coefficient	-	0.02 to 0.2	0.0843	0.0843
REVAPMN	Threshold depth of water:shallow aquifer to deep aquifer	mm H2O	0 to 1000	867.1680	867.1680
RCHRG_DP	Deep aquifer percolation fraction	-	0 to 0.25	0.0822	0.0822

5.1.3 Management scenarios

The role of crop rotations in assessing economic and environmental impacts of agricultural production systems is increasingly acknowledge by integrated agricultural land use models (Schönhart *et al.*, 2009). The integration of remote sensing-based crop rotation data can considerably reduce uncertainties regarding the management in regional agro-ecosystem modeling (Waldhoff *et al.*, 2017).

Techniques for enhancing the quality of available ground truth, improving the accuracy of small area but high value crops, improvements to spatial resolution and cropping intensity and rotational analysis are being investigated (Boryan *et al.*, 2011).

Due to the lack of data and/or statistics, there is a need for generalization.

Two different project setups were addressed. Both differed only in the Land Use input information: DLU vs CFD. Nitrogen fertilizer is primarily applied as Ammonium-polyphosphate (APP) and Anhydrous-ammonia (AA). Calculations are made following the Tri-State Fertilizer Recommendation (Vitosh *et al.*, 1995) based on previous crop and yield at county level. Conservation tillage has been widely adapted in the watershed for corn, while for soybean crops no tillage practices are the most frequent (Rice, 2005). The two management scenarios can be found at the Supplementary material section A1: management strategy using DLU as land-use input, and management strategy using CFD as land-use input.

5.2 Importance of hydrological watershed characteristics for CSA definition

Hypothesis 1 is based on the addition of morphological watershed characteristics in a targeting technique for a better identification of CSAs within a catchment.

Stream order, nearest drainage distance of each cell/pixel and stream network dilution/enrichment effects are the characteristics which have been added to the analysis.

5.2.1 Stream order

Headwaters are where waters meet the land. Those headwaters are instrumental in conditioning the natural and unnatural inputs from the landscape into forms that downstream ecosystems and human systems are adapted to utilize (Bishop *et al.*, 2008). Downstream quality status might reflect the status for upstream water contribution within a river network. Headwater, intermittent and ephemeral streams are a part of the tributary system (via hydrological connectivity) that cumulatively are contributing to the hydrological and ecological functional integrity of downstream waters (Nadeau and Rains, 2007).

The importance of headwaters and low-order streams for downstream quality has been widely studied and proven in literature (Bao-qin *et al.*, 2005; Kang *et al.*, 2008; Weaver *e al.*, 2001). This demonstrates the importance of considering the influence of headwater on the transport, but also on the supply and fate, of water and solutes in watersheds and their intrinsic connections to landscape processes and downstream waters (Alexander *et al.*, 2007). Since this study relates to nitrate hotspots, it is important to consider the stream order for controlling nitrogen export from watersheds by headwater streams (cf. Peterson et al., 2001). There is also evidence of the connection to distant sources of nitrogen located upstream and the nitrogen in downstream receiving waters that show a quick response to changes in these sources (Boyer *et al.*, 2002; Howarth *et al.*, 1996).

The stream order system used is the method introduced by Strahler (1957) (Figure 5). In the Strahler system, upstream orders 1 or 2 are usually located on higher terrain where agricultural cropland is not so intensive. Mainly grazing animals are located there, but in this study livestock is not relevant, since 72% of the area is dedicated to crops.

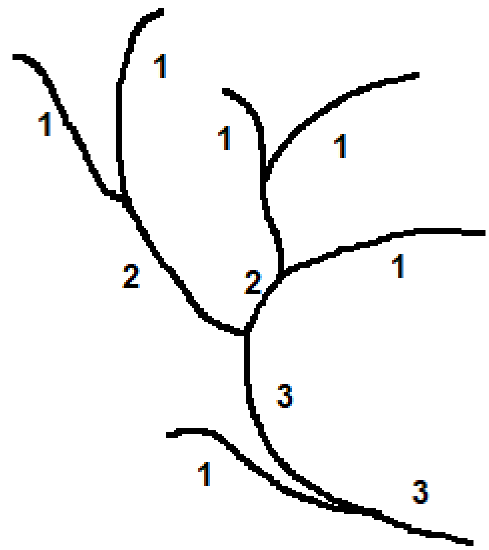


Figure 5. Scheme for Strahler's ordering

5.2.2 Cell distance to drainage stream

The effect of a given crop on nutrient export to a stream would intrinsically depend on its location in a watershed (Molnat and Gascuel-Odoux, 2002). The proximity to a stream has a dramatic effect on the actual nutrient delivery to the stream (Heatwole *et al.*, 1987). The distance to the nearest stream is considered by calculating it from the DEM for each pixel in the watershed to the closest water-draining body. This component reflects indirectly the travel time for draining to the nearest stream, which accounts for the likelihood of nitrate uptake by plants/microorganism and denitrification processes if conditions are favorable.

Denitrification may also occur in the rich soils and subsoils of the Corn Belt but tile drainage appears more important in intercepting the downward movement of NO_3^- (Spalding and Exner, 1993). Therefore, nitrate pollution mitigation is efficiently achieved by riparian areas (Bernard-Jannin *et al.*, 2017). Denitrification is the main process involve in the removal of nitrate in river basins and an important buffer from agricultural land which limits aquatic ecosystem pollution. Still, the understanding of denitrification hotspots (for example, riparian zones), their total removal capacity, and their role in a landscape context at the drainage basin scale are still challenging (Pinay *et al.*, 2015).

The states of Illinois, Iowa, Indiana, Missouri, Arkansas, Kentucky, Tennessee, Ohio, and Mississippi collectively account for 75% of the N and P delivery to the Gulf - 86% of the N from corn/ soybeans. However, it must be considered that the nutrients from these states include contributions both from large cities and agricultural lands that border large rivers enhancing nutrient transport to the Gulf (Alexander *et al.*, 2008).

Through using an ArcGIS operation, the flow direction (Figure 6) was obtained. The distance of pixel n to the river network following the flow calculation is calculated. The distance of pixel *n* is calculated as the distance accumulated for pixels, following the flow direction, between pixel n and the stream. For the Pythagoras theorem (Tesfa *et al.*, 2009), the pixel resolution of 30 m x 30 m and the difference of altitude from cell to cell from the DEM are used as input data for the formula:

$$distance\ pixel_n = \sum_1^n \sqrt{(a^2+b^2)} \tag{3}$$

for flow direction equal to 64, 16, 4 and 1: a = 30, b = altitude (n) – altitude (n-1),
for flow direction equal to 128, 32, 8 and 2: a = 30√2, b = altitude (n) - altitude (n-1)

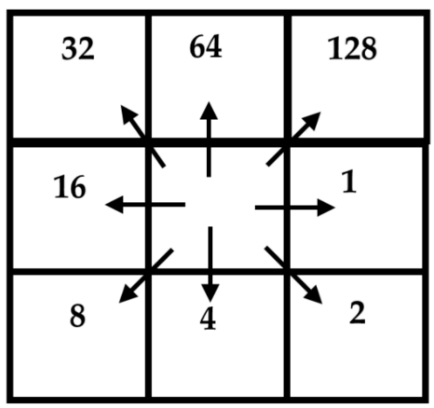


Figure 6. Flow direction code in ArcGIS tool

For this novel technique approach (HosNIT), several extra data (besides loading) are required. The 30-m resolution was nominally selected as the finest scale considered, given that it is common for most spatial datasets used in SWAT modeling (Pignotti *et al.*, 2017).

5.2.3 Stream network morphology: nitrate enrichment and dilution effects

The rate of downstream N export is determined both by the extent of instream processing that N suffers during transport and by levels of N input to the catchment (McLellan *et al.*, 2018). Downstream nitrate concentrations were significantly related to upstream concentrations, and the results indicated that upper basin areas exerted a proportionally large effect on the overall watershed export (Jha *et al.*, 2010). In order to account for nitrate enrichment or nitrate dilution effects at subbasin level from upstream confluences, the nitrate concentration at each outlet is considered. It also reflects in-stream turnover and nutrient decay processes. In aerobic water bodies, there is a stepwise transformation from organic N to ammonia, to nitrite, and finally to nitrate. The amount of nitrate in the stream may be increased by the oxidation of nitrite or decreased by the uptake of nitrate by algae. The conversion of nitrite to nitrate occurs more rapidly than the conversion of NH_4^+ to NO_2^-, so the amount of nitrite present in the stream is usually very small (Neitsch *et al.*, 2011). The SWAT model considers these conversions and the algae uptake.

5.3 BMPs selection for the CCW

Potential BMP effectiveness is site-specific (Giri *et al.*, 2012). Determining the most effective BMP for a specific catchment, therefore, depends on understanding nutrient flow paths (McLellan *et al.*, 2018). Considering resources are limited and constraint, it is not possible to implement conservation practices in every candidate location in a catchment (Chiang *et al.*, 2014).

Farmers' engagement is essential for successfully implementing conservation practices/BMPs in any watershed. In a study of adaptive targeting (Kalcic *et al.*, 2015) in west-central Indiana, 14 producers and landowners were survived, and results indicated which practices were most palatable to farmers. In our study, a selection from this result is made. Cover crops are the "most convincing" practice for farmers, although low rainfall and cool temperatures during autumn present challenges to establishing cover crops in the northern Corn Belt successfully (Strock *et al.*, 2004). Also no-tillage is accepted among producers.

In order to check the influence of monocropping practices on water quality, the transformation of monocrop to rotations was also selected and studied.

The conservation practices simulated in the study are the introduction of cover crops into corn-soybean rotations and monocrop practices, the *Zerotill* (nº4 in SWAT till.dat file) routine in SWAT instead of *Fldcge15* (nº6), and the avoidance of monocropping practices for the identified CSAs through HosNIT.

5.3.1 Cover crop

Cover crops are grasses, legumes or small grains which are grown between cash grain crop production periods in order to conserve and improve the soil. The most common cover crops in Indiana are fall-seeded cereals, such as cereal rye or wheat, and fall-seeded annual ryegrass (Mannering *et al.*, 2007). Increased interest in restoring water quality in ecosystem resulted in important efforts to tighten N cycling within the soil–crop–soil interface, minimising nitrate flows into freshwater bodies (Thapa *et al.*, 2018). The inclusion of cover crops in a rotation has benefits in terms of reducing nitrate-N and other nutrient from leaching, improving soil structure, supplying nutrients to the following crop and improving weed control (Shah *et al.*, 2017). Interest in cover crops has been permanently increasing among producers in the eastern Corn Belt. Despite the potential benefits of cover crops, farmers need to manage them carefully to avoid or reduce the risks to crop production (Kladivko *et al.*, 2015). In most cases, the main idea is to minimise soil erosion while preventing nitrate and other nutrient from leaching, but also to increase organic matter, to improve soil biology and to suppress weeds. From a producer's point of view, cover crops should have benefits on the succeeding crops in terms of yield, reduced nitrogen fertiliser inputs, improving soil structure, increasing soil organic matter and infiltration rate (Shah *et al.*, 2017).

Since this study concerns water quality regarding nitrate pollution, the introduction of cover crops in the rotations is added in the SWAT management files. In the supplementary material, section A1 for CFD, cereal rye was added after harvesting the cash crop (SWAT code: 30). The implementation of winter cover crops plans should be established in catchments according to local traits and agronomic characteristics for reducing nitrogen loss (Lee *et al.*, 2016).

Cover cropping in the off-season months offers a potential solution for avoiding nitrate leaching losses because it increases the amount of time the land is covered with vegetation which grows. Growing cover crops will remove water and N out of the soil profile through transpiration processes and N uptake (Strock *et al.*, 2004). For several reasons, cereals like rye or wheat are Indiana's most popular cover crops. They are relatively easy to establish and rapid growing; seed is readily available and not very expensive (Mannering *et al.*, 2007). Since this incorporation is challenging, cereal rye gives a good window opportunity for planting and a reliable establishment for the CCW. Reliable establishment means there is generally enough time for the cover crop to survive to benefit the soil and the following cash crop (Kladivko *et al.*, 2015). The Midwest Cover Crops Council offers the possibility through a Cover Crop Decision Tool (CCDT) to select the best cover crop according to several parameters, which are: location of the fields (at county level), the presence of tiles when low permeable soils, the current cash crop (for this study either corn or soybean), its planting dates, and preferred goals/conditions. The first selected goal is a cover crop, a nitrogen scavenger, followed by a need for weed fighter (weed control in no-tillage corn is more complex than in reduced or conventionally tilled) and the last is a soil builder. With all these conditions, cereal rye is the first option for corn as previous crop (Figure 7) and soybean (Figure 8). Cover cropping with rye reduced drainage discharge relative to winter fallow, although the magnitude of the effect varies with annual precipitation (Strock *et al.*, 2004).

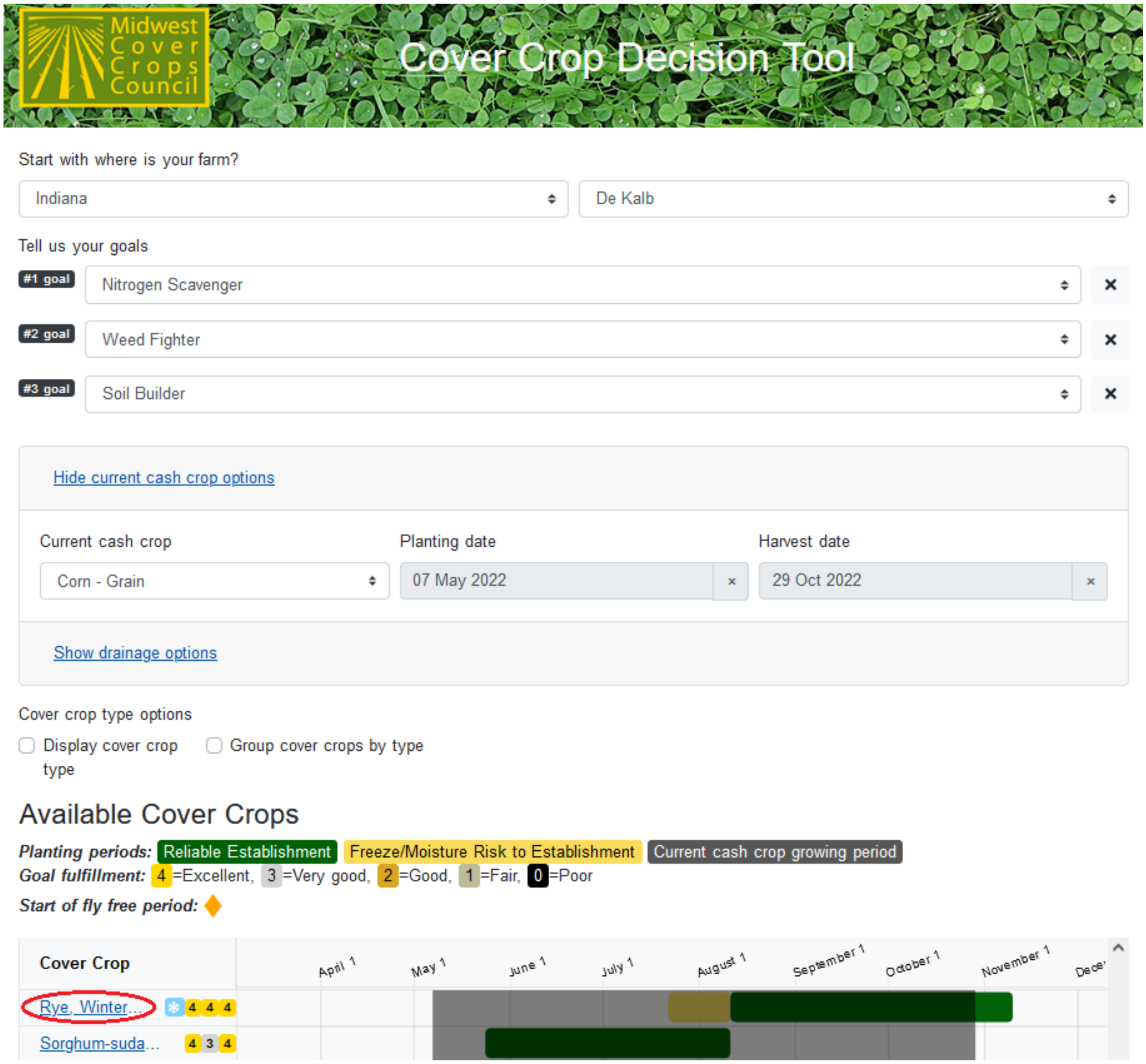


Figure 7. Cereal rye as the best cover crop after corn for the CCW according to the CCDT

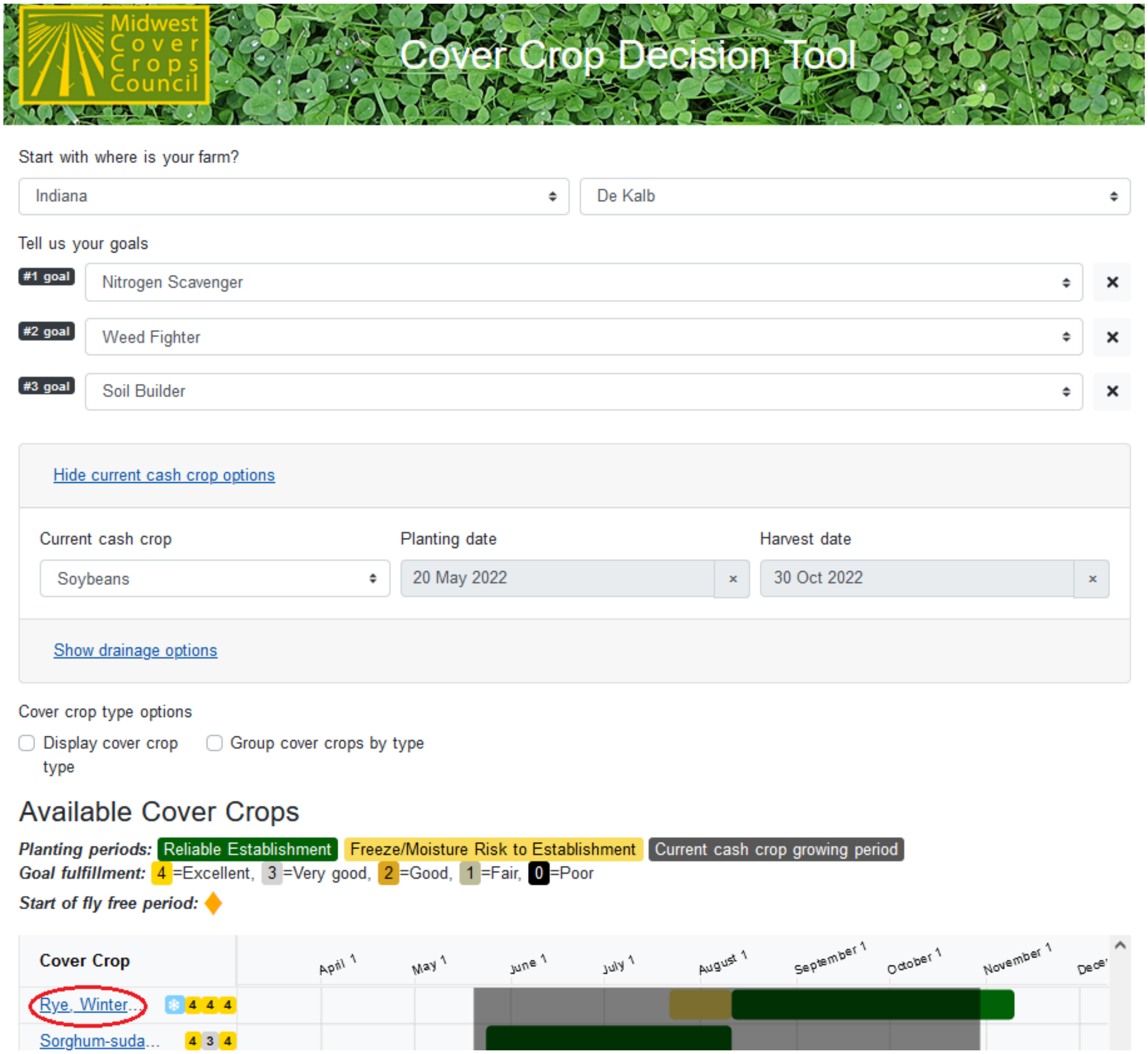


Figure 8. Cereal rye as the best cover crop after soybean for the CCW according to the CCDT

5.3.2 Tillage management

Tillage is defined as the mechanical manipulation of the soil in order to manage crop residue, prepare seedbed and incorporate amendments, preparing a seedbed, control weeds, and avoid surface compaction and rutting (Dejong-Hughes and Daigh, 2017).

Farmers can choose between conventional tillage (with different implements to work with) and conservation tillage. This last, “conserves” soil by reducing erosion. In the Midwest, the erosion caused by water is the major concern, whereas western regions of the US are more susceptible to wind erosion (Sandbrook, 2015).

No-till is a type of conservation tillage, and one of the BMPs implemented and studied in this research. No-till is the complete absence of any type of tillage practice with the objective of leaving the soil as undisturbed as possible during the entire year. Most no-till planters have residue managers, finger coulters and double disk openers that move some residue from the row and improve seed to soil contact (Dejong-Hughes and Daigh, 2017). No-till also reduces rill, sheet and wind erosion. The practice works helps to improve soil organic matter content, reduces CO_2 losses from the soil and soil particulate emissions, increases plant-available moisture and provides food and escape cover for wildlife (Lal and Unger, 2005).

The no-till system effectively increases soil water infiltration and reduces evaporation from soil and water runoff. The water availability for crops is increased, offering the opportunity to improve general soil functioning and crop performance. The principles are equally helpful for both rain-feed and irrigated cropping conditions. Under rain-feed (CCW regime), no-till greatly contributes to minimising the yield impacts caused by water stressing periods allowing to obtain higher and less variable crop yields (Peiretti, 2005).

Also, the crop residues covering the topsoil create a favourable environment for a significant increase in biological activity that further improves the soil and the general agro-ecosystem functioning (Peiretti, 2005). (Huang *et al.*, 2021) on a regional study to attempt tillage effects on crop water productivity (defined as the ratio of crop productivity to evapotranspiration) in the Midwest, indicated that conservation tillage can be a viable approach to enhance crop water productivity in corn and soybean cropping systems.

Although no-till has been promoted as an alternative land management practice to conventional tillage, its impact on water quality, especially nitrate loss, remains controversial (Daryanto *et al.*, 2017).

In a study of optimisation of BMPs for diffuse sources (Maringanti *et al.*, 2011), tillage practices did not affect the percentage reduction in sediment and total N load. Some studies (Daryanto *et al.*, 2017; Huang *et al.*, 2021) suggested that, although no-till and reduced tillage might decrease surface runoff, they could also increase subsurface drainage and nutrient loss from grain crops via leaching. These results indicate that conservation tillage should be complemented with additional water and nutrient management practices to enhance soil water retention and optimise nutrient use in the cropland of the region. It is then important that no-till is complemented with cover crops to improve its environmental quality benefits. Complementary management that enhances the overall environmental benefits of no-till is, therefore, crucial (Daryanto *et al.*, 2020), and cover crops will help tighten nutrient cycling in the no-till system.

The controversy is explainable since in literature studies can be found reporting that nitrate is reduced under no-till management. Khan *et al.* (2017) considered that minimum tillage enhances the availability of nutrients to the plants and is therefore considered a phenomenon more appropriate to minimise the leaching of nutrients along with water.

In a tiled-drained Midwest watershed, Motsinger *et al.* (2016) found that the no-tillage management operation in SWAT performed the best in reducing nitrates discharge from the watershed. This is thought to be caused by the improved soil structure that does not disturb the soil. In the Supplementary Section A1 for CFD, the tillage practices were changed to zero till (SWAT code: 4).

Also, in a continuous corn system (Drury *et al.*, 1993), where the primary loss of N from the corn production system was through tile drainage, conservation tillage did reduce these losses somewhat, as there were lower volumes of water lost and lower concentrations of nitrate in tile drainage. Further, the increased yield and N uptake in grain resulting from the conservation tillage systems reduced the amount of nitrate available for leaching. It is interesting to note that the increase in N uptake in grain in conservation tillage systems over conventional tillage was roughly similar to the reduction in nitrate leaching losses.

The selection of no-till as a BMP to study at the CCW was challenging and risky since its performance at the identified CSAs might increase the nitrate concentration due to the different and contrary results found in the literature. The incorporation of cereal rye in winter was, then, crucial.

No-till management also has water quality benefits for sediments, P and herbicides that might be lost via runoff and end in surface waters.

5.3.3 Monocrop avoidance

Corn (*Zea mays*) and soybean (*Glycine max*) production form an integral part of the global economy, but yields are constrained by biotic and abiotic factors linked to short rotations and long-term monocultures (Strom *et al.*, 2020). Wang and Ortiz-Bobea ((2019) examined the market drivers of corn monocropping in the US Midwest by empirically analysing crop rotation responses to market fluctuation from 2005 to 2014. They observed an increase in corn monocropping in the Midwest (Indiana, Illinois, and Iowa) from 2005–2009 due to the biofuel boom and how corn prices affected the farmers' decision to shift to monoculture. In the 10-years study of the Wisconsin Integrated Cropping Systems Trial, Posner et al., 2000) found that the average concentrations of nitrate and nitrite-N in the groundwater under the cash grain systems mirrored the levels of purchased inputs used in them. Continuous corn, with its relatively heavy applications of inorganic N, leached the most nitrate on average and led to well water nitrate concentrations nearly two times the safe level for drinking water. The no-till corn-soybean rotation leached less, hovering around the enforcement standard, and the low-purchased input corn-soybean-wheat/red clover system leached slightly less. Continuous corn was expected to be the highest purchased input system in the trials, relying on manufactured fertilisers and chemical and mechanical weed and pest control (Posner *et al.*, 2000).

Rotation, a very old practice in agriculture, was adopted since the beginning of sedentary agriculture, starting from the empirical evidence that the yields decreased in the case of cropping (monocropping) for many years (Gomez-Lopez *et al.*, 2019). Large potential reduction in N leaching could be achieved in numerous intensive cereal regions of the world where cropping systems are usually based on very few crops, mainly cereals (Beillouin *et al.*, 2021)

Diversifying cropping systems improves environmental health and has the potential to reduce the risk of climate change-related threats (Bowles *et al.*, 2020). The two-crop rotation breaks up some pest cycles and reduces corn's need for N fertiliser (Posner *et al.*, 2000). The technologies that have traditionally fostered the transition toward monoculture are mechanisation, the improvement of modern varieties, and the development of agrochemicals for soil fertilisation and pest and weed control.

Governmental trade policies of the past decades have promoted the acceptance and use of these technologies. The result today is fewer but more extensive and specialized farms with more intensive capital requirements (Emanuelli *et al.*, 2009).

For the CCW, when implementing BMPs at identified CSAs, monoculture is considered, and shifts in cropping rotations. Adopting crop diversification from intensive and simplified farms represents an important step towards sustainability (Gomez-Lopez *et al.*, 2019).

5.4 BMPs combination: scenario analysis

Three different scenarios are simulated in SWAT at the identified CSAs (Table3). The land use selected for this analysis with BMPs is the CFD since, from our point of view, it represents more realistically crop patterns and practices taking place across the watershed. New management crop practices (Chapter 4.3) were implemented at the identified hotspots. The SWAT model was run for the period 2005-2020 with a warm-up period of 3 years. It was run three times, once for each scenario. HRUs identified as CSAs were changed in their management files in SWAT according to the scenario conditions.

Table 3. BMP scenarios simulated in SWAT at identified CSAs

Scenario	Monocrop	Cover Crop	Tillage	% of CSAs targeted
1	To corn-soybean rotation	NO	Conventional Till	15
2	with Cover crop	YES	No-Till	100
3	To corn-soybean rotation	YES	No-Till	100

5.5 New methodology: Combination of Plan-based methods (HosNIT) and Process-based methods (Parsimonious optimization)

Establishing or protecting special areas as riparian zones or large catchment portions that mitigate impacts of human land use on water quality may be not financially possible and/or politically complicated, specially areas whose land is privately owned. In these cases, it is essential that scientists and stakeholders identify areas within watersheds where protection would improve water quality at their most, and prioritize them for protection (Dodds and Oakes, 2008).

This novel methodology consists of a combination of a Plan-based method for CSA identification (novel HosNIT methodology) with a subsequent Process-based method (Parsimonious approach) for BMP implementation in the CSAs previously identified.

5.5.1 Plan-based method: HosNIT

HosNIT is a finer targeting technique since it identifies nitrate hotspots (CSAs) by considering the nitrate export rates (leached, lateral, and runoff), nitrate outlet concentration from hydrological models such as SWAT and intrinsic morphological characteristics of the watersheds. In HosNIT, the placement of BMPs is based on the targeting approach (hotspots) identified as a result of a comprehensive procedure, but with the difference that not just the export of nitrate is used as a parameter of identification. Hotspots are characterised both spatially (30 m by 30 m) and temporarily (monthly) in order to account for spatial and seasonal variations. It also adds watershed geomorphological characteristics to the analysis, providing a better understanding and a more refined targeting for BMPs. The components considered are:

1. Nitrate export rate: defined as the sum of nitrate being leached and present in lateral flow and runoff per HRUs kilograms (kg) per hectare (ha).
2. Stream order: in order to consider the influence of headwaters in downstream waters. Subbasins with stream order 1 and 2 are considered for analysis in HosNIT because of their risk to get impaired due to its low-flow property in stream networks and the importance of their impact downstream when receiving “clean or polluted” waters from upstream.
3. Nitrate outlet concentration, simulated with SWAT at each delineated subbasin.
4. Distance to the nearest stream: represents likelihood of nitrate uptake and denitrification, and indirectly, travel time.

There are two consecutive steps:

1- HosNIT assumes that pixels with the highest values of nitrate export, located near the stream and draining into streams of order 1 and 2 are most likely to get impaired waters within a given watershed. In order to account for the concepts of “high” values of nitrate export and “near” to the stream, two thresholds were applied. We selected pixels with agricultural land-use for the analysis since the watershed is predominantly agricultural and receive nitrate inputs from fertiliser. Information for these selected pixels regarding two different variables: “Distance to stream” and “Nitrate export” is extracted.

To account for the nitrate export and the different nitrate concentrations at the outlets of each subbasin, the SWAT model (version 664) was used. After calibration and validation of the SWAT model for the period 2008 - 2016, nitrate export rates (kg/area) and nitrate outlet concentration (mg/l) are obtained and used as input data for HosNIT for all subbasins within the watershed. The nitrate export rate is transformed to kg/pixel. Different stream orders from the river network were obtained through GIS tools.

A boxplot is a standardised way of displaying the distribution of data. A boxplot for the two variables was generated to know how “near” agricultural pixels are from their draining stream and how “much” nitrate is exported. Threshold-values are obtained from these two boxplots in order to select potential areas that are the first hot spot (in red) likelihood location (Figure 9). Areas under tile drainage and areas with no drainage are differentiated since tiles shorten distances, and nitrate decay decreases substantially. Therefore, on pixels under tile drainage, no threshold is applied to the variable distance.

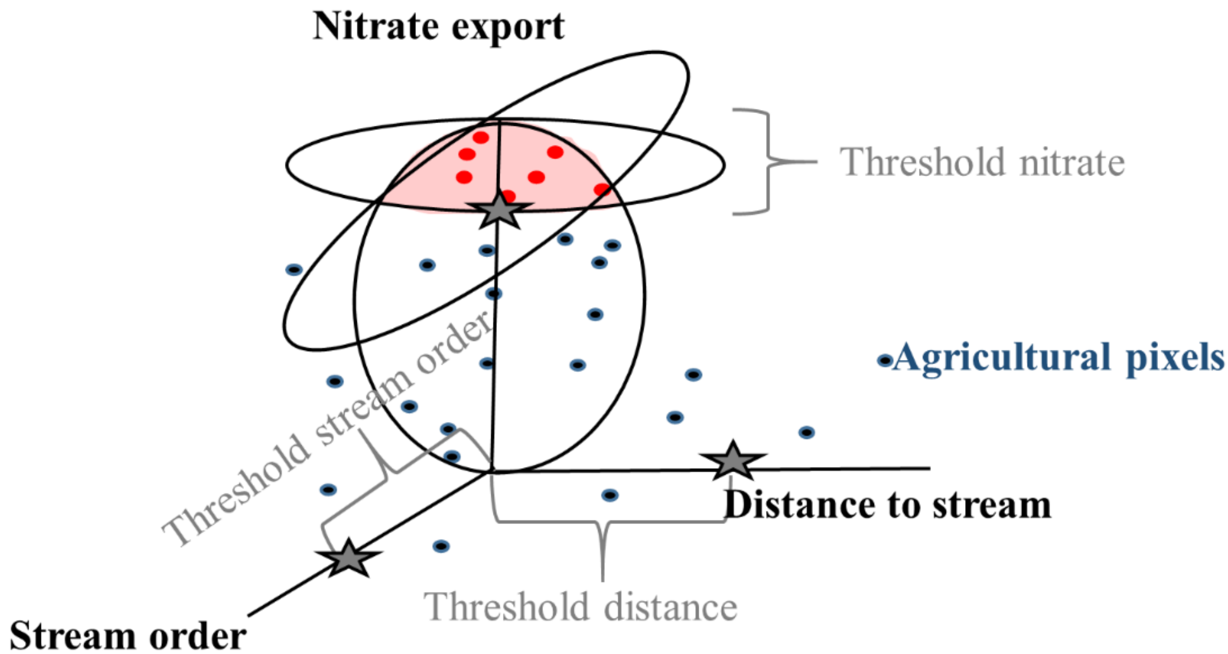


Figure 9. Conceptual scheme of pixels as first-potential hotspots (in red)

Teshager *et al.* (2017) also used SWAT-simulated threshold-values based on the distribution of each pollutant's loads at the HRU level. In our study, threshold-value´s decisions are made from the data distribution (box plots) for the two variables: nitrate and distance. For nitrate export, agricultural pixels within the interval from the first quartile (Q1) up to the farthest outlier are considered, accounting for 75% of the highest values of the data. For distances, the interval from the lowest outlier up to the third quartile (Q3) is used, accounting for 75% of the nearest distances. The variable distance and stream order are not dynamic. They just affect the spatial variation of the hotspots. In order to account for seasonal variations over the months, the monthly average (period of 2008 - 2016) of simulated nitrate export is considered for each HRU. During this first step, each month of the year is considered, having 12 different boxplots to contemplate seasonal dynamics. The boxplot which shows the highest nitrate export average is selected (March for our case). In this way, the highest exports in the basin are considered. Then, the Threshold-Value Q1 - related to nitrate export - is obtained from the month of March. The first potential pixels to target (CSAs) will be those which encompass a whole HRU area for facilitating a future BMP implementation.

In this first step, for a pixel to be selected as a “potential CSA“, it has to fulfil three conditions simultaneously: drain into a stream of order 1 or 2, be in magnitude concerning nitrate export no smaller than the lower quartile (Q1) of the boxplot for March regarding nitrate export, and be in magnitude concerning distances to stream no greater than the upper quartile (Q3).

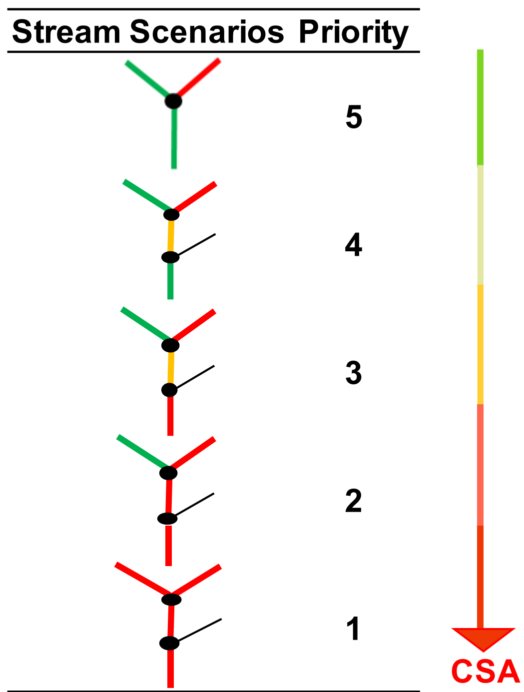
2- The second step accounts for enrichment or dilution effects from upstream subbasins, which could mitigate/improve or lower water quality.

Once first potential CSAs are preliminarily selected, the subbasin to which they belong is taken into consideration to account for the water quality of the stream they drain. The subbasins to which these pixels belong are checked from the point of view of mitigation or enrichment effects downstream to find if their subbasins are mitigating or impairing waters downstream. Decisions are made based on the simulated nitrate concentration at each outlet of the subbasins. This step of the workflow checks whether these potential selected pixels are having an impact on their corresponding outlets or are just not reflected in water quality measurements due to mitigation effects from confluences. Classification of these two different types of subbasins is made from the environmental threshold with a guiding concentration of 5.6 mg nitrate-N/l to reflect a level of concern (EUROSTAT, 2012) where algal blooms are associated with the loss of ’desirable’ plant and animal species affecting biodiversity.

The simulated daily nitrate concentration at each subbasin’s outlet is analysed to see how many days each subbasin has exceeded the environmental threshold during the studied period (over-threshold days´ variable), obtaining a picture of the “most polluted” and the “cleanest subbasins”. A boxplot is then obtained from all the data regarding the number of days exceeding 5.6 mg nitrate-N/l at each subbasins´ outlet for the DLU and CFD scenarios.

For differentiating the two types of subbasins, the over-threshold days ‘variable for the CCW corresponds to the lower quartile (Q1) of this boxplot. Subbasins that have exceeded the environmental threshold of 5.6 mg nitrate-N/l on more days than the Q1 threshold-value are considered “non-mitigators of pollution”. In contrast, those subbasins with values lower than Q1 are classified as “mitigators of pollution” when converging with their respective confluence in the CCW stream network since they are “cleaner” and contribute to dilution of nitrate when converging with confluences. Possible theoretical scenarios of confluence effects downstream and priority areas for BMPs placement (from 5 to 1, being 1 the worst case scenario/CSA, so the first priority area to act) are shown in Table 4. Pixels from the first step above will be definitely considered a CSA when the interaction of assigned polluted streams with their respective confluences results in a stream of priority ≤ 3 from Table 4 criteria.

Table 4. Mitigation and enrichment scenarios for stream network and priorities for CSA identification



The combination of the two steps will lead to the likely areas of pixels (CSA) impairing waters the most. The hypothesis assumes that targeting these hotspots at headwaters (stream orders 1 and 2) will improve the current water quality situation not just at the specific subbasin, but by taking advantage of confluence effects downstream, getting an overall water quality improvement within the watershed. The first and second steps were both performed for the two land use scenarios, DLU and CFD. In (Wang, Ma, *et al.*, 2018), nitrate losses are classified at the county scale in China into four categories quantiles (25%, 50%, 75%) of N losses. Their N and P losses are categorised as hotspots if they fall within the range of the top 25%.

5.5.2 Process-based method: Parsimonious approach

The application of mathematical programming and optimisation techniques to spatial analysis offer significant decision support in various circumstances where the production of solutions optimising certain objectives can be defined by users or decision makers (Meyer *et al.*, 2009).

To enable cost−effective selection and placement of BMPs, alternative BMP scenarios must be compared according to the functions of cost and diffuse pollution control (Veith *et al.*, 2004). As discussed in several papers, optimisation of multifunctional aspects is suitable to provide major orientations on changes (e.g. Meyer *et al.*, 2009). This study considers two factors: economic and environmental performance (costs for BMP implementation and nitrate concentration at outlets) in a cost-effective strategy management. Management approaches should consider the spatial location of sources of pollution in order to choose the most appropriate BMP that will achieve the required environmental targets while being economically and socially viable (Udias *et al.*, 2016).

5.5.2.1 Costs of estimation

Calculations are made individually per each Scenario and the Baseline model. Costs are calculated, first, per hectare (ha), then per HRU until obtaining a total result (total dollars at watershed level of implementing Scenarios 1, or 2, or 3 on the CSAs). The cost results are compared to the Baseline Scenario and are presented in $ per ha.

From Langemeier *et al.* (2020) seeds costs (Table 5) are calculated for average productivity soil. Units given are $/acre which are later transformed into $/ha.

Table 5. Seed acquisition costs

Operation	Units	Corn	Soybean
Seeds	$/acre	111	67

The operation management costs are obtained from (Langemeier, 2019) (Table 6). Units are $/acre and again converted into $/ha for calculations.

Table 6. Operation management costs

Operation	Units	Corn	Soybean
Planting	$/acre	Conventional:17.49, No-till:17.45	No-til:17.34
Tillage system: No-till	$/acre	0	0
Tillage system: Conventional (Plow and field cultivator)	$/acre	Chisel plow:14.3, Field cultivator:11.63	0
Application nitrogen fertilizer	$/acre	Spraying liquid:6.72, Side-dress AA:10.05	0
Application phosphorous fertilizer	$/acre	0	Broadcasting bulk dry fertilizer: 6.18
Herbicides application	$/acre	Self propelled sprayer:6.73	Self propelled sprayer:6.73
Harvesting	$/acre	Combine and haul to bin:37.52	Combine and haul to bin:33.56

The costs for AA, 10-34-0, Aatrex and Roundup (Table 7) were obtained from (Agricultural Statistics Board NASS-USDA, 2009), the Agricultural Prices 2008 Summary.

Prices for fertiliser AA is obtained as an average for the period 2003-2014, 10-34-0 for the period 2003-2008 and P fertiliser for 2008-2014. Aatrex and Roundup for 2005-2008.

Calculations are again made following the Tri-State Fertilizer Recommendation (Vitosh *et al.*, 1995) based on previous crop and yield at county level.

Table 7. Nitrogen and phosphorus fertiliser and herbicides costs

Operation	Units	Corn	Soybean
Fertilizer Nitrogen	$/ton	AA:615, 10-34-0:351	0
Fertilizer Phosphorus	$/ton	0	TSP(46% P2O5):662
Herbicide	$/l	Aatrex:3.44	Roundup:8.76

Some assumptions are taken for simplification purposes, contributing to no extra costs.

- No grain is kept as stock. Selling grain directly from the field at a moisture level above that needed for quality grade is convenient (Edwards, 2014). Indian farmers usually have small holdings. They do not have the financial capability to retain their surplus produce till favorable market price and have often to sell their product, immediately after the harvest (Noogle and Hormann, 2020).

- Not shredding of corn stalks.
- Not surfactant added to herbicide. Roundup is a glyphosate-based herbicide. Many glyphosate products come “fully loaded,” meaning they are formulated to include a surfactant (Armstrong and Lancaster).

Net returns (i.e., a comparison of costs and benefits) can be used to measure the economic impacts resulting from the introducing cover crops. Economic can be higher crop yields and lower nitrogen application rates. Adoption costs include seed costs, planting costs, termination costs with changes in fertiliser costs (Hughes and Langemeier, 2020). For the adoption of cereal rye as a cover crop in scenarios 2 and 3, the net return of 7.04 $/acre from a study in central Indiana (Hughes and Langemeier, 2020) is used.

Yields are also considered as the percentage of yield lost/gain compared to the baseline scenario. The percentage of yield variation is calculated for corn, soybean and winter wheat for the baseline and scenarios 1, 2, and 3.

From USDA's NASS-Indiana Field Office (Part of the Great Lakes Regional Field Office) (Indiana Field Office, 2014), the average price (dollars per bushel (bu)) for the period 2008 - 2020 is considered (Table 8) to financially quantify any lost in yields affecting farmers’ income.

Calculations are made with the yield lost/gain per HRU and the prices converted to $/kg.

Table 8. Average price for the main crops studied

Crop	Average price	Unit
Corn	4.47	$/bu
Soybean	10.73	$/bu
Winter wheat	5.35	$/bu

5.5.2.2 Environmental performance

Water quality can be measured in two different forms - by pollutant concentration or pollutant load. Both ways provide information of environmental significance, but each has limitations (Cahn and Hartz, 2015). This study considers nitrate loads in HosNIT (kg exported to the system). Still, for surface waters, nitrate concentration at outlets makes it easier to compare and more “visually” understandable for baseline variations. Also, the city of Fort Wayne takes its drinking water from the St. Joseph River downstream of its confluence with the CCW (Rice, 2005) and drinking water quality standards are globally given in this form which is selected for the optimisation part in this study.

Then, the nitrate concentration at each outlet for all subbasins within the CCW is considered to account for the environmental performance of BMPs at the identified hotspots through HosNIT. CSAs (HRUs in SWAT) change their management file according to the scenario simulated. The SWAT model is run daily for the baseline scenario and scenarios 1, 2, and 3 for the period studied, and the nitrate concentrations are obtained on a daily scale. Same as with HosNIT, and for consideration of temporary variation, spring is taken as reference since it is the period where the maximum export of nitrate is registered. The idea is to check whether a reduction at the subbasin level is obtained through implementing BMPs on the CSAs and, in the end, at the outlet of the watershed.

Per scenario, a season average of nitrate concentration for each subbasin is obtained. Then, relative change is calculated for a comparison of each scenario to the baseline scenario.

5.5.2.3 Parsimonious approach

To address the current algal bloom problem in Lake Erie, one solution is to determine the most cost-effective strategies for implementing agricultural best management practices (Liu *et al.*, 2019). An (environmental and economic) optimised solution is obtained for the CCW for the BMPs selected and being spring the referent for seasonal considerations of nutrient export. The constraints incorporated in the optimisation approach include costs of BMP implementation and pollutant (nitrate) concentration reduction at the subbasin scale.

At each subbasin, a unique scenario is selected for the optimized solution, so the scenario applied in each CSAs/HRUs is the same at the subbasin level (there are no different scenarios for the HRUs within a subbasin for pragmatically use in running SWAT).

The scenario selection is based on the efficiency of pollutant reduction per 1-dollar cost of the BMP implementation. So, the maximum nitrate concentration percentage reduction by every $ spent on BMPs implementation is desired.

Once each subbasin has its corresponding scenario, this optimised solution is run in SWAT for the period of study 2005 - 2020. Total nitrate concentration reduction is quantified at the outlet of the CCW (watershed scale).

The finest detection of hotspots of nitrate through HosNIT allows a more simplistic and straight forward implementation of BMPs considering costs and maximum nitrate reduction at surface waters.

5.6 Preliminary check for identified CSAs: Sensitivity of HosNIT to fertiliser reduction rates

There is no literature identifying the total CSA pollutant contribution at the catchment scale, and there is no quantitative assessment of program effectiveness if CSAs are actively targeted (White *et al.*, 2009). In order to test the sensitivity of HosNIT to identified CSAs, several fertilizer reduction scenarios were analysed (Table 9).

The amount of fertiliser containing nitrogen (APP, AA, Elemental N and Dairy manure) for the different crop rotations was reduced by 5%, 10%, 20% and 50% compared to the initial baseline scenario in the identified CSAs for DLU and CFD. These values were selected to check a slight reduction of nitrate input to a more critical one for crops.

Each CSA was an HRU in SWAT, where the fertiliser reduction was applied in the management file.

Table 9. Fertiliser reduction scenarios according to types and crops

Crop	Baseline		5% reduction		10% reduction		20% reduction		50% reduction	
	APP	AA	APP	AA	APP	AA	APP	AA	APP	AA
Corn (in soybean) kg/ha	130	160	123.5	152	117	144	104	128	65	80
Corn (in monocrop) kg/ha	133	203	126.35	192.85	119.7	182.7	106.4	162.4	66.5	101.5
Corn (in winter wheat and soybean) kg/ha	130	160	123.5	152	117	144	104	128	65	80
	Elemental N		Elemental N		Elemental N		Elemental N		Elemental N	
Winter wheat (in corn and soybean) kg/ha	33	100	31.35	95	29.7	90	26.4	80	16.5	50
Winter wheat (in alfalfa) kg/ha	30	100	28.5	95	27	90	24	80	15	50
	Dairy Manure		Dairy Manure		Dairy Manure		Dairy Manure		Dairy Manure	
Alfalfa (in winter wheat) kg/ha	40000	30000	38000	28500	36000	27000	32000	24000	20000	15000

6 Results and discussion

6.1 Calibration and validation

The calibration and validation are on a daily step, and it has been used the adjusted NSE with the +-5 days window for loads, as mentioned in Chapter 4.1. The adjusted NSE has been previously used in literature (Femeena et al., 2018) together with recommended performance ranges from Moriasi *et al.* (2007). The same authors (Moriasi *et al.*, 2015) reviewed and established new performance evaluation criteria for recommended statistical performance measures for watershed- and field-scale models. This paper establishes ranges for model performance measures of R^2, NSE and PBIAS. Results for the CCW of the statistical indexes of R^2, NSE and PBIAS for both scenarios, for stream flow and nitrate loads, are shown in Table 10.

The previous review (Moriasi *et al.*, 2007) about these statistical model performance indicators did not specifically include R^2 but mentioned that for R^2, typically, values greater than 0.5 are considered acceptable in literature (Santhi et al., 2001, van Liew et al., 2003). When using more ambitious ranges from (Moriasi *et al.*, 2015) for streamflow and loads (nitrogen), calibration can be judged as satisfactory and good for streamflow and very good and good for loads in both land use scenarios (DLU and CFD). For validation, it is not satisfactory for flow and good for loads. Typically, model performance is poorer for relatively finer temporal resolution for evaluation than for longer resolutions (e.g., daily vs monthly or yearly) (Engel *et al.*, 2007). The performance guideline is on a monthly scale. Therefore, sometimes unsatisfactory performance may still be satisfactory. There are specific performances which are unacceptable beyond certain reasonable ranges. Thus, in this article (Moriasi *et al.*, 2015), $R^2 < 0.18$, NSE < 0.0, PBIAS $\geq \pm 30\%$ for flow, and PBIAS $\geq \pm 70\%$ for nutrients represent unacceptable model performance. None of these ranges appears in our model for calibration and validation.

According to Moriasi *et al.* (2007), in general, monthly model simulations can be judged as satisfactory if NSE > 0.50 and if PBIAS ±25% for streamflow, PBIAS ±55% for sediment, and PBIAS ±70% for N and P. Considering that the performance at the watershed outlet is daily for calibration and validation, it can be described as good for both lands uses, DLU and CFD; and for the three statistical indexes tested (R^2, NSE and PBIAS), also taking into account the uncertainty of the spatial distribution of the location of tile drains. CCW is a heavy tile-drained area.

The R^2 values of both land-use scenarios of streamflow and nitrate loads are over 0.59 for calibration and over 0.48 for validation. NSE ranged between 0.58 and 0.61 for calibration and between 0.46 and 0.57 for validation, respectively.

PBIAS also describes a very good model performance in streamflow for both scenarios and for calibration and good for validation (van Liew *et al.*, 2007). Loads of nitrate range between -37.80 and -47.20 in calibration and validation.

Table 10. Daily calibration and validation results for flow and nitrate loads. DLU (upper) and CFD (lower) scenarios

DLU	**Calibration**			**Validation**		
Metric	R^2	PBIAS	NSE	R^2	PBIAS	NSE
Stream flow (m^3/s)	0.60	-8.30	0.58	0.48	-20.20	0.46
Nitrate loads (kg/d)	0.72	-37.80	0.61	0.76	-47.20	0.55

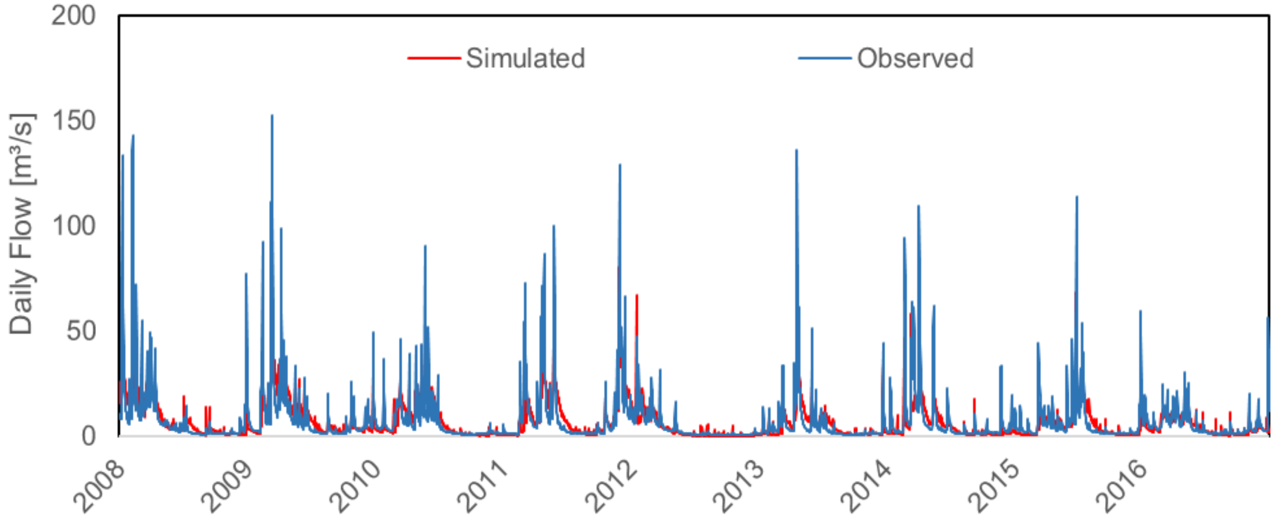
CFD	**Calibration**			**Validation**		
Metric	R^2	PBIAS	NSE	R^2	PBIAS	NSE
Stream flow (m^3/s)	0.60	-6.20	0.58	0.49	-17.00	0.47
Nitrate loads (kg/d)	0.71	-40.30	0.58	0.78	-46.20	0.57

A day-to-day simulated and observed hydrograph are presented in Figure 10, and simulated and observed loads in Figure 11.

The calibration period is from 2008 to 2012, and validation is from 2013 to 2016.

In general, during the study period baseflow conditions are well represented and slightly over-estimated in the simulation, being peaks normally under-simulated except for the flow in 2012, which was considered a very dry year. During the simulation period precipitation varies from 670 to 1218 mm (2008: 1083 mm, 2009: 1161 mm, 2010: 867 mm, 2011: 1218 mm, 2012: 670 mm, 2013: 925 mm, 2014: 896 mm, 2015: 969 mm and 2016: 912 mm).

Under-estimation of the peak flows may be a consequence of the location of climatic stations. If an event has taken place at the gauge, it is probably that the intensity has not been well represented. The assignment to each subbasin of the rain gauge nearest to its centroid does not guarantee that the gauge selected is the most representative of the precipitation in the subbasin. If more than one rain gauge is available in the subbasin, precipitation data are lost (Galván et al., 2014). Figure 3 demonstrates that the gauge station USGS is almost equidistant to the climatic stations of Garrett and Columbia. There is just one station (Garrett) within the CCW, and its furthest point is the USGS station, where discharge data is obtained. Load peaks are also underestimated for both scenarios, which follow the pattern for the flow. Still, it also may be possible that the amount of agriculture and/or fertilisation levels in the CCW were underestimated, and more fertilisation was applied by farmers than our calculation from the guidelines in the Tri-State recommendations (Vitosh *et al.*, 1995).



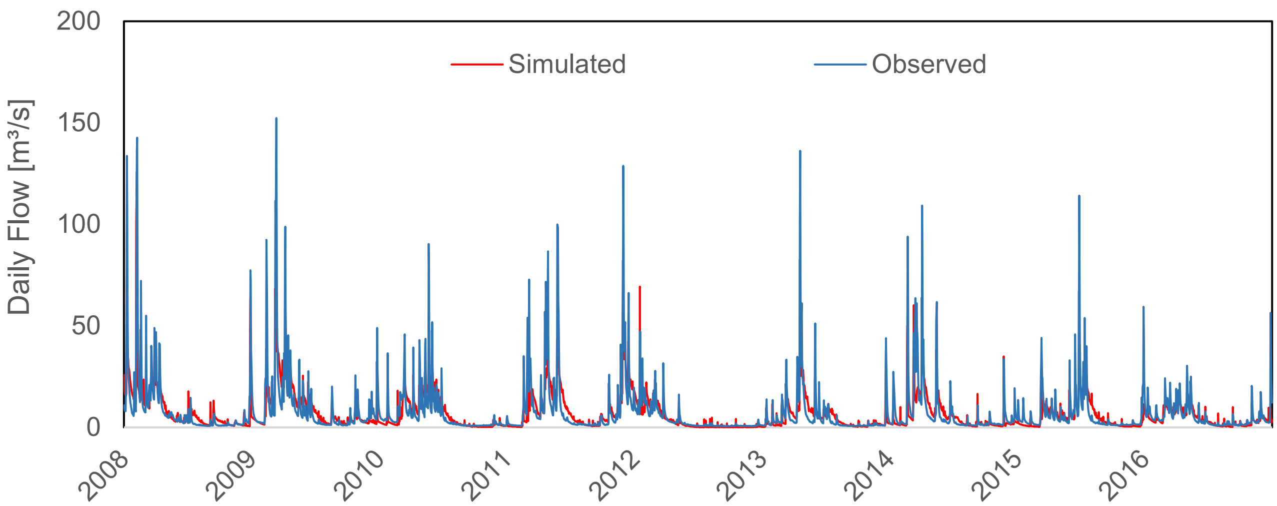
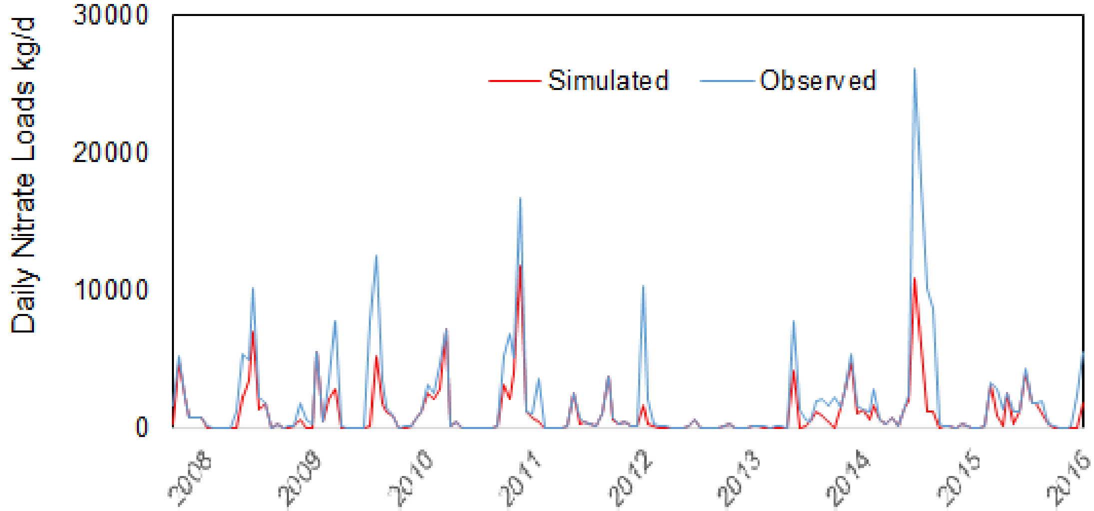


Figure 10. Comparison of observed and simulated daily flow at the watershed outlet for the baseline 30-m CCW for DLU (above) and CFD (below)Conceptual scheme of pixels as first-potential hot spots (in red)



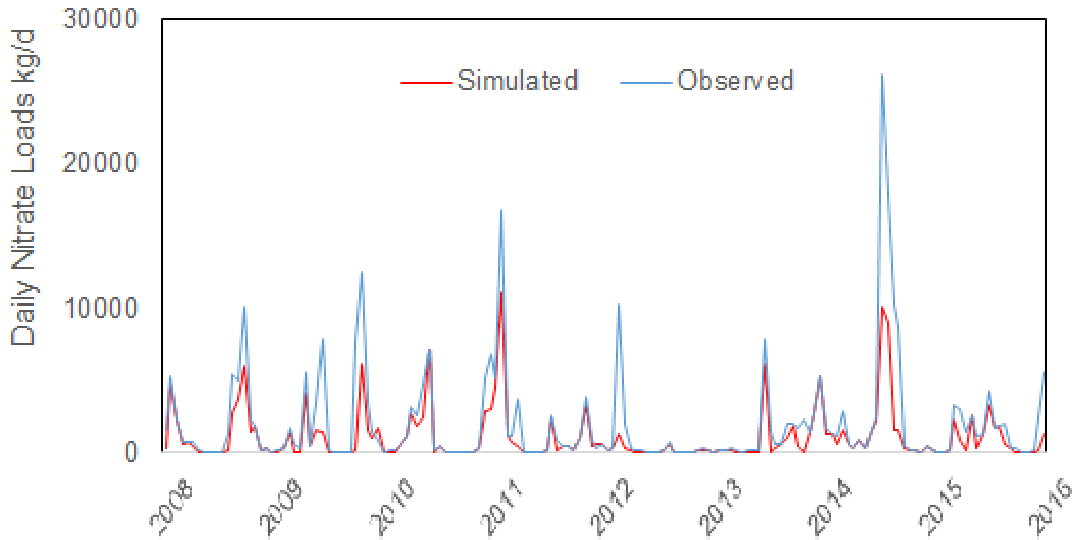


Figure 11. Comparison of observed and simulated daily nitrate loads at the watershed outlet for the baseline 30-m CCW for DLU (above) and CFD (below)

Table 11 presents basin-level SWAT values for significant water and nitrate components. This water balance budget and the importance of tiles in the watershed might also explain some performance in the calibration and validation results. As mentioned before, the assumption of the spatial location for tiles is made due to the lack of this type of data. It can be appreciated that runoff and lateral flow are not the main pathways for water in the CCW, which corresponds, for both scenarios, to the low value of nitrate yield compared to nitrate being leached. This is probably due to the general flat slopes across the terrain.

The main pathway is water that percolates and becomes groundwater. But, it is also important to notice the value of water reaching the stream from tiles, 44 mm and 39.3 mm for DLU and CFD, respectively. Even if these values could be, apparently, masked by their numbers, it has to be highlighted that these are averaged values for the entire watershed, meaning that some areas/HRUSs are exporting a considerable amount of water/nitrate since tiles eject nitrate directly to the stream. This critical factor of tiles is “spatially unknown” and has an important weight in water and nitrate budgets. The calibration of heavy-tiled watersheds, such as the CCW is challenging, especially for nitrates.

Table 11. SWAT water and nitrate parameters for annual basin values for DLU and CFD scenarios

Parameter	DLU	CFD	Units
SURFACE RUNOFF Q	45.0	41.8	mm
LATERAL SOIL Q	6.9	6.1	mm
TILE Q	44.0	39.3	mm
TOTAL AQ RECHARGE	244.3	242.6	mm
NO3 YIELD (Surface Runoff)	1.9	1.6	mm
NO3 YIELD (Lateral flow)	0.0	0.0	kg/ha
NO3 YIELD (Tile)	1.9	1.9	kg/ha
NO3 LEACHED	17.2	17.0	kg/ha

6.2 Spatio-temporal variation of hotspots with HosNIT due to different crop rotation scenarios (DLU vs CFD)

The analysis is made for the period 2008 - 2016. Continuous simulation of multi-year crop rotations yielded results of slightly higher quality compared to the simulation of single years (Kollas *et al.*, 2015).

In order to test the sensitivity of the HosNIT method, the influence of the four different fertiliser reduction scenarios (cf. Table 9) at the HRU level on the water quality was observed through the CCW`s outlet response for the two different scenarios: DLU and CFD.

The two different land-use inputs also make a difference in relation to the percentage of the watershed to target (hectares of identified CSAs) and the average of how many days each subbasin has exceeded the environmental threshold during the studied period (over-threshold days variable).

In Figure 12 (Soybean (SOYB)), the percentage of the difference in land use in CFD with respect to DLU is shown. The difference between the two land uses encompasses a total area of 10.7%, with the distribution specified in Figure 12. A 9.7% out of the 10.7% belongs, in the same proportion, to monocrop soybean and the practice of incorporating winter wheat as a cover crop in a corn-soybean rotation. In CFD, the practice of soybean/corn monocrop was detected since, in those pixels, at least seven years (in a period of 9 years, reference 2008 - 2016) were soybean/corn cultivated.

A portion of 4.8 % of the agricultural land was classified as monocrop soybean. On the other hand, even though cropping corn usually provides higher economic returns compared to soybean, it is also more expensive to produce and to harvest (Ubilava, 2008). Then, the CFD scenario adds less nitrate input to the watershed than the DLU since, for the four crop patterns in Figure 12, DLU assumes a corn-soybean rotation in the period of study, and the continuous corn practice shows a small share. The farmers' adoption of either rotating or continuous corn is largely determined by the expected prices of corn and soybean (Ubilava, 2008).

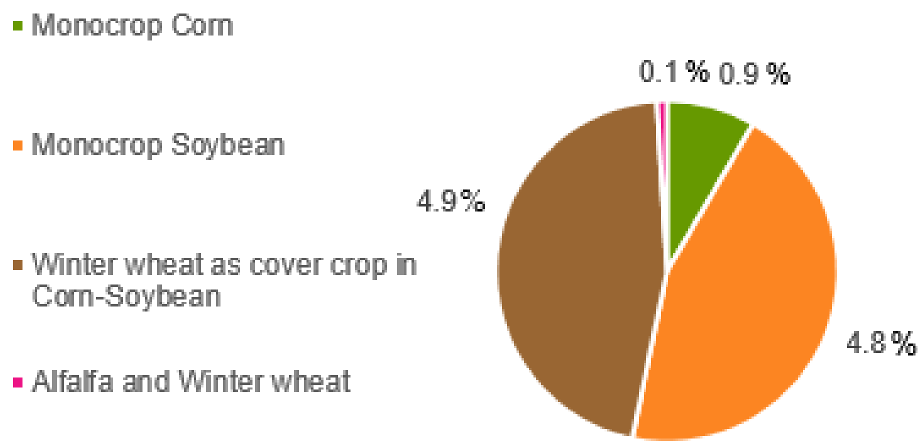


Figure 12. Percentage of land use difference in CCW in CFD respect to DLU.

These spatial differences reflected in the land-use input part of the model have an impact on the hotspot distribution. Different HRUs will become CSAs.

The designation of CSAs is based on the criteria described in the Methodology (Chapter 4.5). The results presented are for the threshold of the nitrate export obtained in March (month of the maximum nitrate export), for distances, the interval up to the Q3, accounting for 75% of the nearest distances, and for the differentiation of streams being mitigators or non-mitigators of pollution considering the threshold of 5.6 mg nitrate-N/l concentration at the outlets.

It has accounted for the worst-case scenario, trying to include as much data as possible without making an unfeasible analysis. Probably, with the change of the criteria, hotspots may vary spatially. Assuming these thresholds and establishing multi-criteria specifications for CSAs definition may, accurately, depict hotspots of nitrate where BMPs implementation will improve water quality at their most.

Table 12 presents the three parameters selected to account for the differences in DLU and CFD. These are the targeted area (total CSA area), the Over-threshold days` variable and the outlet response to fertilizer reduction (50% and summer) in nitrate concentration.

Table 12. Response differences-DLU and CFD scenarios

Parameters	DLU	CFD
Targeted area (% watershed)	14.8	9.3
Over-threshold days ‘variable	28	24
Outlet response nitrate	7	7.1

One of the most relevant differences is the targeted area (% watershed), described as the total area of the watershed, which is considered a CSA. For DLU, 14.8% of the total watershed is considered a CSA, and for CFD, 9.3%. Identifying proper rotations and not assuming a specific rotation of soybean and corn translates in the CCW into a reduction of 5.5% of the total area of the watershed to target through BMPs.

The Over-threshold days ‘variable considers a subbasin as a “mitigator of pollution” if it has not exceeded the threshold of 28 days above the environmental threshold in the DLU scenario and 24 days in the CFD. The value of 28 and 24 days corresponds to the Q1 of the boxplot in Figure 13. In this way, a criterion for differentiation is achieved for checking any dilution effects from the confluences. The Over-threshold days ‘variable is used in the second step of HosNIT, once potential first cases of CSAs are determined. The idea behind this parameter is to verify if preliminarily identified areas are having an impact (on water quality) at their corresponding outlets or if mitigation effects from the upper part of the catchment are masking them.

Again, the selection of the Q1-value for this parameter encompasses the majority of the data and accounts for an ambitious threshold.

Following the Table 4 criteria, priorities are established to finally classify an HRU as a CSA.

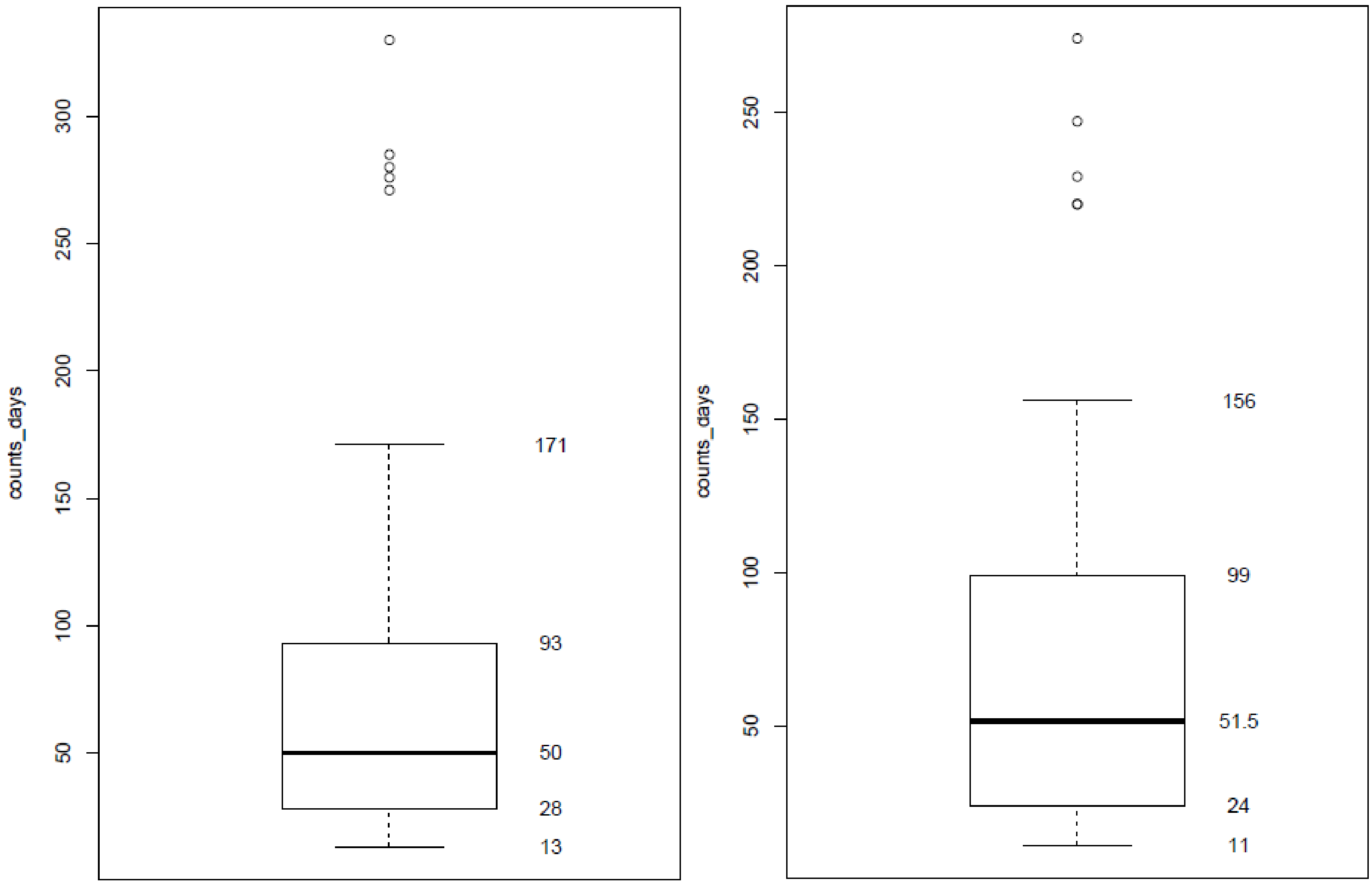


Figure 13. Boxplot for the total of CCW subbasins of days exceeding the environmental threshold for DLU (left) and CFD (right)

Figure 14 shows (for the baseline scenario) each subbasins difference (in days) and stream order (SO). The difference (X axis) is calculated as the total number of days that each subbasin has exceeded the environmental threshold in the CFD scenario minus the total number of days that each subbasin has exceeded the environmental threshold in the DLU scenario. Subbasins near the grey-discontinuous line (0) mean no difference between the scenarios for nitrate outlet concentration above 5.6 mg N/l in the number of days exceeded. These subbasins have a lower amount of pixels which have been transformed from DLU to CFD because a different crop practice was identified. In the case of the outlet of the CCW (subbasin 69), the difference is small and close to the zero line. Negative values account for a higher number of days exceeding for DLU, the opposite for positive values. Some subbasins, especially for the first stream order (Figure 15) (low discharge), are more sensitive to the land use input.

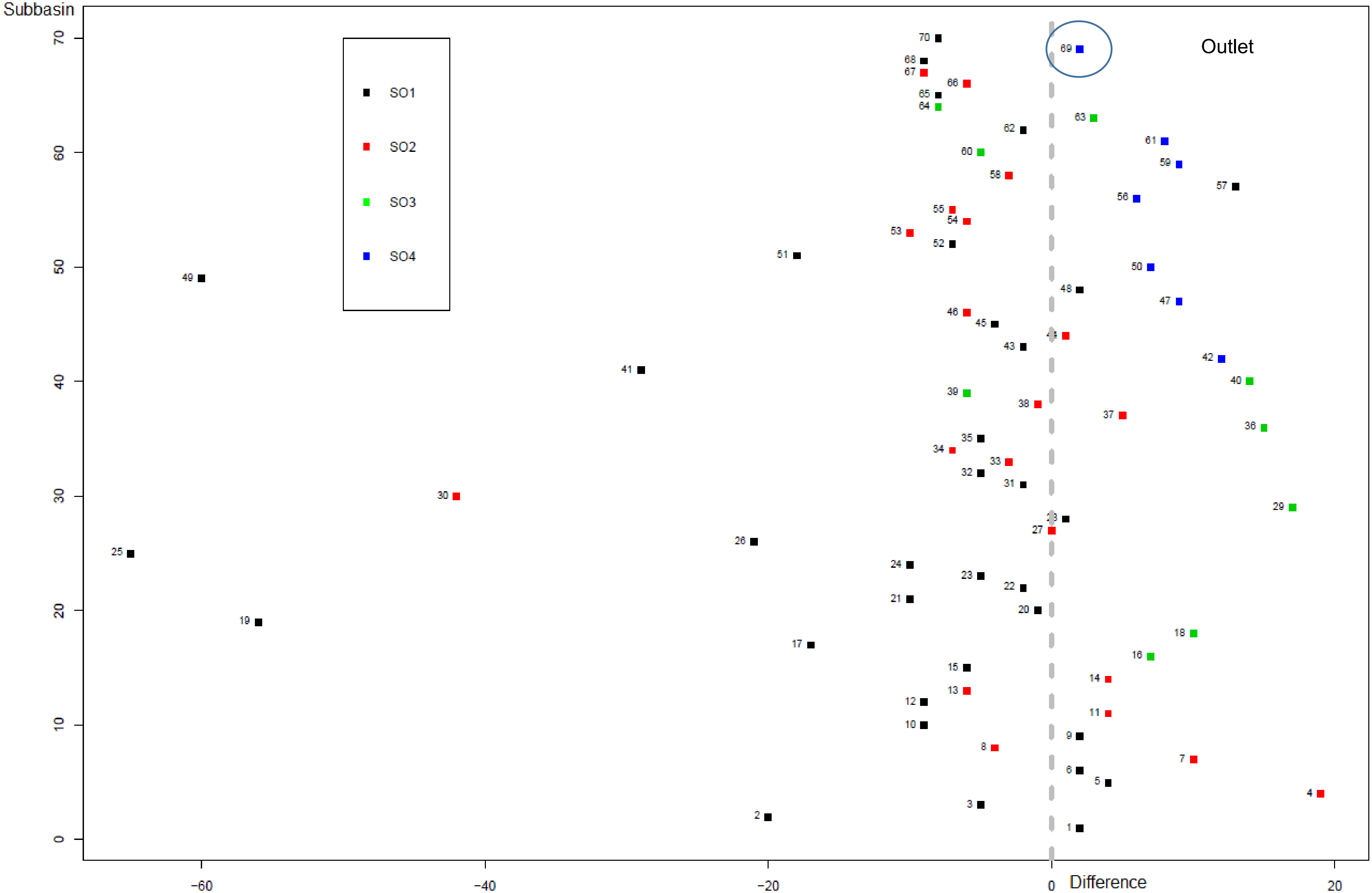


Figure 14. Difference (in days) per subbasin and stream order of each subbasin (CFD-DLU)

Subbasin 30 results from a conjunction of Subbasin 25 and Subbasin 26, even if stream order is not 1, this conjunction of polluted streams impacts on it.

Subbasins with the most extreme values in Figure 14 (Subbasin 25,49,19,30,41) of difference are subbasins under tile drainage and (mostly) type of soil IN5. Also, Subbasin 25 has the 70% of its soil under artificial tile. Changes in the crop rotations directly affect the stream water quality since tiles flush out nutrients. Incorporating a cover crop in CFD has a strong impact on water quality.

Although Soil IN25 and IN19 are also tiled, Soil IN5 (Figure 2) is differentiated in the DDRAIN (Distance to sub-surface drain) parameter in SWAT (Table 1). The Ksat (Saturated Hydraulic Conductivity of Soil) is the infiltration rate once the ground has reached 100% saturation. The infiltration rate has become constant and a critical parameter in the design of artificial tiles. At 940 mm, Soil IN5 has 50% content of clay, and Ksat equals 0.56 mm/h, in order to let water in the tile, DDRAIN was set at 730 mm (which means 27% upper than IN25 and IN19). Since nitrate is quickly transported via the tile drains has fewer options for being taken up or denitrified. The subbasins with Soil IN5 are more susceptible to land use changes with any extra fertilizer addition: as monocrop corn or transforming monocrop soybean into a corn-soybean rotation.

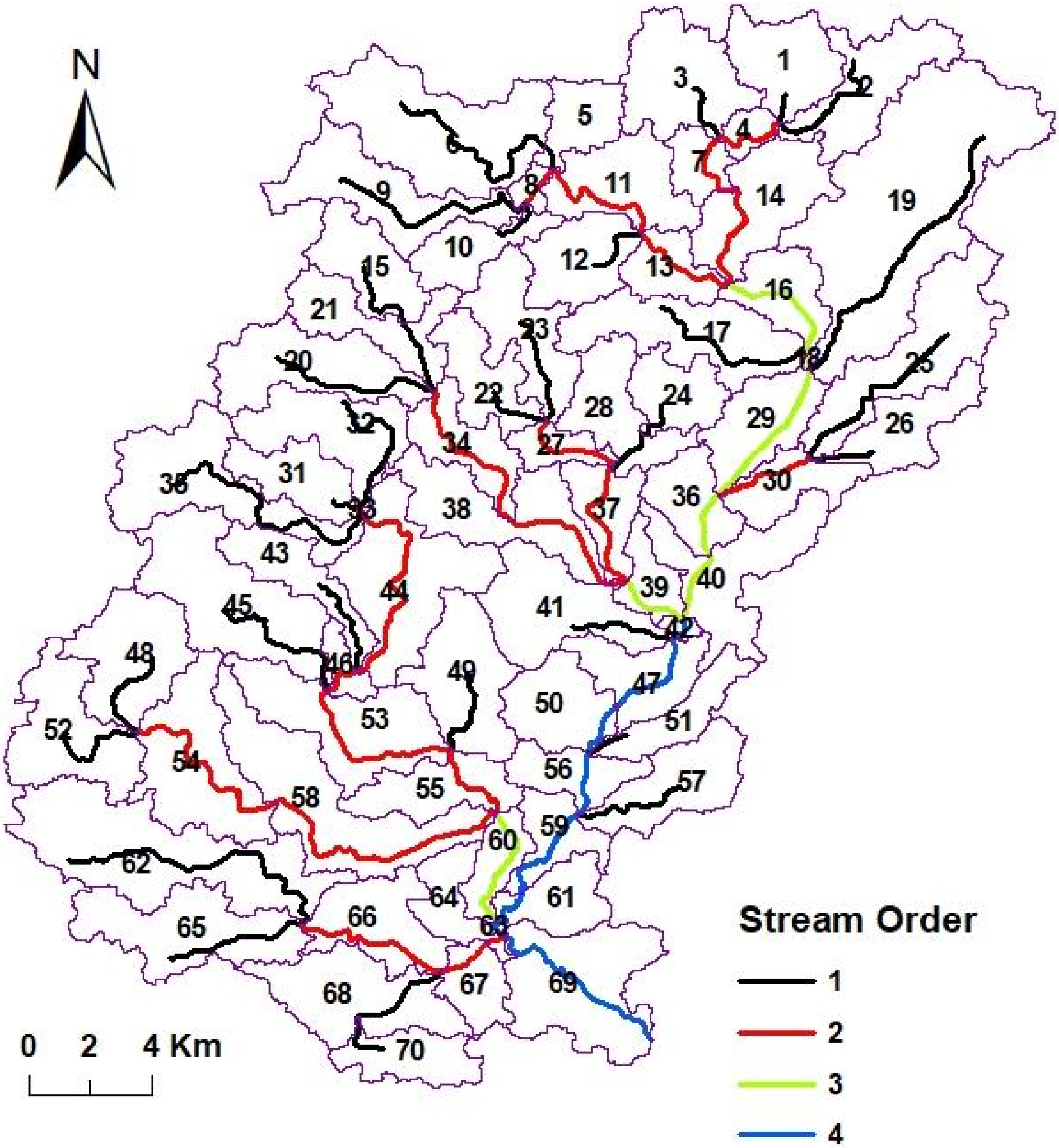


Figure 15. Subbasins and stream order in CCW

The parameter of the outlet response to nitrate reduction (%) is defined as the reduction of the nitrate concentration in the outlet of the CCW as a consequence of fertiliser reduction in hotspots. It is calculated for the different seasons and the subbasins with CSAs in their area and the subbasins with a downstream benefit for both land-use inputs.

The fundamental strengths of SWAT are flexibility in combining upland and channel processes and simulation of land management (Arnold et al., 2012b).

Table 12 gives the outlet response of the whole watershed for DLU and CFD for the summer season. Moreover, it depicts a fertiliser reduction of 50%, with a total of 7% for DLU and 7.1% for CFD nitrate concentration reduction as compared to the baseline scenario. CFD shows approximately the same nitrate concentration reduction at the outlet compared to DLU, considering that this last targets 5.5% of less area of CCW as a CSA. The largest reduction was obtained by summer and 50% application of fertiliser.

Figures 16 and 17 show the specific case of a 50% fertiliser reduction during the summer season. Subbasins with coloured pixels indicate the spatial identification of the CSAs and the reduction of nitrate concentration at their respective outlets, with a maximum of 33% (purple colour in the legend). Dotted subbasins are subbasins with a reduction in their respective outlets (in numbers) due to downstream effects and without any reduction of fertiliser at their subbasins (stream orders 3 and 4). The main differences in the results can be observed between monocrop soybean and the use of winter wheat as a winter crop after the harvest of corn/soybean. Monocrop soybean adds four times less nitrate in 9 years than the corn-soybean rotation. Incorporating winter wheat as a cover crop in the corn-soybean rotation during the winter season has benefits studied and shown in the literature. Cover crops are able to reuse nutrients that might otherwise be lost into water during the winter and spring (Mannering *et al.*, 2007).

Identifying proper rotations in fields translate into more accurate rates of nitrate exports within the watershed, which means finer and more precise CSA identification.

The other maps for other seasons and different fertilizer reduction ranges are included in the Supplementary Material section A2.

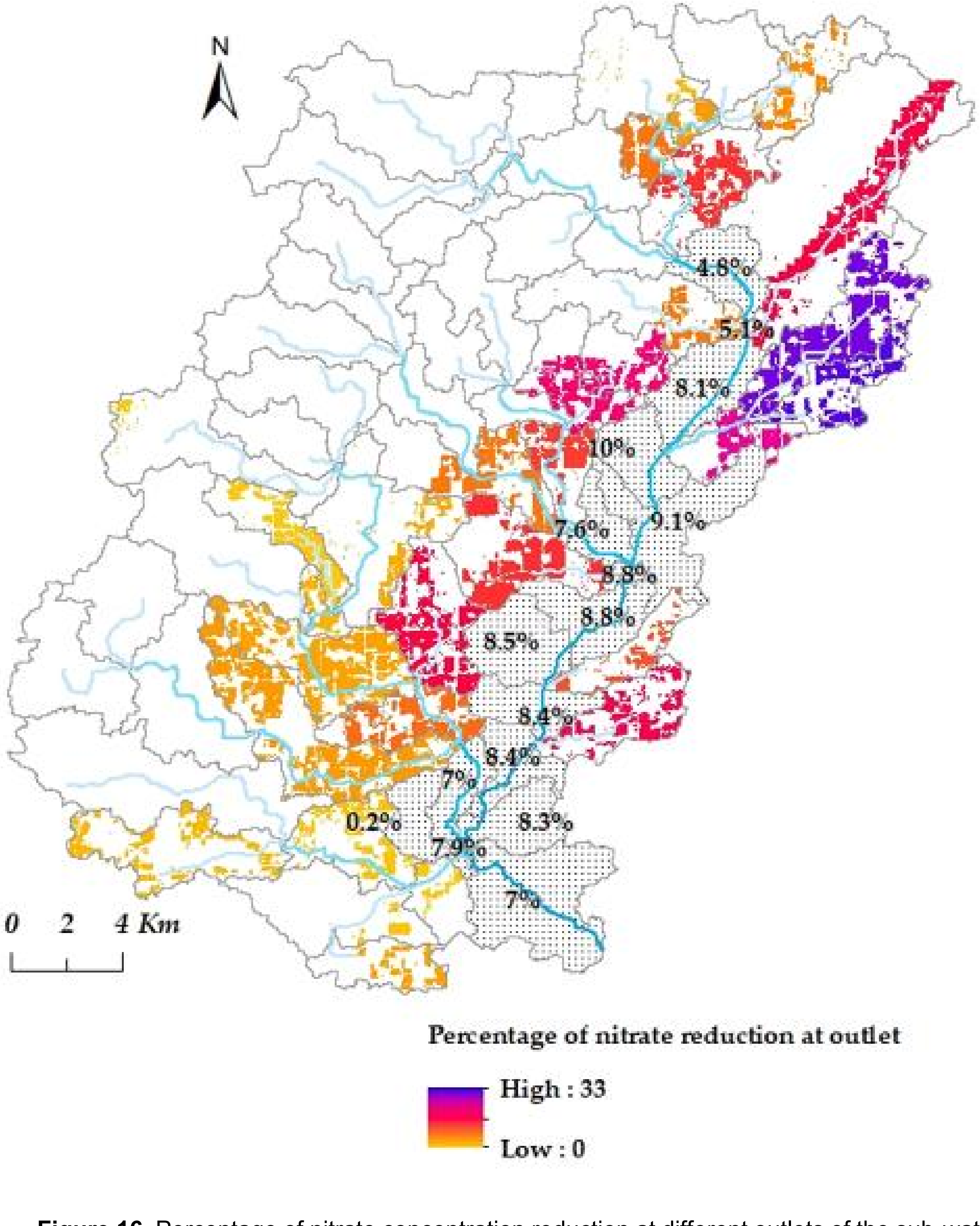


Figure 16. Percentage of nitrate concentration reduction at different outlets of the sub-watersheds for the Cedar Creek Watershed (CCW) in summer with a 50% of fertilizer reduction at CSAs. DLU scenario

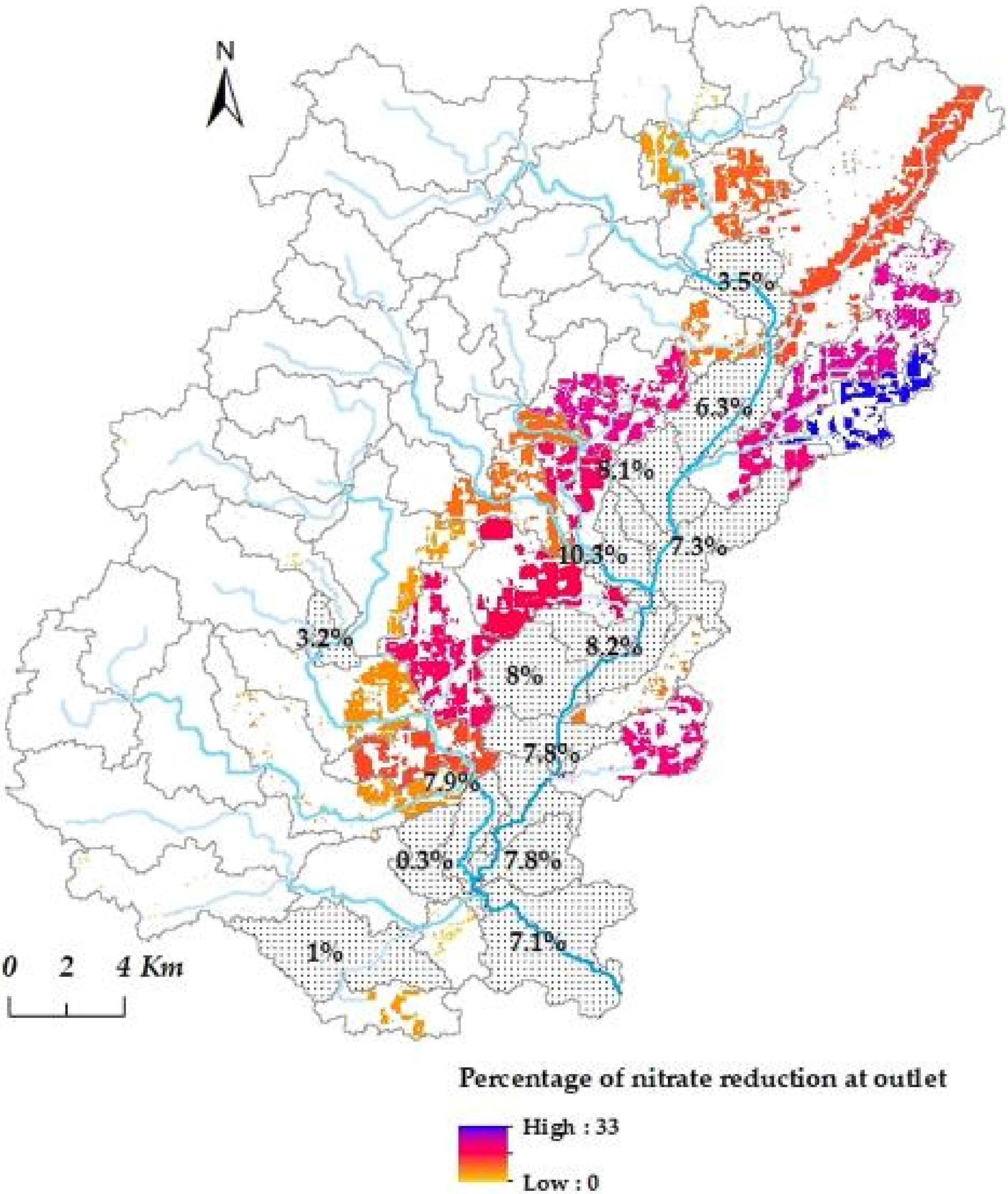


Figure 17. Percentage of nitrate concentration reduction at different outlets of the sub-watersheds for the Cedar Creek Watershed (CCW) in summer with a 50% of fertilizer reduction at CSAs. CFD scenario

In order to calculate the different reductions in nitrate concentration, daily SWAT model runs from 2008 until 2016 were carried out for the baseline scenario and the four different fertiliser application rates. Nitrate concentrations at outlets for each subbasin were obtained. An average was calculated for spring (days of March, April and May), summer (days of June, July and August), fall (days of September, October and November) and winter (days of December, January and February) according to the seasons' definition by the World Meteorological Organization (WMO) (WMO, 2010). Then, the four application rates were compared to each season's baseline scenario for DLU and CFD scenarios. Figure 18 presents the results for the DLU and CFD scenarios at the CCW outlet. The variation in nitrate concentration at the final outlet of the CCW verifies the importance of these areas (CSAs) in water quality downstream.

Since fertiliser reduction affects both loads and the hydrology remains the same (constant) for all scenarios, it is assumed that the variation in the concentration relies on a variation in loads. Therefore, the nitrate concentration outlets give information about their corresponding drainage area related to reducing nitrate inputs at hotspots. Results then are assumed to be independent of the discharge variable.

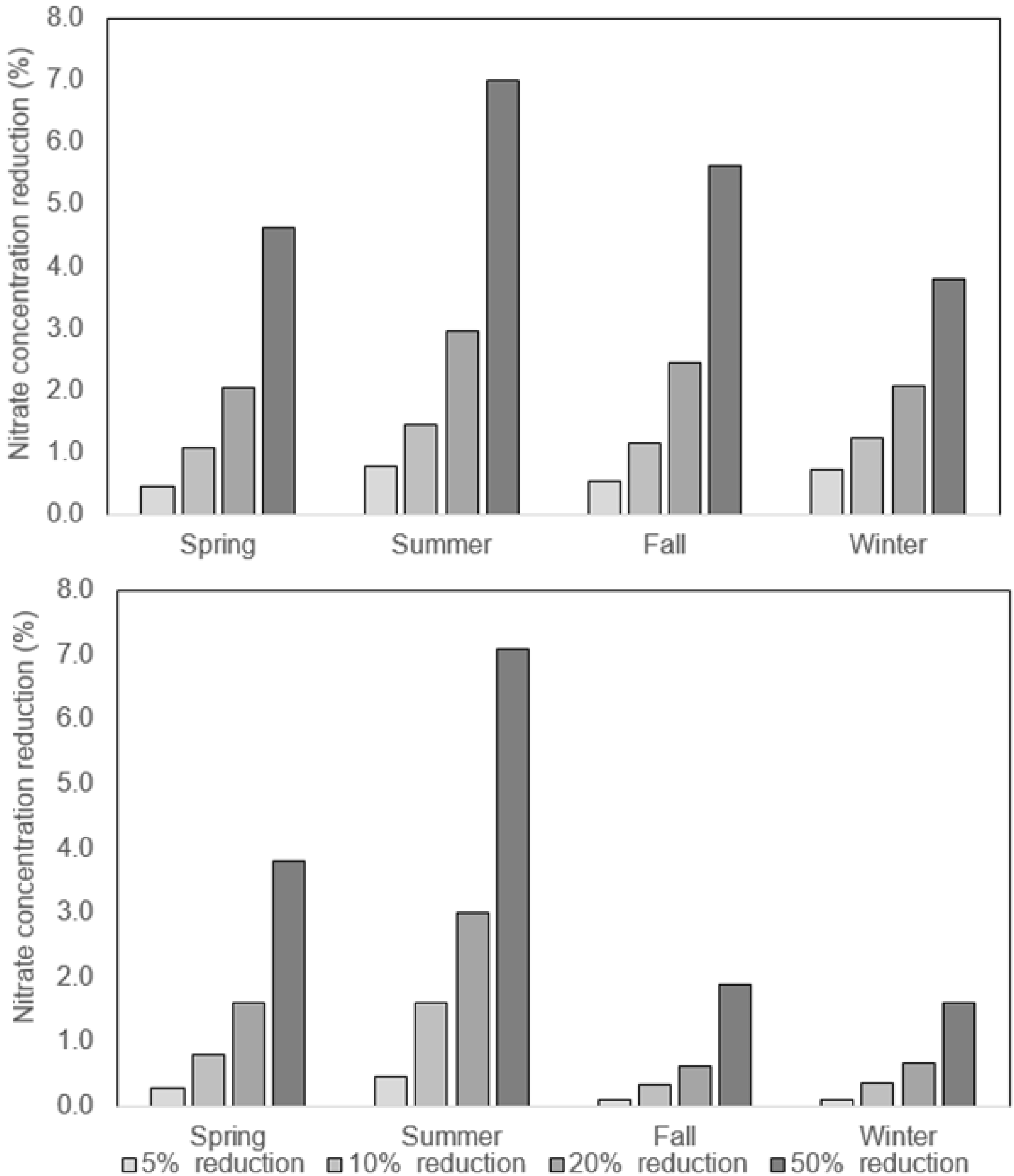


Figure 18. Nitrate concentration reduction in percentage at the outlet of Cedar Creek Watershed (CCW) for every season with the four different fertilizer reduction scenarios for the DLU (above) and CFD (below)

The identification of more realistic crop patterns (CFD) results in a different spatial distribution of hotspots across the watershed, affecting, in some cases, different subbasins. These different patterns in the land use input affect the nitrate export rates. When the land-use input corresponds to the CFD scenario, the total area considered a hotspot is 5.5% less than the DLU scenario. Still, both achieve approximately the same reduction in nitrate concentration in the CCW outlet for all seasons and all fertiliser application rates, except for the fall and winter seasons compared to the baseline scenario. The incorporation of a winter cover crop in the CFD scenario positively impacts the nitrate export rate (decreases), especially in fall, after the harvest of corn or soybean. Quantitative variations were found regarding the effects of the DLU and CFD scenarios on nitrate reduction at the outlet. Therefore, the difference between CFD and DLU for this season and the 50% reduction scenario is notable since less nitrate is available in fall to be "mitigated".

Regarding the different outlet behaviour of DLU and CFD for nitrate reduction, quantitative variations are found (Figure 19). The percentage of variation for each season (i) with each different fertiliser application rate (j) is calculated as subtraction of DLU and CFD reduction:

$$\textit{Percentage of variation}(\%)(i,j) = \textit{DLU reduction}(\%)(i,j) - \textit{CFD reduction}(\%)(i,j) \quad (4)$$

The red line in the graph below represents no variation in the percentage. The differences mentioned above for fall and winter are visually explained, while for the two other seasons, the difference in nitrate reduction in the outlet of CCW for DLU and CFD is < 1%.

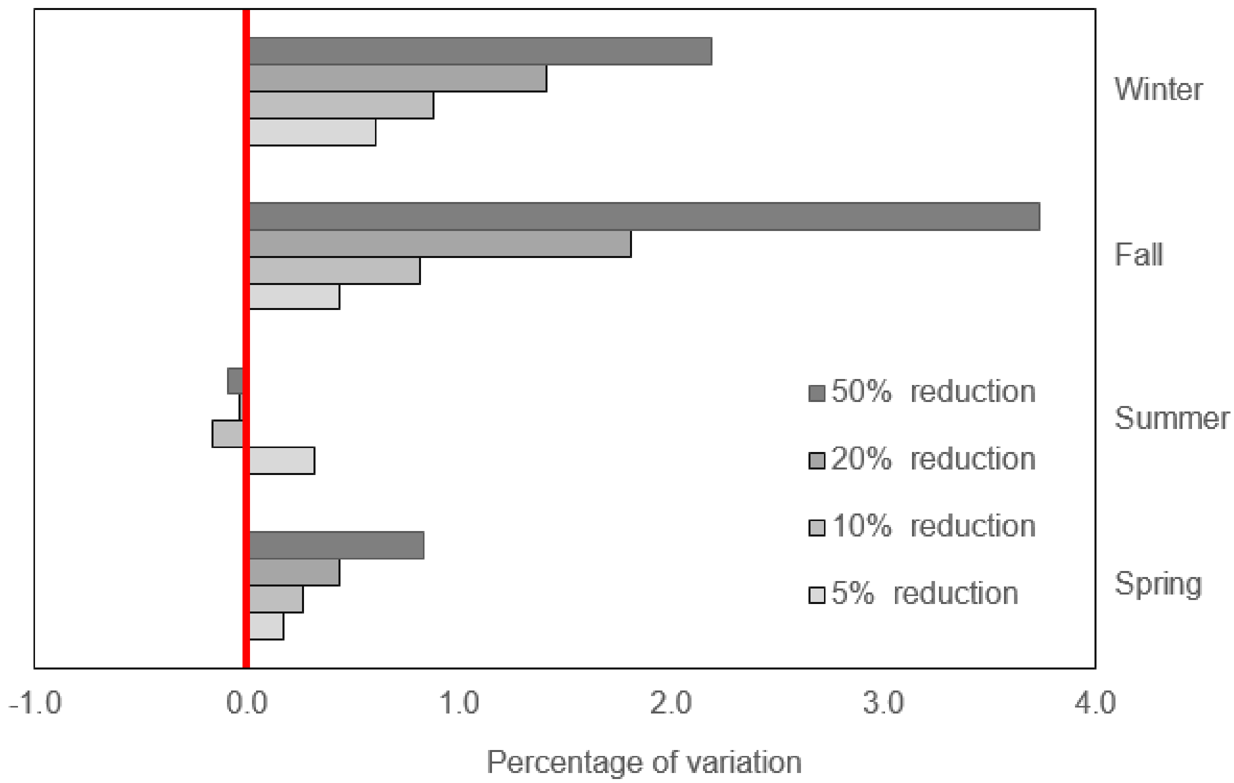


Figure 19. Percentage of variation (DLU-CFD) of nitrate concentration outlet for CCW

The summer season obtained the largest nitrate reduction at the CCW outlet in both scenarios (DLU and CFD) and for all different fertiliser rates. The most relevant crops in CCW are corn and soybean. With reduced fertiliser application, the plant is forced to obtain more nitrate from the soil pool. The months of June, July and August coincide with the largest nitrate uptake in corn (Hanway, 1966) and soybean (Hanway and Thompson, 1967). The nitrate export decreases compared to the baseline scenario due to the extra uptake from the soil to supply the drop in fertiliser.

Northeast Indiana is dominated by a pothole landscape with many closed depressions being scattered throughout a watershed (Smith *et al.*, 2008), this may affect the location of the hotspots. It is important that SWAT simulates tile flow and pothole landscapes that are common in much of the Corn Belt and Great Lakes states (Du *et al.*, 2005). In the SWAT 2012, a subroutine simulates depressional areas that do not drain to the stream network (potholes) and impounded areas such as rice paddies. The output.hru file identifies potholes and parameters that affect nitrate and water quality, such as:

- POT_TILE: Average daily outflow to main channel from tile flow (depth [mm] over entire HRU)
- POT_VOLX: Maximum volume of water stored in the pothole (depth [mm] over entire HRU)
- POT_VOL: Initial volume of water stored in the pothole (depth [mm] over entire HRU)
- POT_NO3L: Nitrate decay rate in pothole [1/day]

For simplification purposes, it has not been considered potholes, but it still is important to be aware of their uncertainty in the spatial hotspot distribution. HosNIT is a methodology applicable to any watershed where main CSAs of nitrate need to be detected, and potholes are a particularity for the watershed studied. Moreover, potholes located up to 5 km away from a drainage ditch are farmed as a combination of surface and subsurface drainage that can be used to sufficiently remove excess water during the growing season (Smith *et al.*, 2008).

6.3 BMPs choice: costs and environmental contribution

Best management practices are routinely used to reduce nonpoint-source pollution resulting from agricultural activities and improve water quality (Bracmort *et al.*, 2006). One of the benefits of having spatially referenced HRUs, that could potentially match farms/fields, is to visualize and identify contributions of different components of water, sediment, nutrient, and crop yields of the subbasins. This in turn provides a platform to simulate implementation of management practices at local scales (Teshager *et al.*, 2017).

For the implementation of BMPs in the CCW, the CFD is used.

Each scenario (see Table 3) is tested at the subbasin level and per season in order to observe the nitrate outlet concentration variation (environmental contribution compared to baseline scenario). There is no combination of different scenarios within a subbasin for simplification purposes.

As mentioned in Chapter 4.3, conservation practices are cover crops (incorporation of cereal rye), the adoption of no-tillage when corn is cultivated, and the avoidance of monocropping (scenarios 1 and 3) incorporating rotations. Conservation practices of no-till and crop rotations are critical to face detrimental effects of monocultures and tillage operations on ecosystem services (Behnke *et al.*, 2020).

It has not taken into consideration any nitrogen credit from the catch crop in winter. Since most crops benefit from the nutrients released by mineralising residues of the preceding crop (Kollas *et al.*, 2015), the environmental contribution probably might be more significant (when considered) since it could lead to a decrease in nitrate fertiliser in the case of corn in spring. SWAT deals with the nitrogen from the catch crop in two different ways: when the management schedule is set in a way that the catch crop is harvested then N is transported away with the harvest product and the residuals are considered as organic matter where N is released via mineralization. If the catch crop is not harvested, then everything is going to be residual and mineralize over time. But this means slow release. In our case, it is directly terminated.

Figure 20 shows the percentage of nitrate outlet variation concerning the baseline (no CSAs) and the area targeted (with land use specification) per each subbasin (where CSAs were identified) in spring.

Figure 21 gives the percentage of nitrate outlet variation concerning the baseline (no CSAs) and the area targeted (with land use specification) per each subbasin (where CSAs were identified) in summer.

Figure 22 shows the percentage of nitrate outlet variation concerning the baseline (no CSAs) and the area targeted (with land use specification) per each subbasin (where CSAs were identified) in fall.

Figure 23 presents the percentage of nitrate outlet variation concerning the baseline (no CSAs) and the area targeted (with land use specification) per each subbasin (where CSAs were identified) in winter.

In these Figures, Scenario 3a represents a 5% reduction of nitrate fertiliser concerning Scenario 3, Scenario 3b represents a 10% reduction of nitrate fertiliser concerning Scenario 3 and Scenario 3c represents a 20% reduction of nitrate fertiliser concerning Scenario 3. It has been observed how the management of fertiliser, as a synergistic complement to the BMPs studied in Scenario 3 affects water quality. Still, in this study, no yield reduction has been analysed for Scenarios 3a, 3b and 3 c, just for Scenarios 1, 2 and 3. It was not the purpose to implement N management together with the three BMPs selected with their corresponding yield calculation loss. Therefore, no function of yield and N fertiliser reduction has been optimised.

In spring (Figure 20), preliminary hotspot detection is based on this season for the CCW (month of highest nitrate export: March). Scenarios behave as expected (i.e. there is a reduction of the nitrate concentration at each outlet where BMPs have been implemented on CSAs at their subbasins), even with the presence of CWPS. March had the highest nitrate export average rate (leached + surface + lateral). Probably the snow melt due to an increase in temperature, the spring rain (see Figure 1) “wakes up” all the nitrate retained during winter, where there is low water movement and soil is bare (no catch crop), and cash crops are not fully developed. The establishment of cereal rye as a cover crop in the other scenarios (2 and 3) improves this specific situation. The uncertainty of the method for accounting for the seasonal variation might be to use this criterion (of the month with the highest nitrate export rate) as input data for nitrate export in HoSNIT.

Scenario 1 is almost a baseline scenario and close to the zero line. This is because the targeted area (BMPs on CSAs) is just 15% of the CSAs.

During the spring season is achieved a reduction of half of the nitrate concentration at outlets of subbasins with greatest peaks. This is translated in that subbasins go below 2 mg nitrate-N/l.

A previous study about nutrient losses from row crop agriculture in Indiana (Smith *et al.*, 2008) revealed that two conservation practices had been implemented in Northern Indiana to reduce sediment and nutrient transport to surface water. During the last 20 years, there has been a significant focus on getting farmers to use no-tillage when planting crops.

By reducing tillage, the soil is less disturbed and will be less able to erode the soil and the nutrients included. By not disturbing the soil, macropores are kept intact, allowing for preferential flow paths, improved root aeration, increased earthworm activity, and improved soil structure to occur (Motsinger *et al.*, 2016).

Improved aeration by increased earthworm activity helps the root to access more macropores, which are reconfigured by tillage practices. These observations suggest that no-tillage may improve crop nitrogen utilisation, but it may also indicate more volatilisation (Motsinger *et al.*, 2016).

Cereal rye grew between harvesting the previous crop (or the last tillage applied) and planting the next crop, absorbs soluble nutrients from the soil and provides a leaf canopy to protect the soil surface from raindrop energy. Temporally cover crops began to effectively reduce sediment and nutrient loads right after planting. When they were terminated and left as residue on fields, the N mineralised from fresh organic N could increase the load of soluble N (Her *et al.*, 2017), but also as a source of starter fertiliser with a decrease in the quantity of fertiliser to be applied by farmers.

In Figure 14, the most sensitive subbasins to land-use change can be identified. These are also the subbasins with the greatest reductions with respect to the baseline scenario when BMPs are applied.

In summer (Figure 21), subbasins that in spring had a decrease in nitrate concentration are facing an increase in the nitrate concentration (especially in Scenario1). It might be an effect of the rain in June together with the fertiliser period of May. Compared to fall, these increases are minor (around 8%) since crops are taking up at their maximum capacity. This factor probably makes the increase for some scenarios goes just between 0 to 10%. If a comparison is made between subbasin 14 and 44, it can be appreciated the importance of changing CSAs under monocrop practices. When introducing soybean into monocrop corn (CSIL) in subbasin 44, Scenario 1 behaves more different than in the other subbasins (getting the better performance). Subbasin 44 has the highest percentage of a CSA under monocrop corn. Monocrop corn is changed to rotation with soybean, this means half of the input of fertiliser for the period of study. It can also be appreciated in subbasin 14 how a small percentage of monocrop soybean (5% out of the 29% targeted) impacts water quality, and Scenario 2 performs the best (which keeps monocropping practices, so no incorporation of corn into soybean is made). The percentage of hotspots in a subbasin under monocrop (CWPS and/or CSIL) is an important parameter to consider. Scenario 2 might appear as the “most environmentally friendly” just because of the avoidance of corn, which implies an extra input of fertilisation by farmers. The CSAs detected by HosNIT are very sensitive areas and, if not properly managed, lead to an increase and an impairment of water (an increase of nitrate concentration).

In fall (Figure 22), the increase in nitrate concentration in subbasins belongs to Scenario 3 and its variants. There is a visually significant difference in Figure 23 between Scenario 2 and Scenario 3, but the only difference among them relies on the conversion to rotation of monocropping hotspots in Scenario 3. Again, these relatively small areas play a big role. Scenario 2 performs properly since the addition of nitrate input of corn was eliminated. An important factor that probably makes this significant difference so relevant: fall coincides with the crop harvest, and cereal rye is just planted, which means very low uptake (crop not yet developed). Also, subbasins with this increase of nitrate concentration in Scenario 3 are all no tiled and belong to soil IN005. IN005 is characterised by the highest HYGRP (hydrologic characteristics of the soil) (STATSGO from 1 to 4): 3.3 of all soils in the study watershed. This code means that this particular soil is naturally very poorly drained. It has the highest clay content, which agrees with having the lowest soil permeability and the highest LL (liquid limit) (percentage of moisture by weight). These characteristics promote nitrate flushed out through the tiles and directly to water without any chance of uptake or immobilisation. Activating these areas through BMP implementation during the harvest season will impact water quality since cereal rye will not be established yet.

Even with this increase of Scenario 3 concerning baseline, Spring is still not overpassed in magnitude (mg NO_3^-/l), so targeting for CSAs identification with the values of March performs well.

In winter (Figure 23), Scenario 2 performs as expected. February reveals the highest surface runoff (double to triple) compared to other months. However, since it is not the primary water path, it makes no impact on water quality via runoff of nutrients (here: nitrate).

Although all conservation practices considered in this study reduce pollutant loads at the source (or in fields) rather than controlling their transport out of fields to the downslope area, it is important to highlight that these reductions at the HRU level will influence water quality downstream.

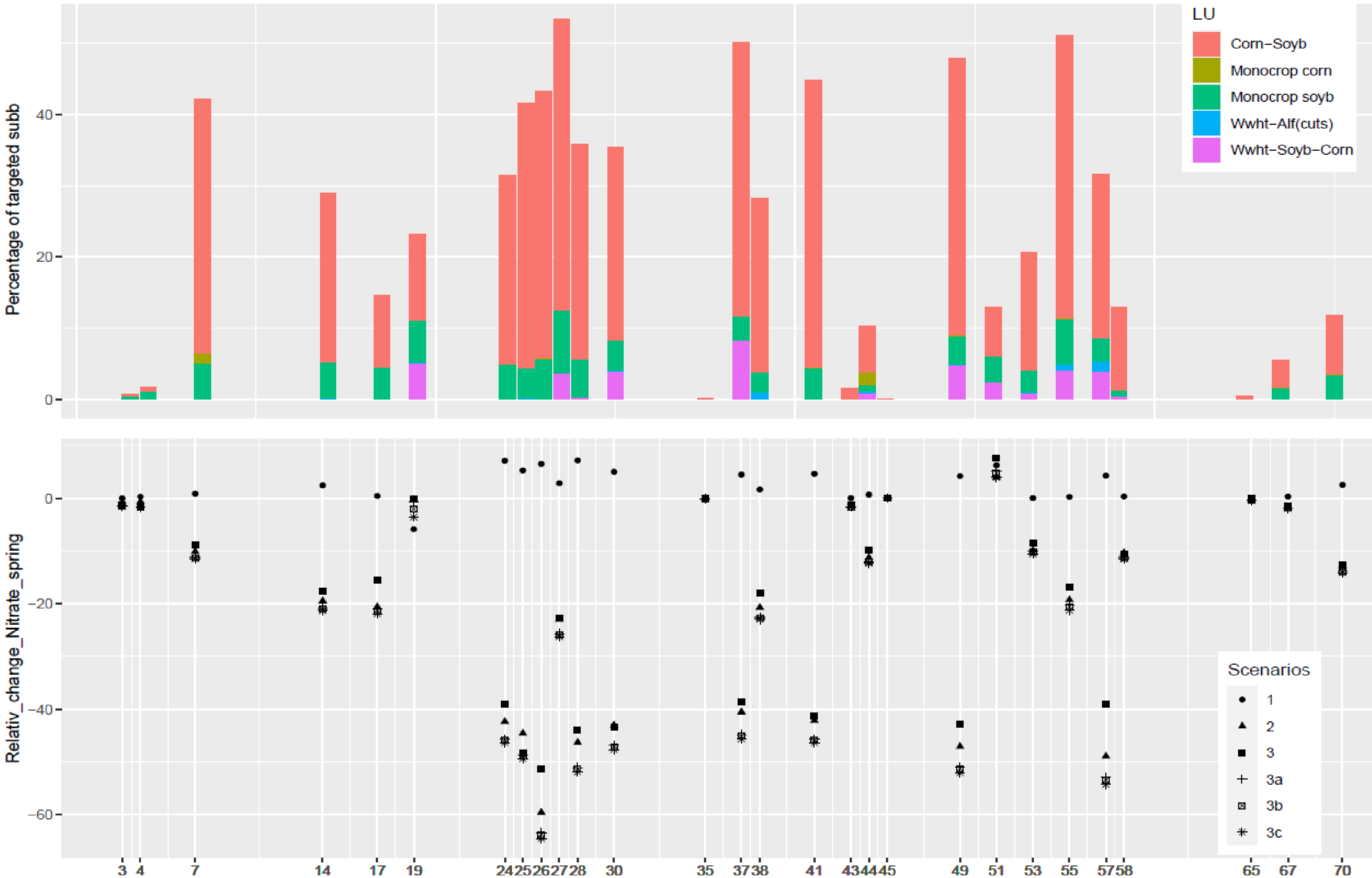


Figure 20. Percentage of nitrate outlet variation and area targeted with its land-use share per subbasin for Cedar Creek Watershed (CCW) in spring.

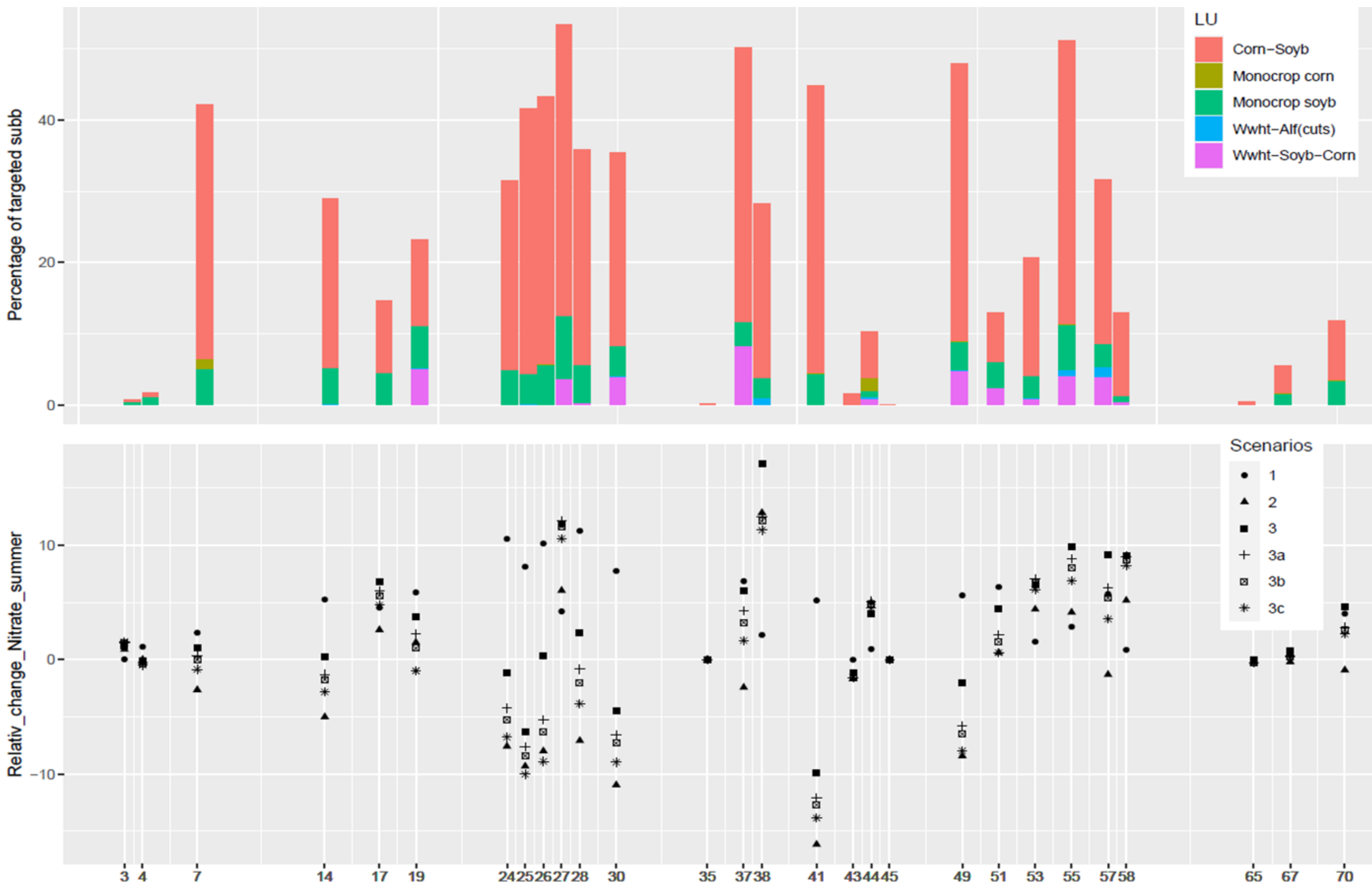


Figure 21. Percentage of nitrate outlet variation and area targeted with its land-use share per subbasin for Cedar Creek Watershed (CCW) in summer.

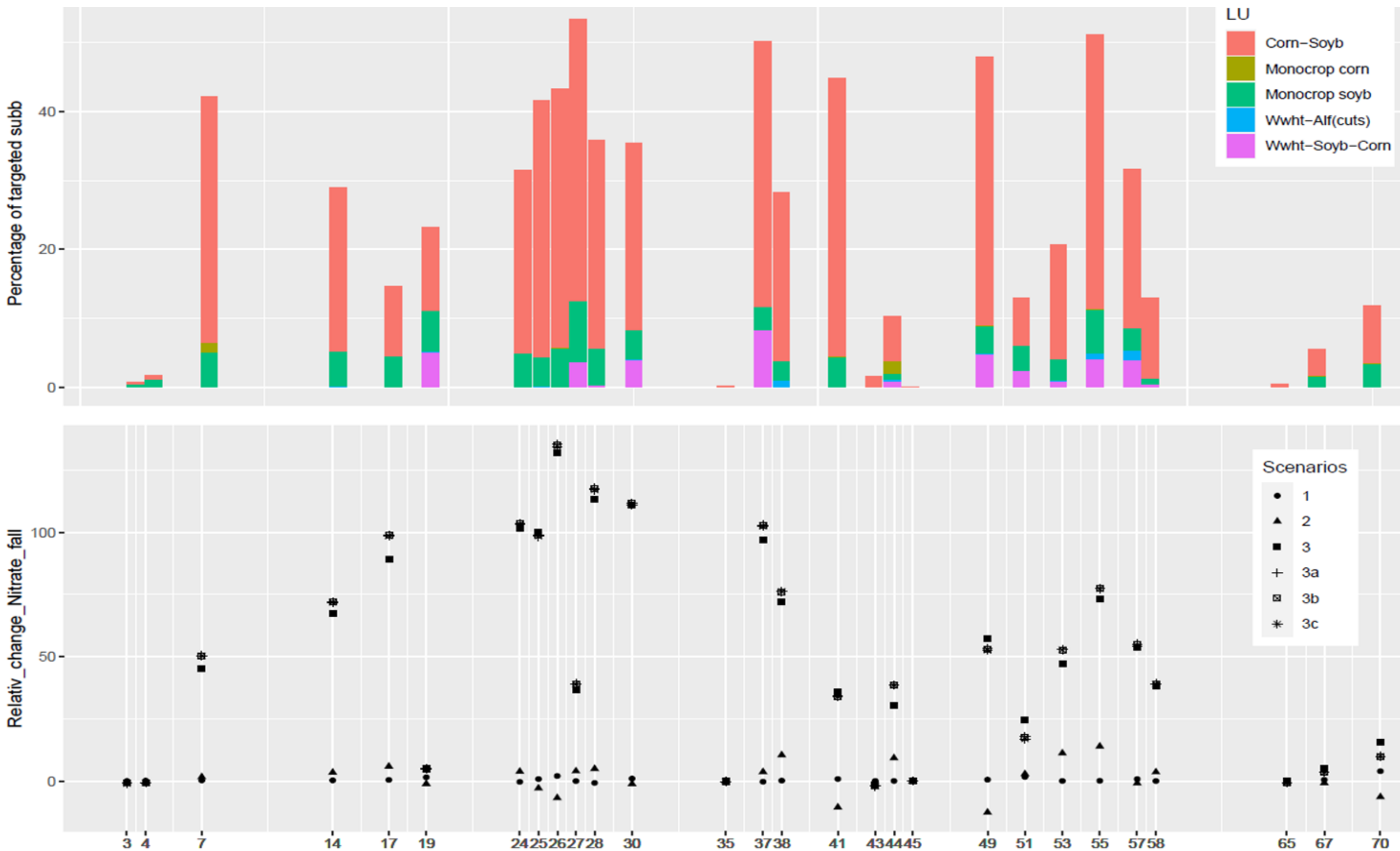


Figure 22. Percentage of nitrate outlet variation and area targeted with its land-use share per subbasin for Cedar Creek Watershed (CCW) in fall.

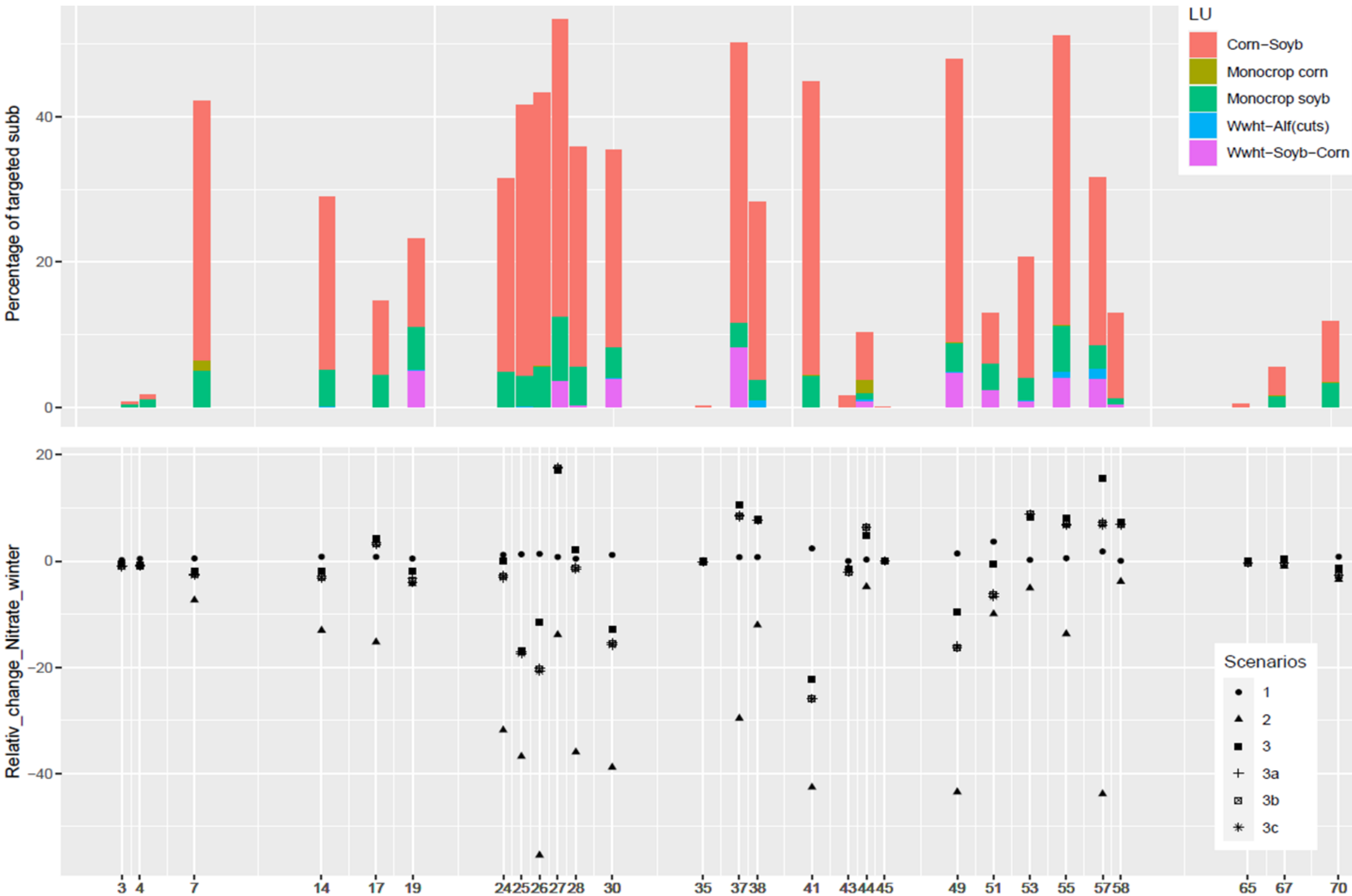


Figure 23. Percentage of nitrate outlet variation and area targeted with its land-use share per subbasin for Cedar Creek Watershed (CCW) in winter.

An analysis of BMPs implementation of SWAT (Motsinger *et al.*, 2016) in a watershed in Illinois and Indiana, which was heavily tiled and with a typical rotation of corn-soybean, described the SWAT tendency, even when the simulation overestimates the flow peak, to underestimate nitrate discharge peaks. These could be due to the inaccurate modelling of pollutants in tile drainage discharge or tile drainage itself. Another source of uncertainty is the SWAT in-stream nutrient transformation routines, which are probably some of the least tested aspects of the model. Limited research and/or review has been conducted with that component. The accuracy of this SWAT component could lead to inaccuracies in HOSNIT estimates.

The identified CSAs react to changes in land use and crop management. Other BMPs could be tested for better performance (decrease of nitrate concentration in fall). No-till could also be controversial: Nitrate losses through underground leaching are higher with no-till than with conventional tillage. Studies by Betts (2018) and Huang *et al.* ((2021) support that additional management practices and strategies are needed to decrease nitrogen loss via leaching from croplands under no-till.

Still, there is an overall reduction in spring (maximum nitrate export rate) which compensates for the fall increase.

Yields are evaluated as an important issue and parameter for farmers. Scenarios of nutrient reduction discharge focus mostly on nutrient reduction at the source, assuming no impact on crop production and without considering the lag time in terms of response to a change in management (Malagó *et al.*, 2019).

Figure 24 provides the calculation results of the average yield (t/ha) for corn, soybean, and winter wheat for the period studied at the watershed scale.

The calculations are made for the baseline scenario and Scenarios 1, 2 and 3, compared to the county-level statistics for these crops.

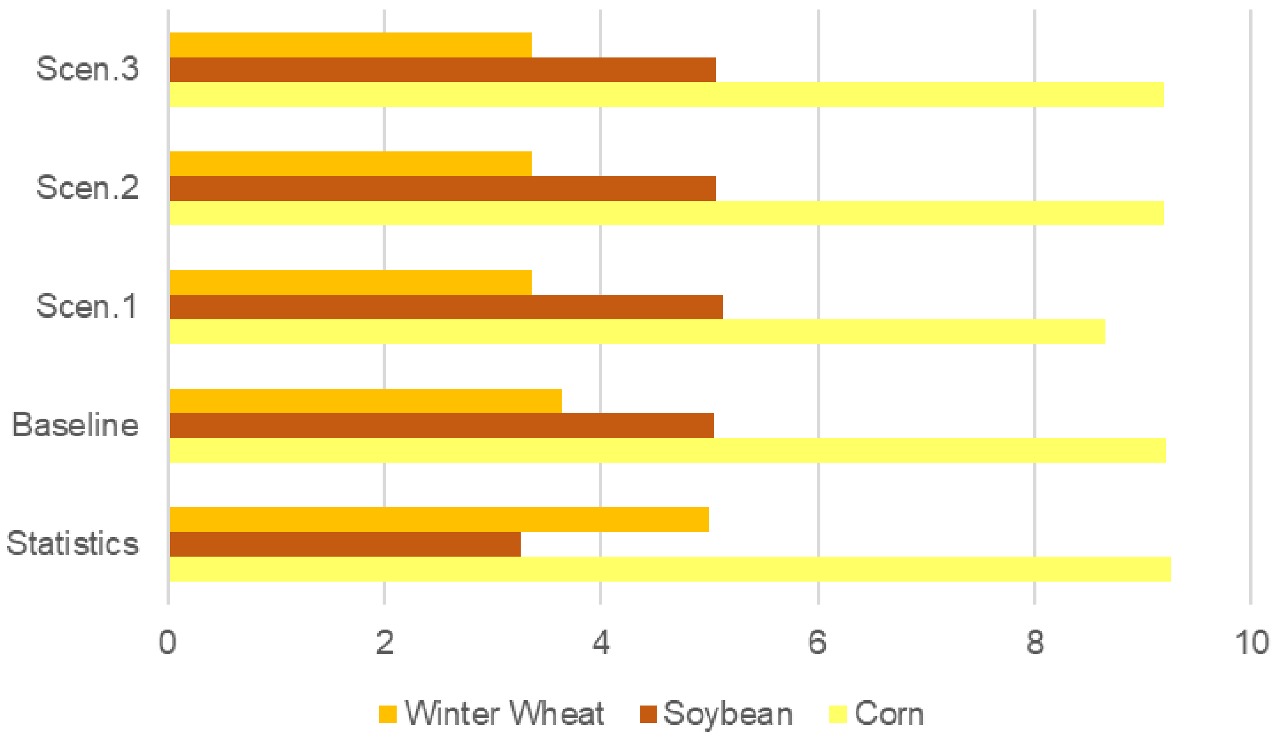


Figure 24. Average yield comparison for statistics (period 2005-2020), baseline scenario and Scenarios 1, 2 and 3 for the Cedar Creek Watershed (CCW).

These changes in yields are considered, in dollars, for the costs in the parsimonious optimization.

Simulated scenarios are performing well for corn compared to the statistics register, underestimating the yield for winter wheat and overestimating the yield for soybean compared to the statistics register.

6.4 Analysis of BMPs scenarios: water quality improvement per dollar spent in BMPs and optimised solution

In 6.3, the environmental contribution of each scenario at each season was presented. But the costs of the scenarios' implementation are also important. As mentioned in 4.5.2.3, the scenario selection is based on the efficiency of pollutant reduction per 1-dollar cost of the BMP implementation. So, it is necessary to look for the maximum nitrate concentration percentage reduction per every dollar spent on BMPs implementation.

Consideration of costs related to implementation and maintenance of each BMP is essential for identifying effective management strategies, and to increase the acceptability by farmers of the selected measures (Udias *et al.*, 2016).

In Table 13, the costs of BMPs implementation are presented for each scenario. The units are dollars per hectare each year. Calculations are made for the period of study and per hectare under the CSAs denomination. Each HRU particularity has been taken into account for crop established and management practices for the years analysed. Costs estimation were explained in detail in section 4.5.2.1.

Table 13. Costs of BMPs implementation for each scenario

Scenarios	$/ha/year
1	24.6
2	8.5
3	13.1

The nitrate percentage reduction (year average: average of all seasons) considering the baseline for each subbasin is also calculated.

In a watershed with many farms and multiple BMPs viable for implementation, it becomes a hard task to select the right combination of BMPs that provide maximum pollution reduction at the most economic cost (Maringanti *et al.*, 2011).

With the nitrate percentage reduction per subbasin and costs per scenario from Table 13, the maximum reduction of nitrate at each subbasins' outlet per $ spent is obtained.

Each subbasin has a more environmental-and cost-efficient scenario (for the selected BMPs). This parsimonious solution is represented in Figure 25 for the watershed and the outlet response to the upstream implementation of the different scenarios. Subbasins with < 0.5% of the area targeted are not shown on the map.

The total reduction of nitrate concentration downstream is 3.7% (outlet for the CCW: subbasin 69).

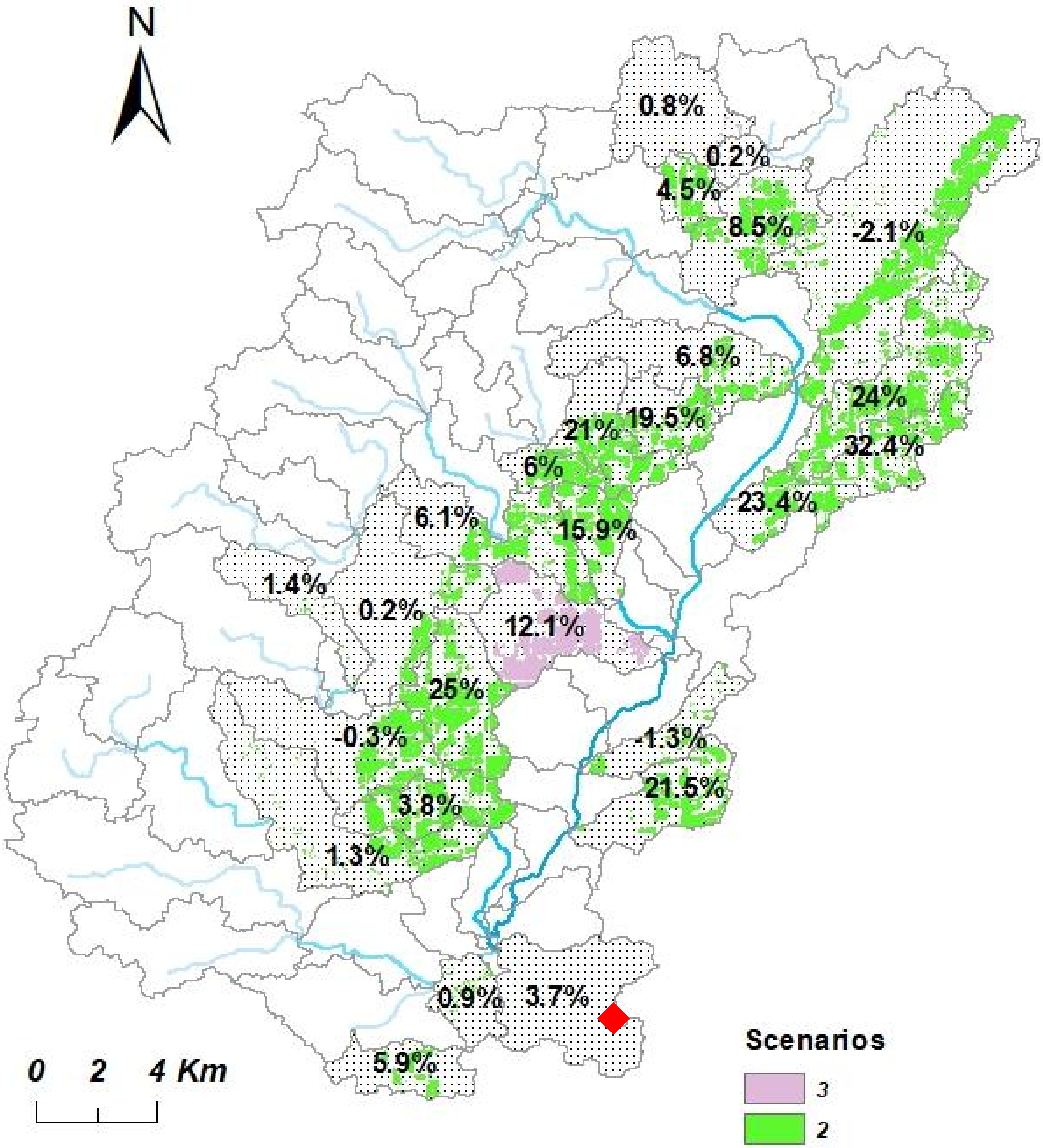


Figure 25. Optimised solution: nitrate outlet concentration reduction compared to the baseline scenario (in %) and outlet result for the Cedar Creek Watershed (CCW).

Optimisation on critical areas can greatly reduce computational time (Liu *et al.*, 2019), and management strategies should also consider the location of sources of pollution in order to choose the most appropriate BMP that will achieve the required environmental goals while being financially viable (Udias *et al.*, 2016)

The negative value (-2.1%) corresponds to subbasin 19. It means an increase in the nitrate outlet concentration for all the years studied. Subbasins 19 and 51 (-0.3%) are the only subbasins where winter wheat and monocrop soybean represent half of the land use targeted. Targeting monocrop soybean impacts water quality -introduction of corn to the rotation- and it is reflected at the outlet of these subbasins.

These are results from selecting these specific BMPs. It has also to be highlighted that the economic function is taken into account. The selection is not just based on the environmental contribution.

In Figure 26, the percentage of nitrate reduction compared to the baseline scenario for the optimised solution and per season is shown for the subbasins depicted in

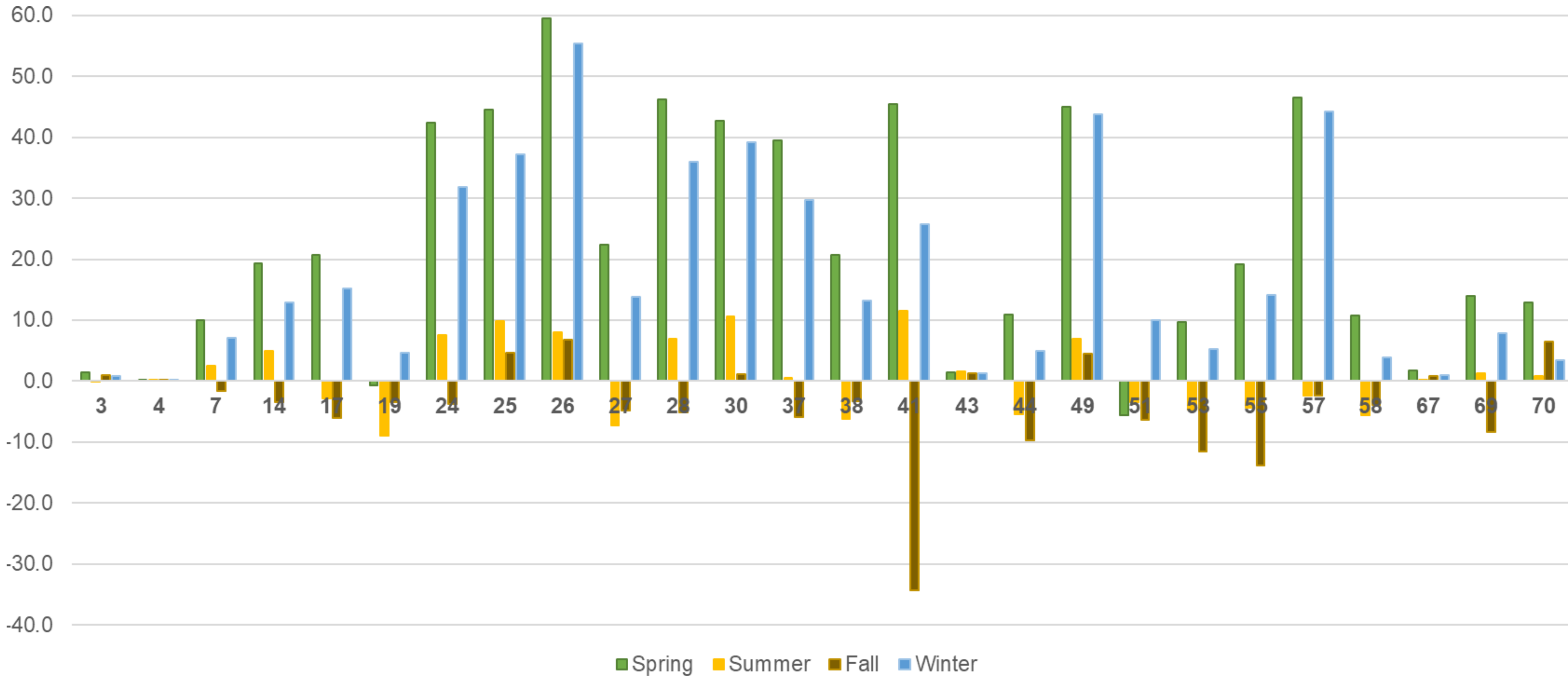


Figure 26. Optimised solution per season: nitrate outlet concentration reduction compared to the baseline scenario (in %) and outlet result for the Cedar Creek Watershed (CCW) (subbasin 69),

The importance of proper BMPs selection for the watershed can clearly be stated. In Indiana, 6 practices were most palatable to farmers and have previously been represented in the watershed model (Arabi et al., 2008; Waidler et al., 2009; Kalcic et al., 2015b). As a first thought, eliminating monocrop practices out of fields might sound environmentally relevant. It is observed that by targeting monoculture in the identified CSAs, a greater impact on the water quality level in the outlet of the respective subbasin is obtained. If initially, a CSA under monocrop soybean (CWPS) is found, combining it with corn for the rotation contributes to an increase in nitrate input which is reflected at the outlet. On the other hand, transforming monocrop corn (CSIL) into a corn-soybean rotation makes the assumption of a rotation being more environmentally friendly, true. For the monocropping of corn in order to maintain yield levels, more inorganic N is required, thereby intensifying the N cycle and causing a dangerous loop (cf. Behnke *et al.*, 2020). Altieri in Emanuelli *et al.* (2009) holds that part of the low resilience to climatic events and the high susceptibility to pests of ecosystems is linked to monocultures. On one hand, habitat simplification has reduced environmental opportunities for natural enemies, interfering with biological controls and thereby fostering the frequent explosion of pests or weeds. On the other hand, homogenous monocultures lack compensation or resilience mechanisms to handle extreme climatic events (droughts, hurricanes, etc.).

These highly sensitive areas verify the importance of managing these spots efficiently in order to improve (and not deteriorate) water quality downstream, but although Scenario 2 is wider extended in the parsimonious solution, won’t be the solution for sustainable farm management. It is important to explore and analyze other BMPs (also structural BMPs) and extract synergies out of their combinations in order to intrinsically account for water quality and sustainable agriculture.

The identified CSAs have a strong impact on their subbasins and, in the end, on the outlet of the watershed.

6.5 Discussion of the hypotheses

There are two hypotheses developed in Chapter 3. Number 1 is related to HosNIT as a finer targeting technique to detect hotspots of nitrate which are impairing water. Number 2 refers to the efficiency of applying optimisation methods (parsimonious approach) to already identified CSAs.

Hypothesis 1: For potential first areas classification, two “extra” components in the targeting technique are taken into account (besides the nitrate export): the stream network and the distance of areas to the stream. The first main assumption is that areas/pixels with high nitrate export, close to the stream and draining in headwaters, need to be (preliminarily) designed as CSAs. After this first filter of pixels, any dilution or enrichment effect from upstream is considered in order to obtain a final list of pixels (HRUs) which are considered hot spots of nitrate.

This finer targeting ends up with very sensitive areas to fertiliser reduction for both land uses. CFD and DLU, as shown in Chapter 6.2, obtain significate reductions in nitrate concentration at the outlet of the watershed (up to 7% in summer with a 50% of fertiliser reduction scenario).

Also, the implementation of BMPs in these specific areas has implications at the water quality level, resulting in an increment or reduction of nitrate concentration at each subbasin, depending on the management selected.

Hypothesis 2: The parsimonious approach relies on the efficiency in nitrate reduction at the subbasin level per each dollar (costs) in the BMP implementation since CSAs are already identified through HosNIT.

Thanks to the optimisation in hotspots, it is possible to avoid long computational times and sophisticated algorithms.

It is used three different scenarios as a combination of three different realistic management strategies for Indiana.

There are different outlet responses per season and subbasins for the scenario implemented (at the subbasin level), but the optimised solution (Chapter 6.4) is for spring since the largest nitrate export is observed.

These areas again react very sensitively to the scenario implemented, verifying the identification of hotspots for the CCW. The watershed obtains an average for all seasons of 3.7% of nitrate reduction (compared to the baseline) for the period studied and the scenarios selected.

The synergy presented in this research between the targeting and optimisation technique can enable the identification of CSAs and be part of the solution for nitrate diffuse sources at agricultural watersheds.

7 Synthesis, conclusions and outlook

7.1 Summary of findings and outlook

Diffuse pollution occurs when potentially polluting substances (such as nitrate) leach into waters as a result of the dynamical behaviour of precipitation, soil infiltration and surface runoff.

Agriculture is one of the main sources of diffuse pollution, and the Midwest area in the US suffers from water quality detriment.

The water quality of the Great Lakes is a crucial concern of people in the surrounding states, as the algal blooms and disease outbreaks have caused the water quality degradation of the five lakes to different levels (Wang, Flanagan, *et al.*, 2018).

Partial restoration of the natural drainage system, disrupted by the installation of drainage tiles, the destruction of riparian wetlands, the channelisation of rivers, and the destruction of Gulf Coast wetlands, could help decrease the response of nitrate flux to precipitation (Donner and Scavia, 2007), but federal and state agencies charged with improving water quality face limited and declining resources to address water quality challenges (McLellan *et al.*, 2018).

There has been widespread implementation of BMPs nationwide. Despite all these activities, agricultural-related water quality problems persist across the U.S. and the effectiveness of BMP implementation strategies at watershed-scale are still not well understood (Teshager *et al.*, 2017).

It is then important to spatially (and temporally: hot moments) identified vulnerable zones where this pollutant is lost (sources of nitrate) in order to implement conservation practices in these critical areas. Structural BMPs can also be applied.

The concept of this study is to apply a combination of plan-and process-based methods in order to extract synergies for both methodologies in identifying hot spots of nitrates and implementing BMPs on them.

Despite demonstrated applicability of the optimisation approach, it has rarely been used in management planning, probably due to the need of excessive computing resources, sophisticated optimisation algorithms, and/or complicated implementation procedures. These requirements made the targeting approach more attractive (Her *et al.*, 2017). HosNIT, as a finer targeting technique, allows for adopting a parsimonious optimisation where the functions of environmental contribution and cost (per dollar spent) on BMPs implementation are considered.

The application of the HosNIT method in a watershed, starting with outputs from the hydrological model SWAT, demonstrates that a more adjusted targeting is possible in the identification of CSAs of nitrate. Limitations are mainly the availability of nitrate measurements and the hard identification of potholes. Quantifying hydrologic and contaminant transport flow paths is very difficult due to alterations of this landscape in the form of surface and subsurface drainage (cf. Smith *et al.*, 2008).

Besides considering nitrate export (loads per HRU) for hotspot detection, HosNIT adds geomorphological characteristics of the watershed to the analysis. Stream orders where the nitrate export drains, accounting for the importance of headwaters in water quality downstream, and distances for these points to their nearest draining stream are also calculated. Based on a threshold system with limiting values obtained from the data distribution (boxplots) for each variable (nitrate export and distance), HosNIT assumes that points with high rates of nitrate export, close to the streams and draining in orders one or two, are most likely to impair waters within a watershed. First potential hotspots identification following the principle of the first step described during the HosNIT methodology is made as a preliminary perspective. Afterwards, it is checked whether these preliminary CSAs effects are being “seen or noticed” in the water quality of the river network (checking nitrate concentrations at each subbasin outlet) or whether they are not affecting the water quality at their respective subbasins. Then, dilution effects from upstream are also considered. Thus, a more comprehensive methodology in hotspots of nitrate detection using a finer targeting technique is presented. In the DLU, this is translated into 14,8% of the area to target, while in the CFD accounts for 9,3%. A maximum reduction of 7% in the nitrate outlet concentration of the CCW is obtained in summer, with a reduction of a 50% in fertiliser application rates. The sensitivity of the method is tested.

The importance of a proper land-use input in process-based models such as SWAT are well known in the scientific community. It is demonstrated how the use of different rotation patterns can lead to the different spatial distributions of the hotspots, putting effort and resources in locations with limited potential for restoration of the watersheds.

Common targeting strategies focus on fields or sub-watersheds with the highest loads, which implicitly assumes that load reductions are proportional to loads. The simulation results showed that the assumption is not always true (cf. Her *et al.*, 2017). Optimising agricultural management practices is imperative for ensuring food security and building climate-resilient agriculture (Huang *et al.*, 2021). This finer targeting from HosNIT allows to implement a parsimonious approach where the optimised solution is directly run in SWAT in order to verify the nitrate reduction at the watershed scale. Instead of sophisticated algorithms, the actual need is to calculate the costs of the combination of BMPs selected (scenarios) at each HRU considered (dollars per hectare) and the environmental contribution (nitrate reduction) at each subbasin of the implementation of the scenarios (simulations in SWAT). With these two parameters, the optimised solution comes from the environmental contribution per dollar spent. For our case study means a year average of 3.7% of nitrate reduction with the optimised selection of scenarios for the studied period.

7.2 Critical evaluation and further improvements

Some degree of uncertainty is inevitable due to several factors, including inherent complexity and variability of hydrological processes, lack of data and measurements at sufficient spatial and temporal resolution for model validation, and limitation of a hydrologic model itself. Consequently, the uncertainty may affect the conservation practice effectiveness estimation. Further study of the uncertainty could improve the reliability of modelling results (Her *et al.*, 2017).

As mentioned before, the threshold in HosNIT to account for the maximum N export rate is taken from early spring, i.e. March. It was decided that, by doing this, the concept of targeting the highest export rate was fulfilled. Still, there was a parallel idea about the analyses of the twelve months and identified CSAs that are active through all months under a yearly threshold.

Another threshold that could be modified in the second step of HosNIT is the 5.6 mg nitrate-N/l at each subbasin outlet for the number of days exceeding it (over-threshold days´ variable). This is a very ambitious goal where the 11.3 mg nitrate-N/l could also be used.

The use of structural best management practices that reduce soil erosion and nutrient loss has been recommended and installed on agricultural land for years. They are expected to be fully functional only for a specific time after installation, after its degradation is likely to no longer provide its services and lead to a reduction in the water quality (Bracmort *et al.*, 2006). It could also be further studied the impact of these types of BMPs and where they might have their maximum removal efficiency since hotspots are already detected through HosNIT.

It could also be added in the Parsimonious optimisation a third function: yields of the main cash crops, and optimise the function of fertiliser reduction as a conservation management (further scenarios 3a, 3b and 3c).

For simplification purposes, it has been analysed the environmental contribution of each scenario per subbasin. There is no combination of different scenarios for HRUs within the same subbasin. Therefore, it might be interesting and worthwhile to implement different scenarios per subbasin. However, this will imply extra computational time and skills, and near/adjacent fields/HRUs tend to behave similarly and also to belong to the same farmers who will apply the same scenarios to their fields.

The concept behind HosNIT could also be extended to other pollutants, such as Phosphorous. In that case, the parameter for nitrate export should focus on different water preferential paths, such as water runoff instead of water that percolates, and the factor of soil erodibility.

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Supplementary Material

A.1 SWAT Management strategy for DLU as land use input, and SWAT management strategy using CFD as land use input

Management strategy implemented in the SWAT model for DLU

Management Strategy_DLU		
	Date	Operation
Corn (in soybean rotation)	1-Apr	Generic spring plowing cultivation
	15-Apr	Field cultivator
	7-May	Fertilizer 10-34-0 (130kg/ha)
	7-May	Pesticide
	7-May	Planting
	25-May	Fertilizer 82-0-0 (160kg/ha)
	29-Oct	Harvesting
	30-Oct	Killing
Soybean (in corn rotation)	20-Apr	Fertilizer 0-100-0 (18kg/ha)
	20-May	No-till
	20-May	Planting
	1-Jun	Pesticide
	1-Oct	Harvesting
	2-Oct	Killing
Winter Wheat	22-Sep	Field cultivator
	22-Sep	Fertilizer 100-0-0 (33kg/ha)
	22-Sep	Fertilizer 0-100-0 (35kg/ha)
	23-Sep	Planting
	10-Apr	Fertilizer 100-0-0 (100kg/ha)
	1-Jul	Harvesting
	2-Jul	Killing

Management strategy implemented in the SWAT model for CFD

Management Strategy_CFD		
	Date	Operation
Corn (in soybean rotation)	1-Apr	Generic spring plowing cultivation
	15-Apr	Field cultivator
	7-May	Fertilizer 10-34-0 (130kg/ha)
	7-May	Pesticide
	7-May	Planting
	25-May	Fertilizer 82-0-0 (160kg/ha)
	29-Oct	Harvesting
	30-Oct	Killing
Corn (monocropping)	1-Apr	Generic spring plowing cultivation
	15-Apr	Field cultivator
	7-May	Fertilizer 10-34-0 (133kg/ha)
	7-May	Pesticide
	7-May	Planting
	25-May	Fertilizer 82-0-0 (203kg/ha)
	29-Oct	Harvesting
	30-Oct	Killing
Soybean (in corn rotation)	20-Apr	Fertilizer 0-100-0 (18kg/ha)
	20-May	No-till
	20-May	Planting
	1-Jun	Pesticide
	1-Oct	Harvesting
	2-Oct	Killing
Soybean (monocropping)	20-Apr	Fertilizer 0-100-0 (18kg/ha)
	20-May	No-till
	20-May	Planting
	1-Jun	Pesticide
	1-Oct	Harvesting
	2-Oct	Killing
Winter Wheat (in corn-soybean rotation)	22-Sep	Field cultivator
	22-Sep	Fertilizer 100-0-0 (33kg/ha)
	22-Sep	Fertilizer 0-100-0 (35kg/ha)
	23-Sep	Planting
	10-Apr	Fertilizer 100-0-0 (100kg/ha)
	1-Jul	Harvesting
	2-Jul	Killing

B

Alfalfa	22-Sep	Field cultivator
	22-Sep	Fertilizer 100-0-0 (30kg/ha)
	22-Sep	Fertilizer 0-100-0 (33kg/ha)
	23-Sep	Planting
	10-Apr	Fertilizer 100-0-0 (100kg/ha)
	1-Jul	Harvesting
	2-Jul	Killing
	1-Aug	Dairy Manure (40000kg/ha)
	10-Aug	Planting
	1-May	Harvesting
	2-May	Dairy Manure (30000kg/ha)
	1-Jul	Harvesting
	5-Jul	Dairy Manure (30000kg/ha)
	15-Sep	Harvesting
	16-Sep	Dairy Manure (40000kg/ha)
	10-Oct	Dairy Manure (30000kg/ha)
	10-Nov	Dairy Manure (30000kg/ha)
	1-May	Harvesting
	2-May	Dairy Manure (30000kg/ha)
	1-Jul	Harvesting
	5-Jul	Dairy Manure (30000kg/ha)
	15-Sep	Harvesting
	16-Sep	Dairy Manure (40000kg/ha)
	10-Oct	Dairy Manure (30000kg/ha)
	10-Nov	Dairy Manure (30000kg/ha)
	1-May	Harvesting
	2-May	Dairy Manure (30000kg/ha)
	1-Jul	Harvesting
	5-Jul	Dairy Manure (30000kg/ha)
	15-Sep	Killing

A.2 CCW maps of HosNIT sensitivity for the rest of seasons and different fertiliser reduction ranges

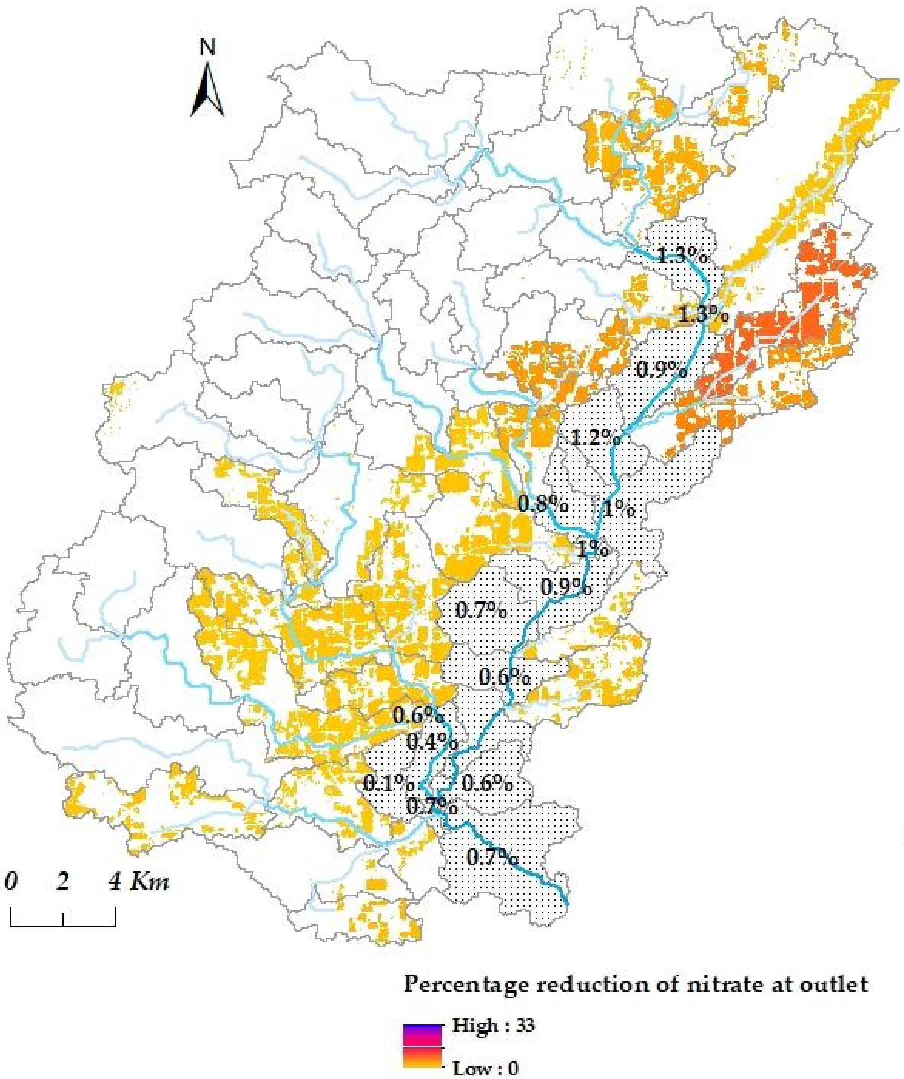

Figure A1. Subwatersheds and winter 5% fertiliser reduction for DLU

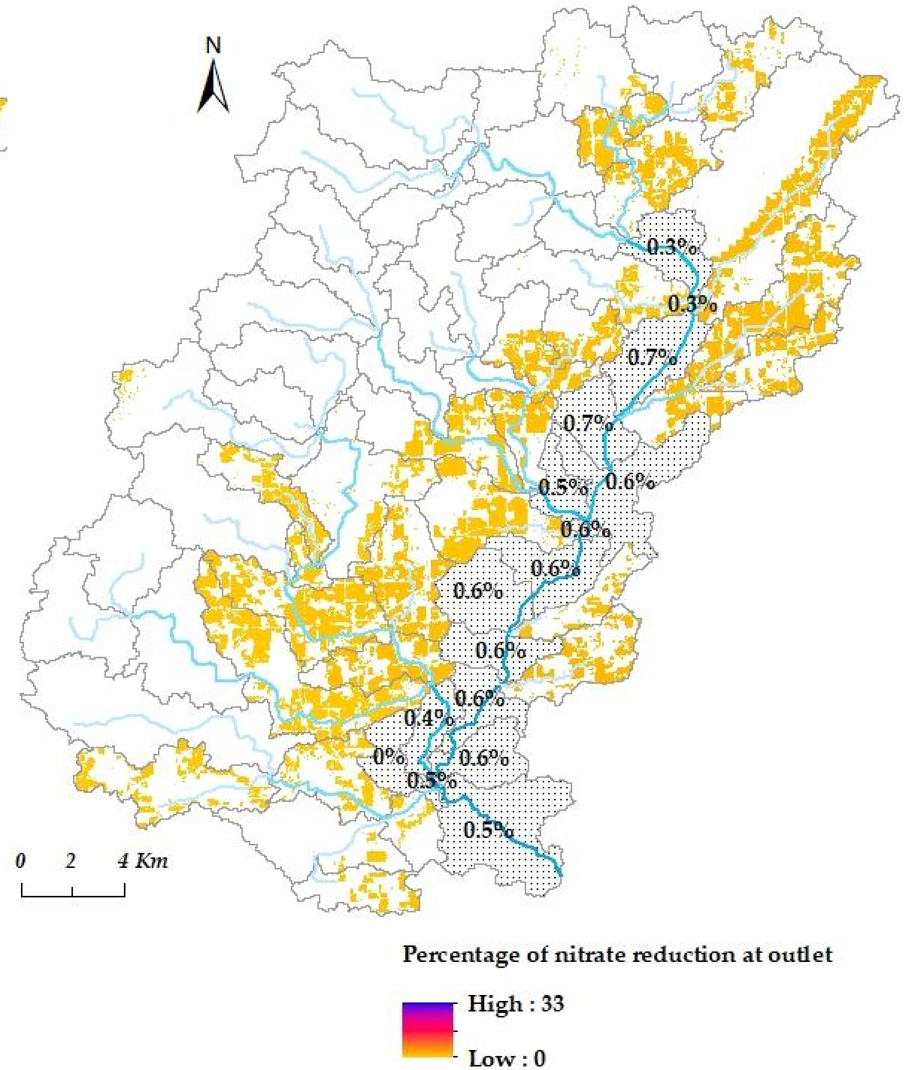

Figure A2. Subwatersheds and spring 5% fertiliser reduction for DLU

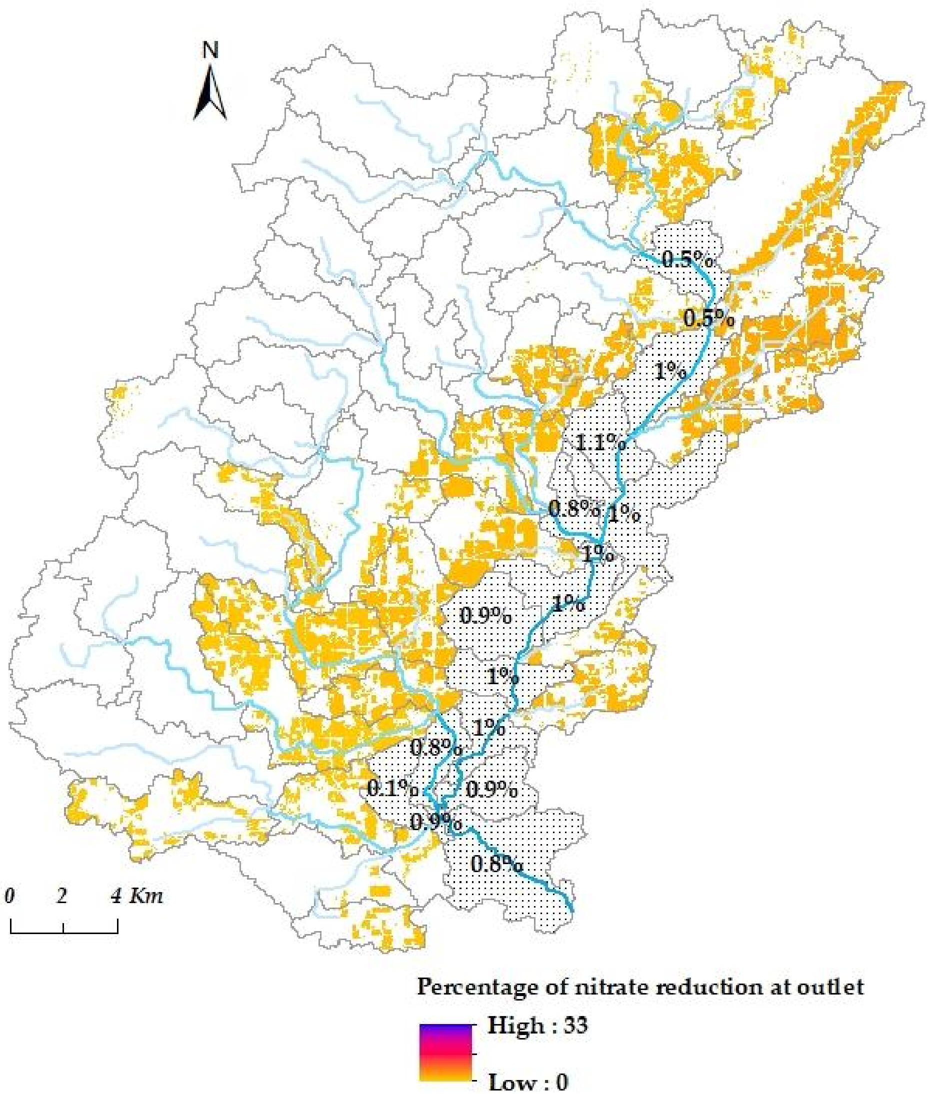

Figure A3. Subwatersheds and summer 5% fertiliser reduction for DLU

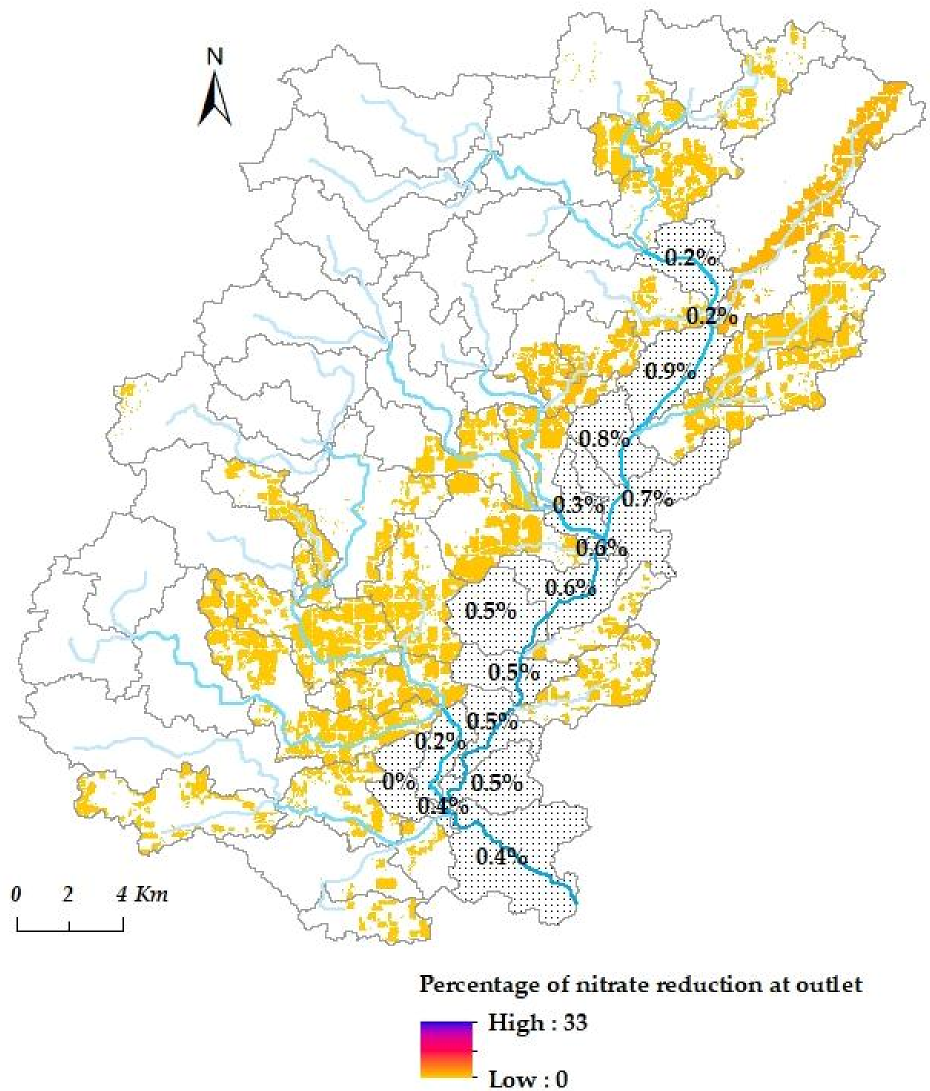

Figure A4. Subwatersheds and fall 5% fertiliser reduction for DLU

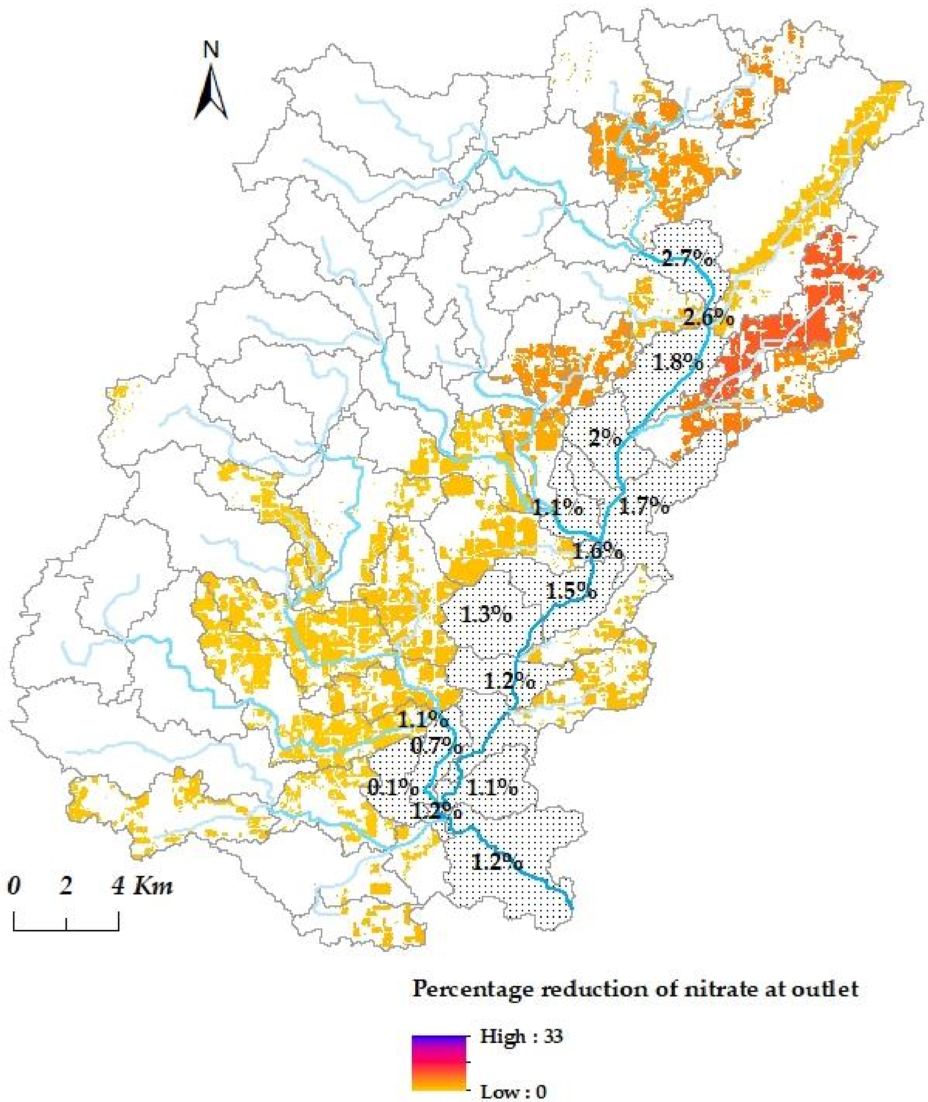

Figure A5. Subwatersheds and winter 10% fertiliser reduction for DLU

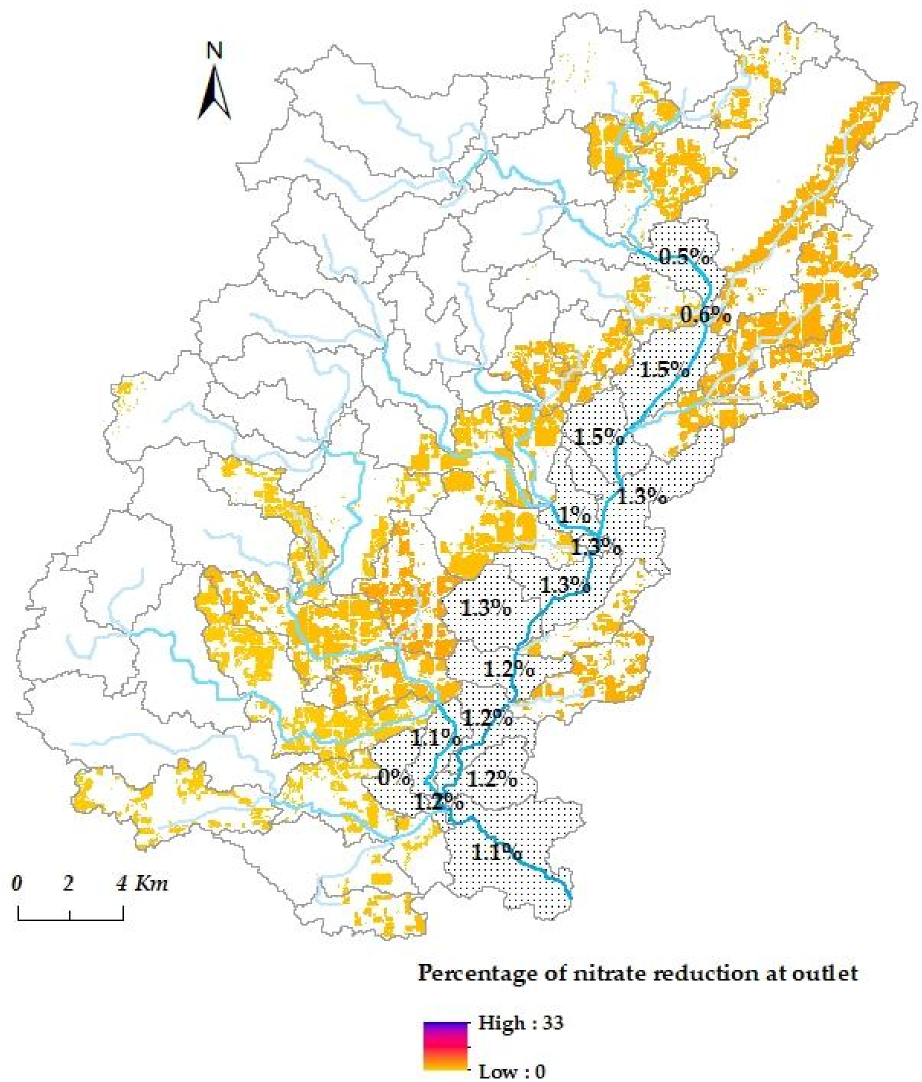

Figure A6. Subwatersheds and spring 10% fertiliser reduction for DLU

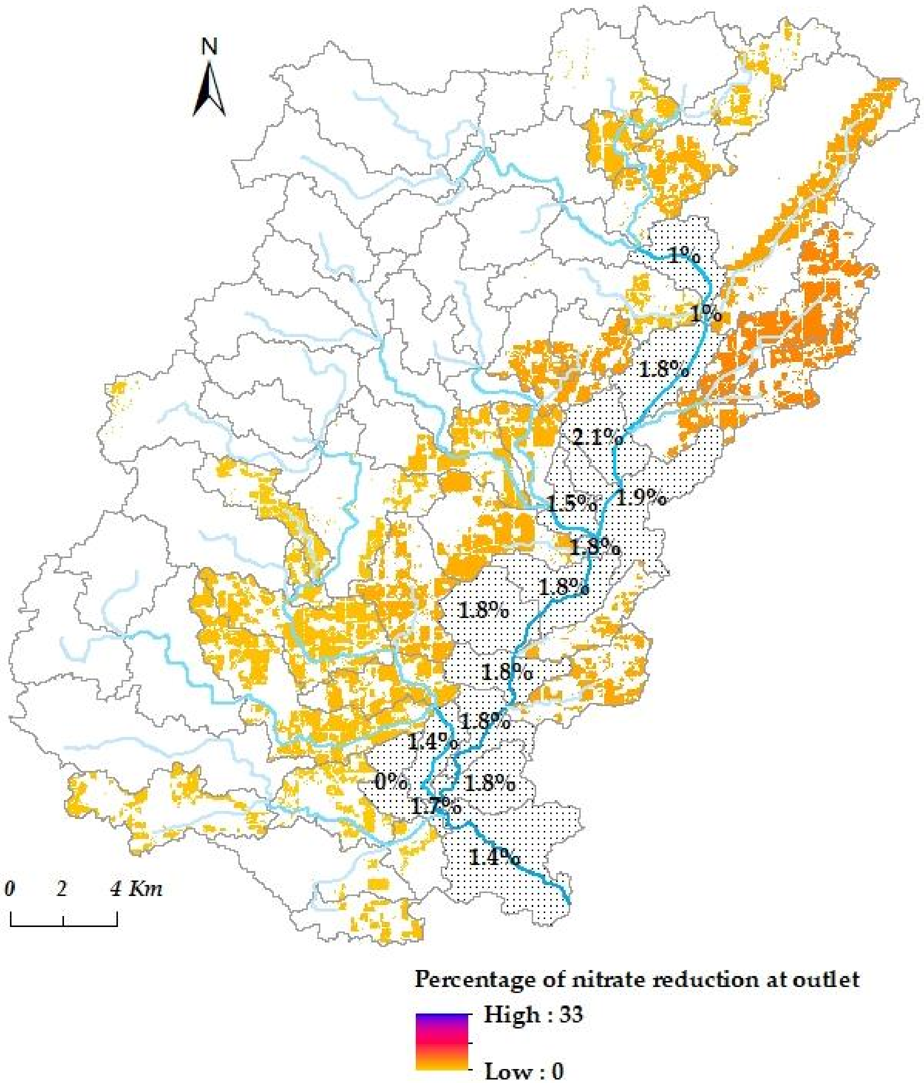

Figure A7. Subwatersheds and summer 10% fertiliser reduction forDLU

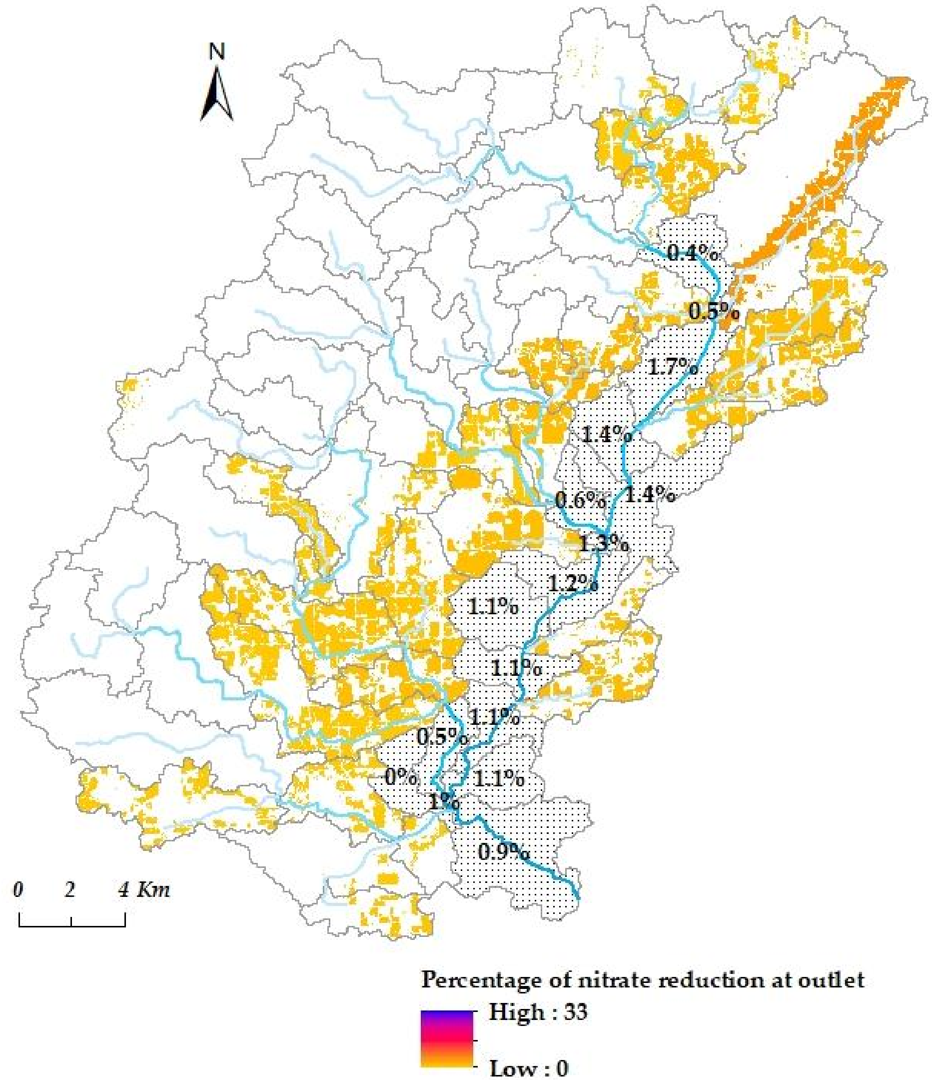

Figure A8. Subwatersheds and fall 10% fertiliser reduction for DLU

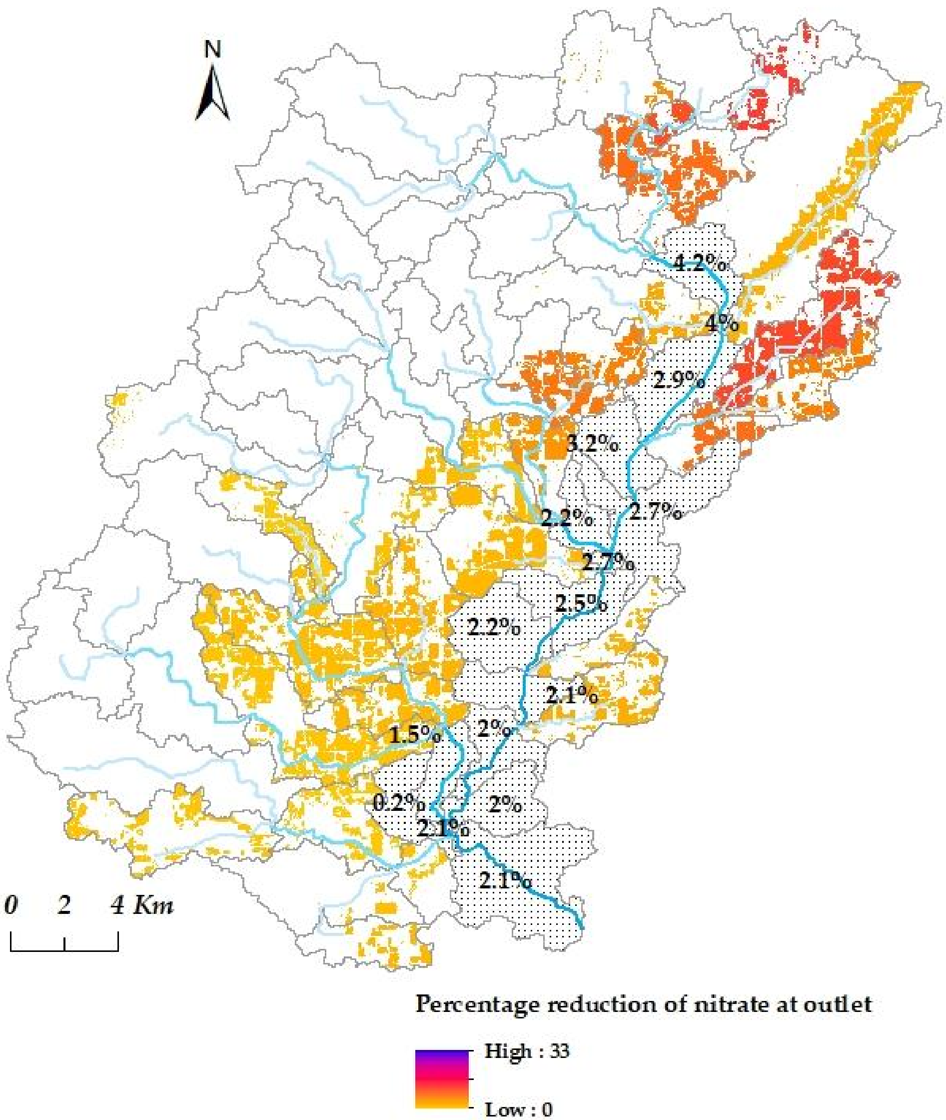

Figure A9. Subwatersheds and winter 20% fertiliser reduction for DLU

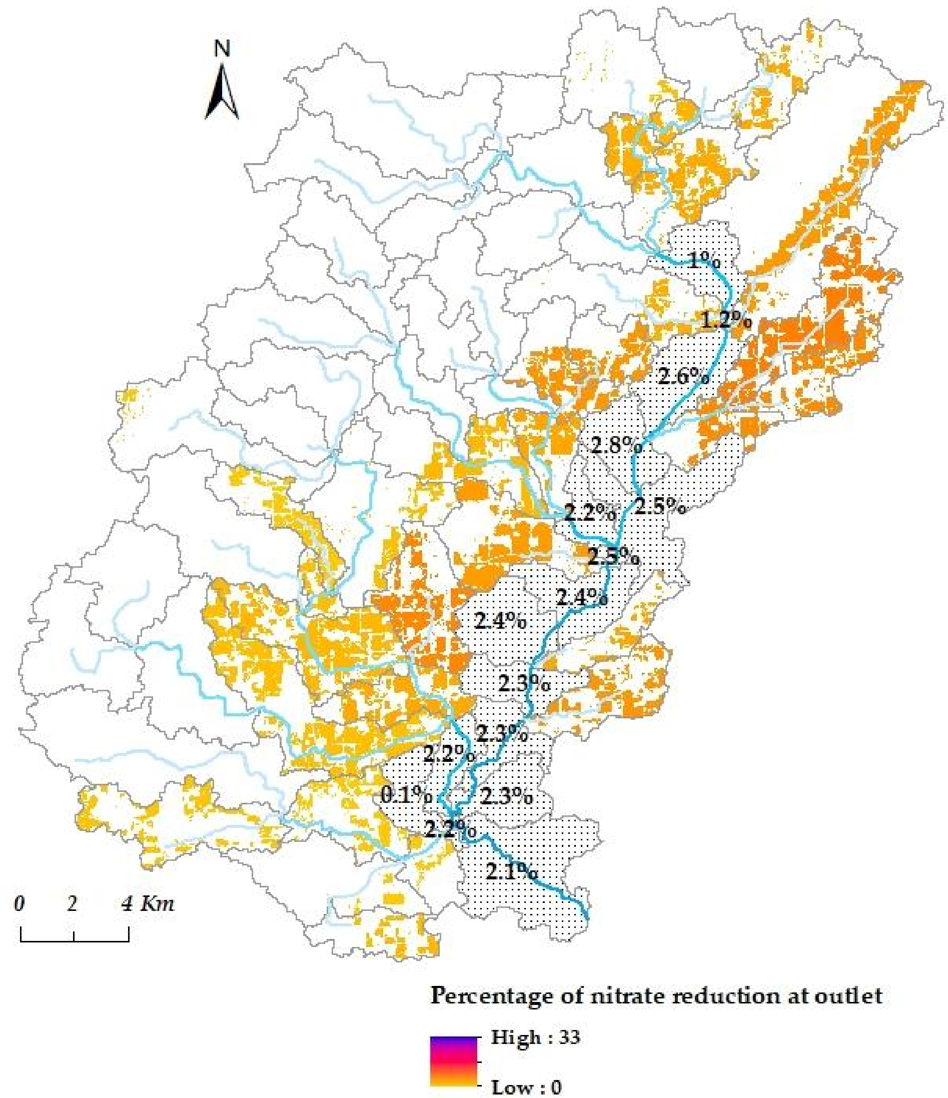

Figure A10. Subwatersheds and spring 20% fertiliser reduction for DLU

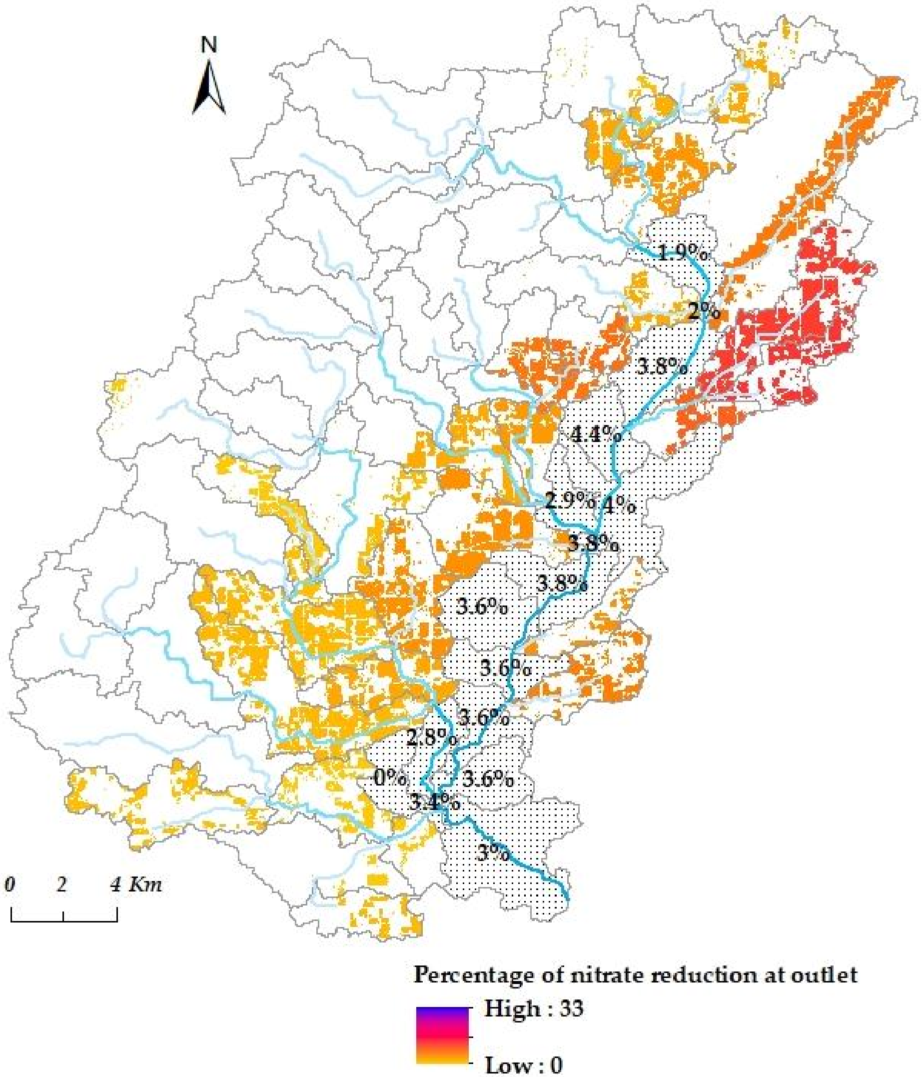

Figure A11. Subwatersheds and summer 20% fertiliser reduction forDLU

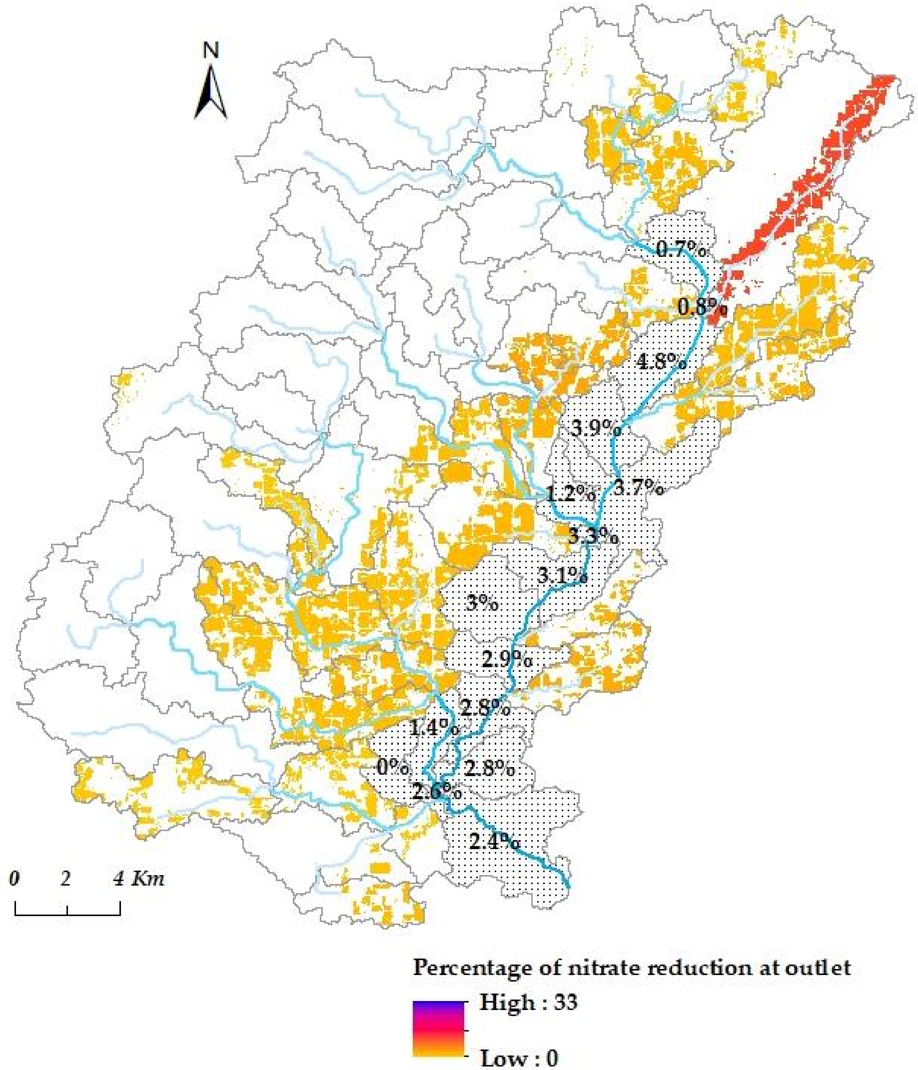

Figure A12. Subwatersheds and fall 20% fertiliser reduction for DLU

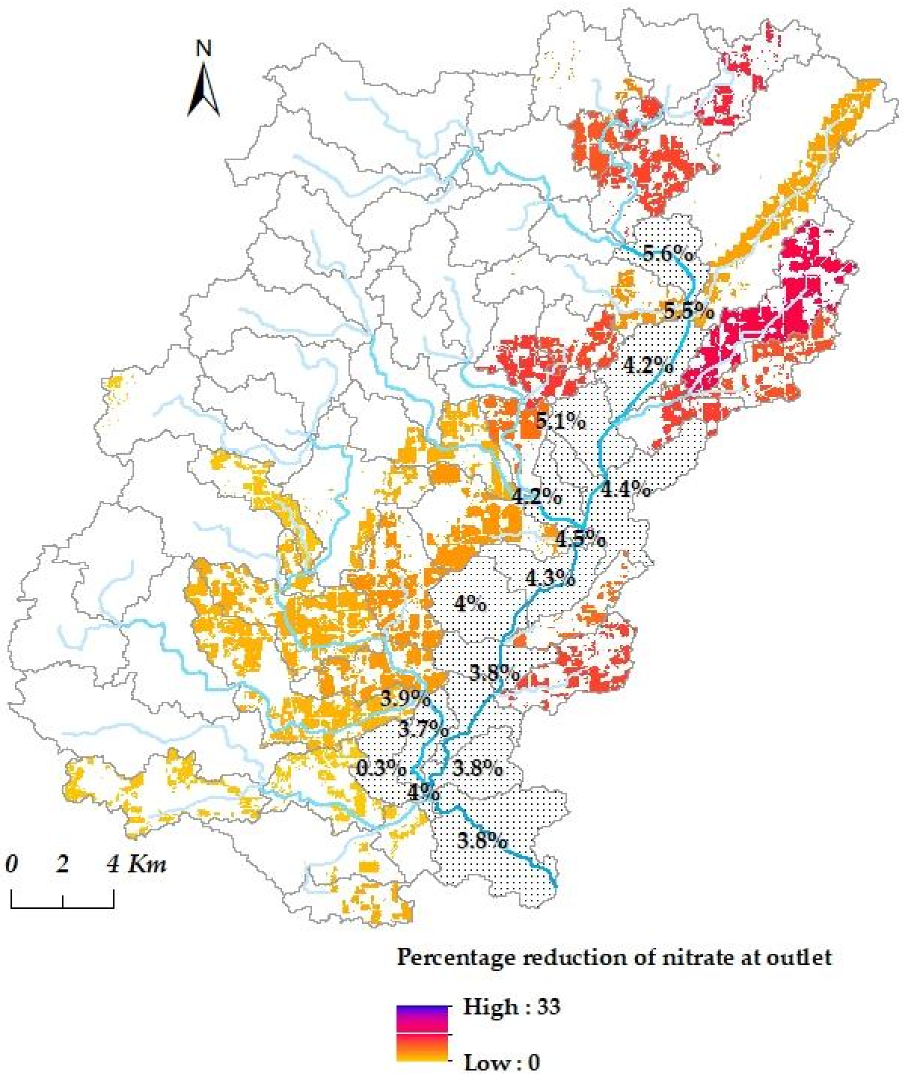

Figure A13. Subwatersheds and winter 50% fertiliser reduction for DLU DLU

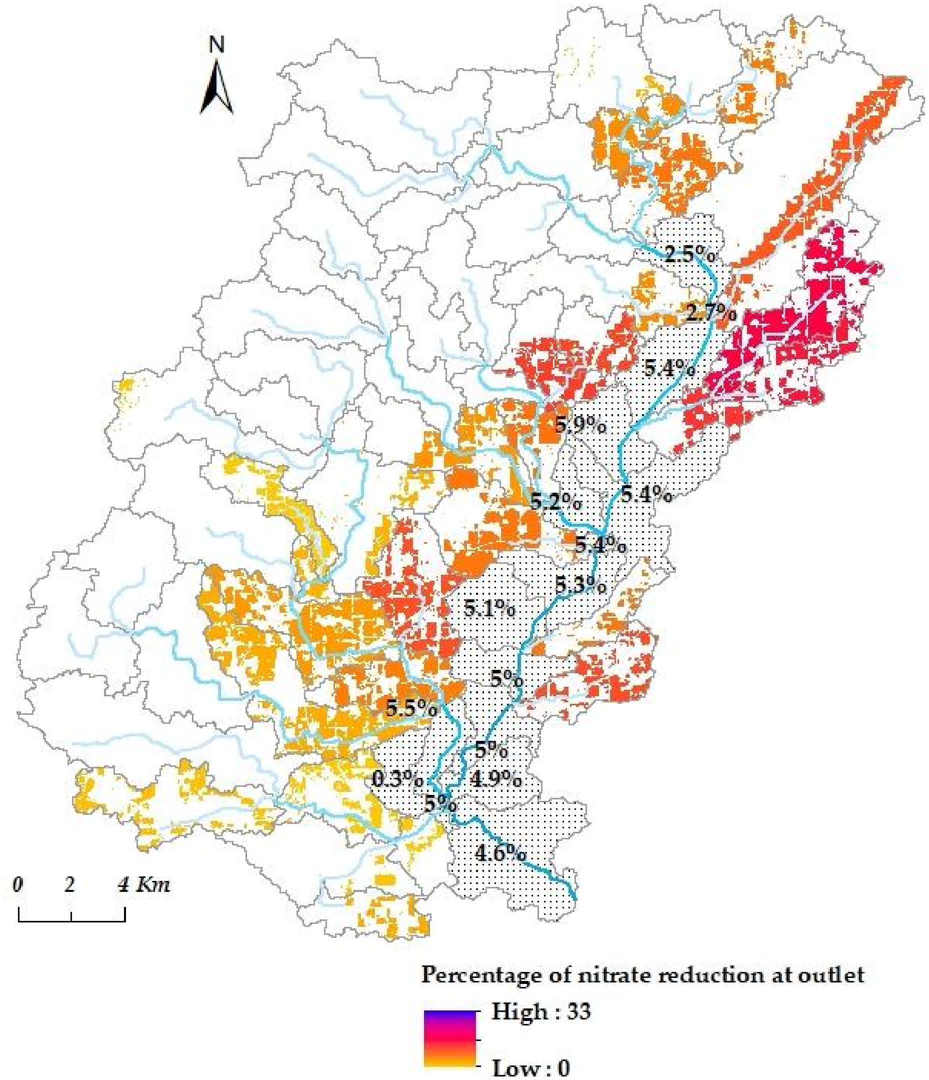

Figure A14. Subwatersheds and spring 50% fertiliser reduction for

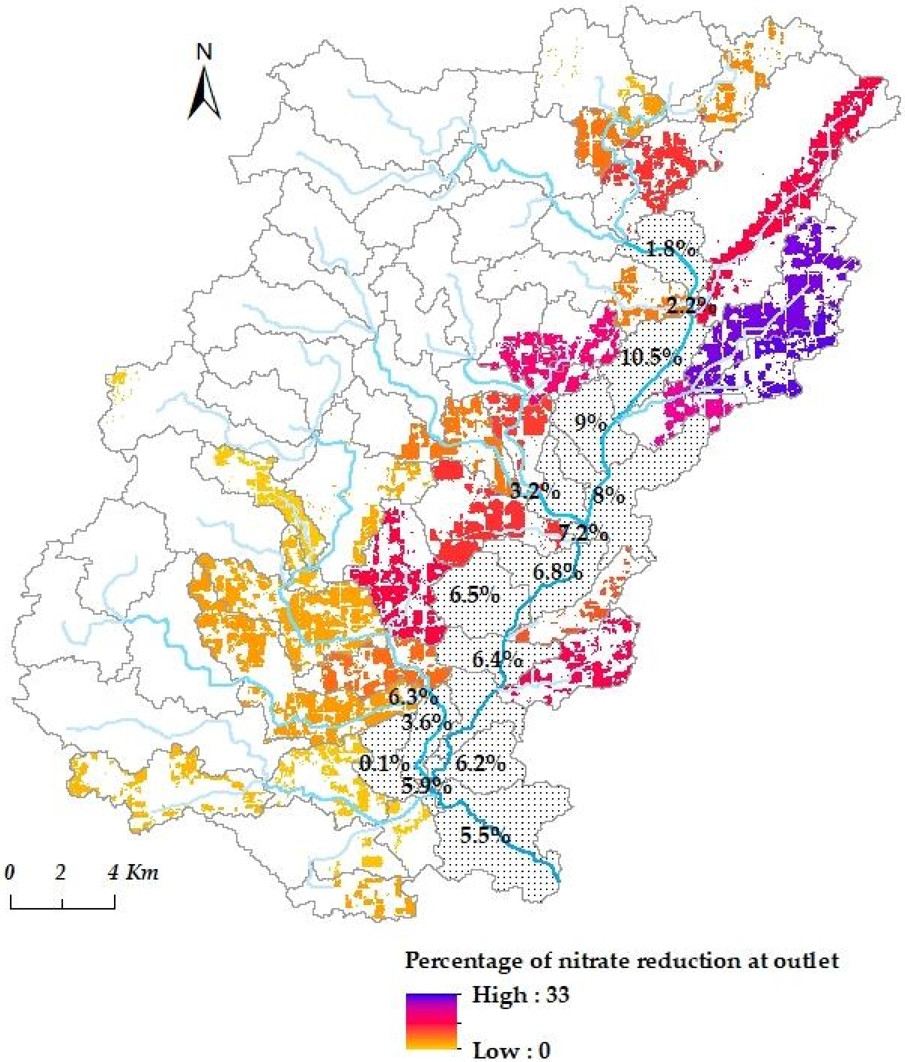

Figure A15. Subwatersheds and fall 50% fertiliser reduction for DLU

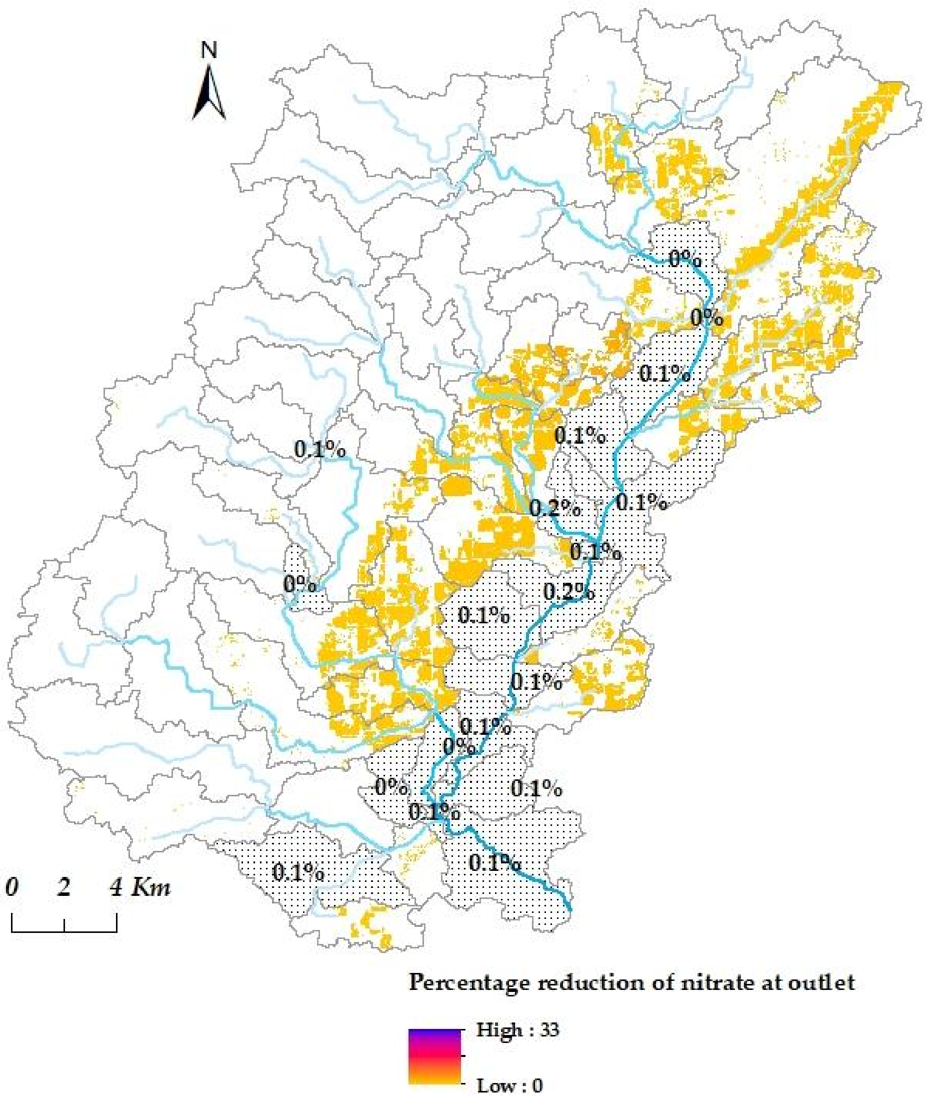

Figure A16. Subwatersheds and winter 5% fertiliser reduction for CFD

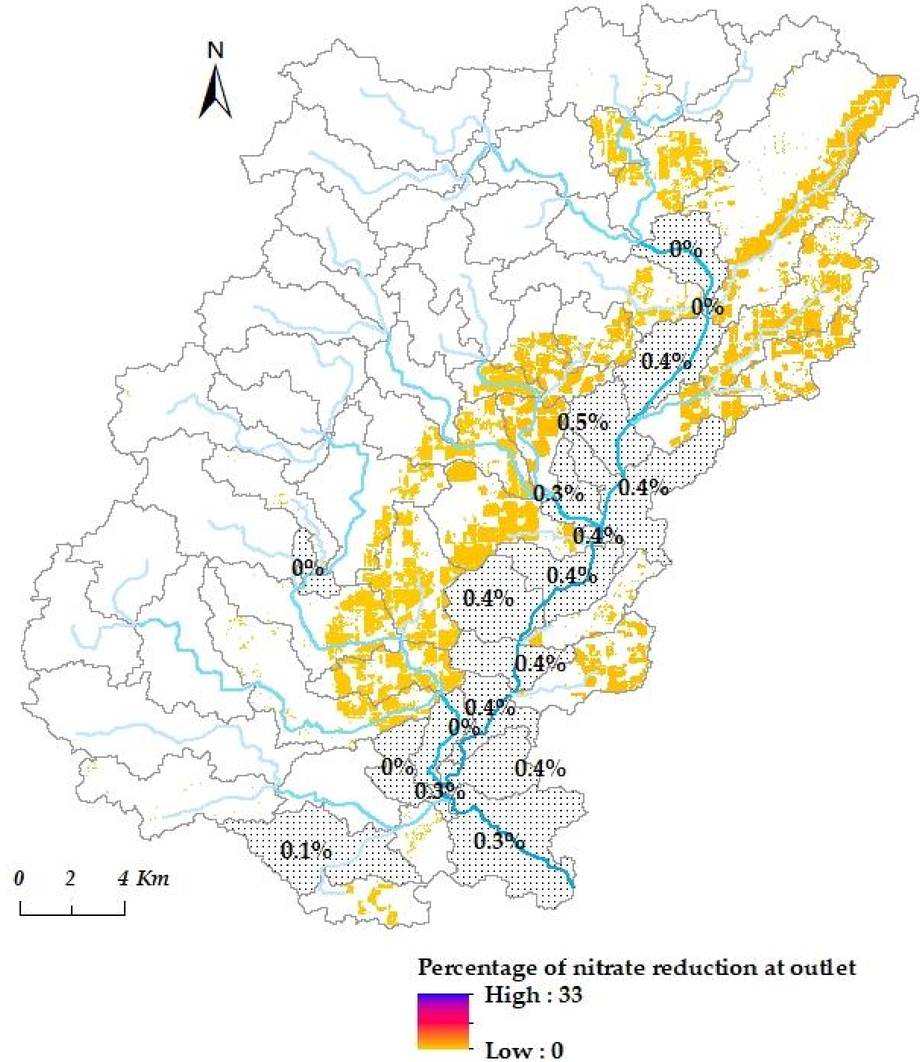

Figure A17. Subwatersheds and spring 5% fertiliser reduction for CFD

L

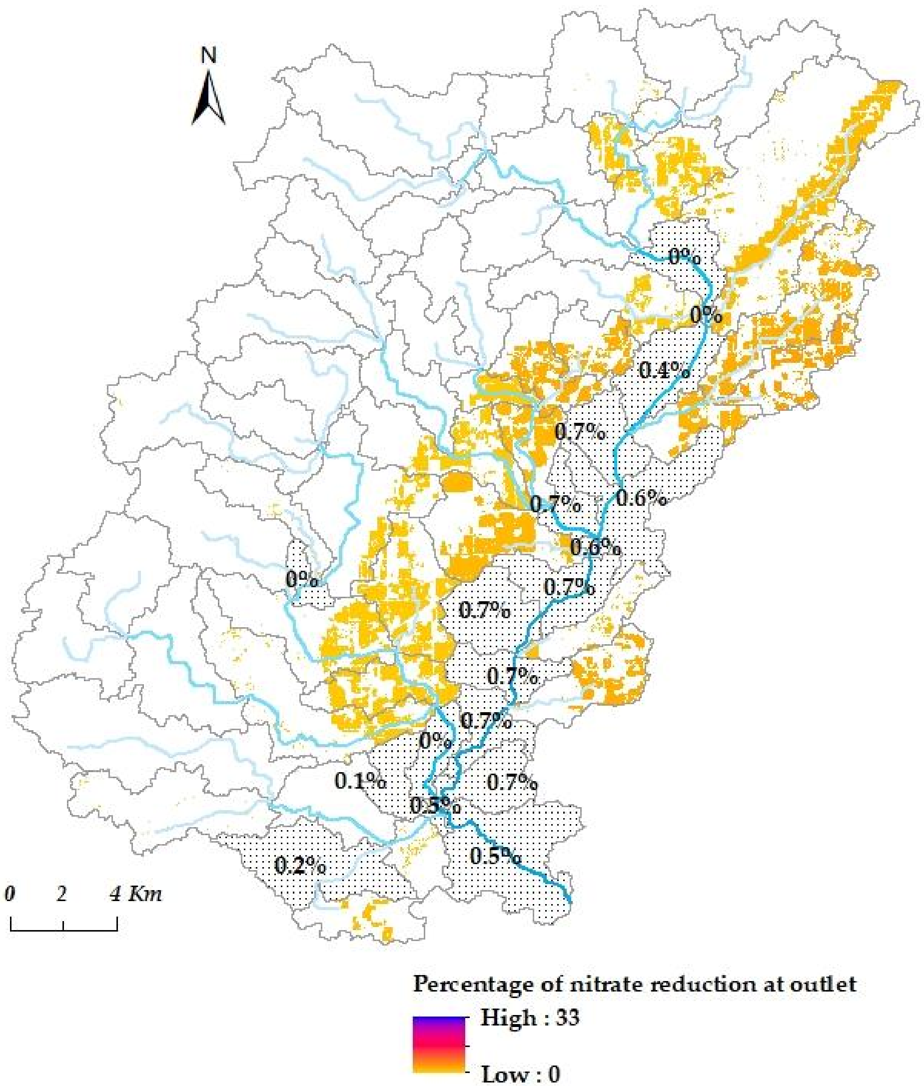

Figure A18. Subwatersheds and summer 5% fertiliser reduction for CFD

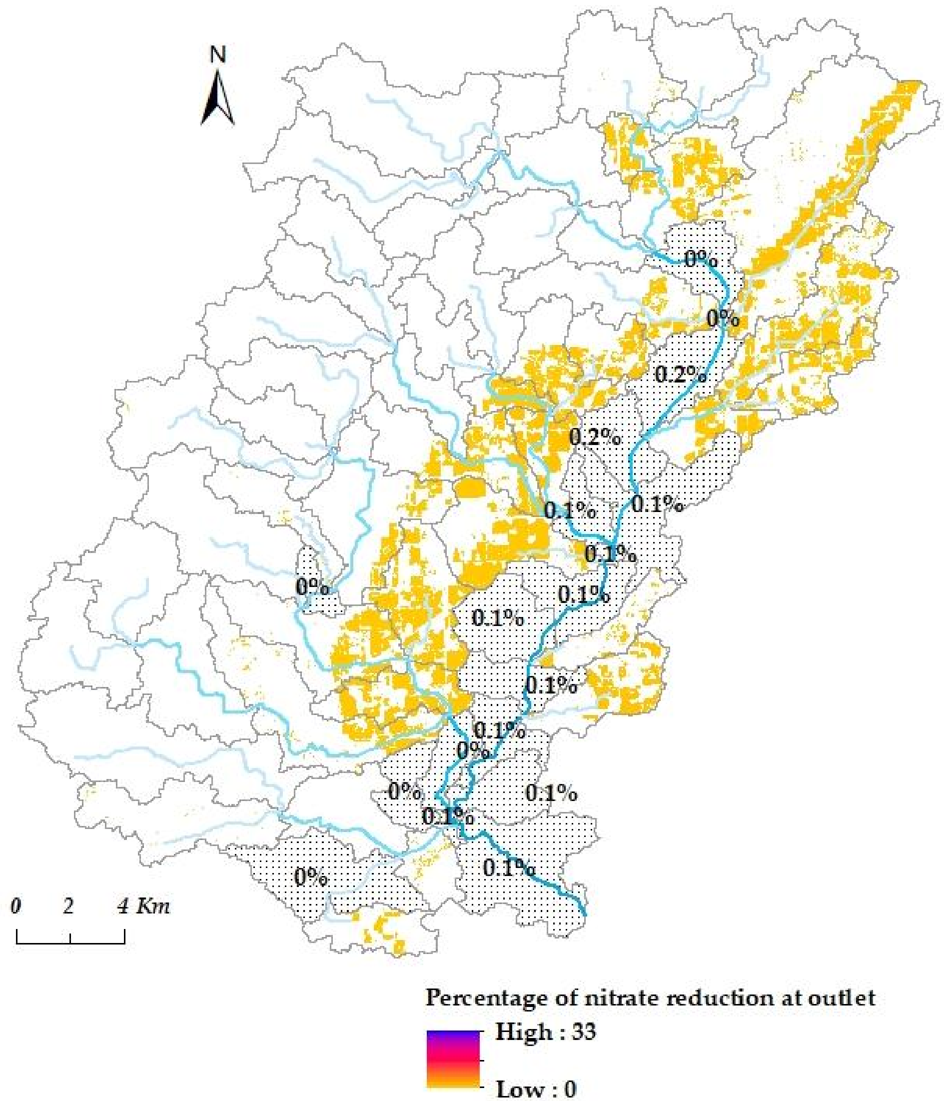

Figure A19. Subwatersheds and fall 5% fertiliser reduction for CFD

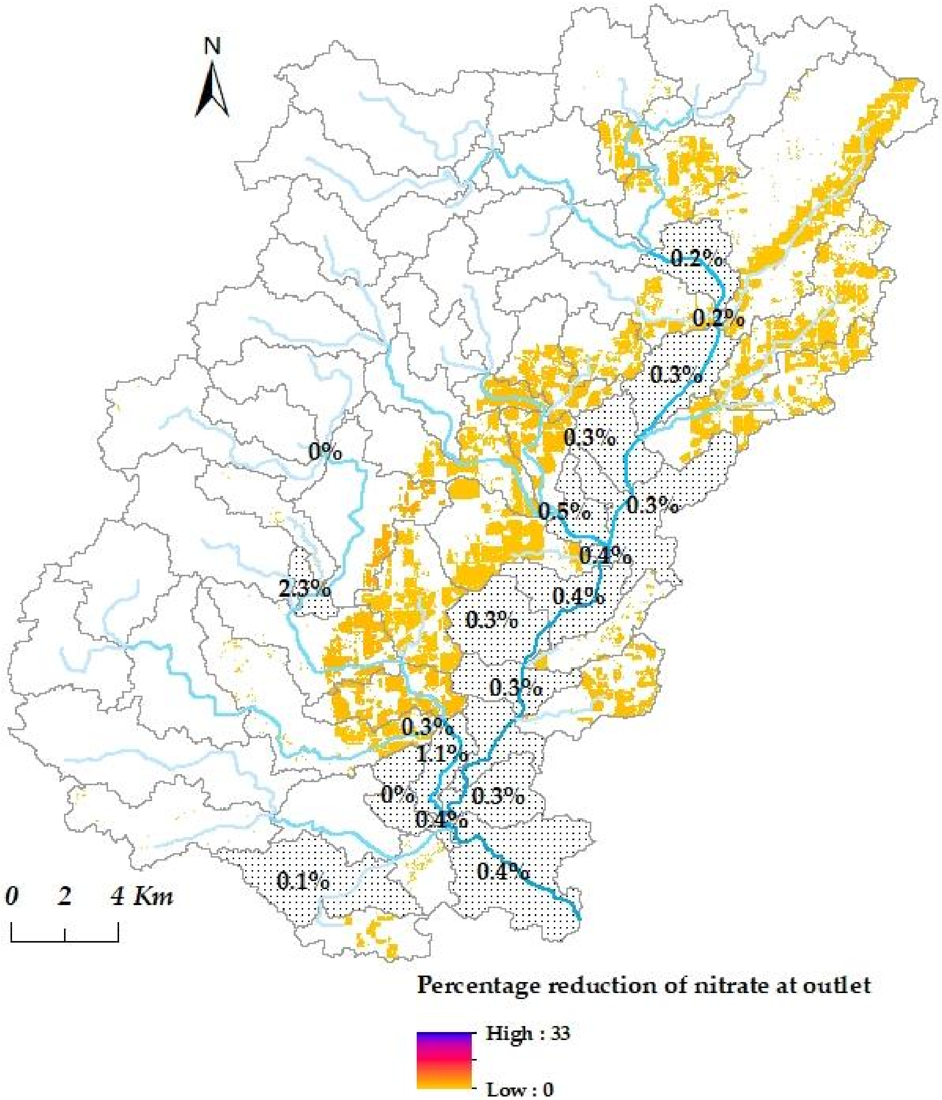

Figure A20. Subwatersheds and winter 10% fertiliser reduction for CFD

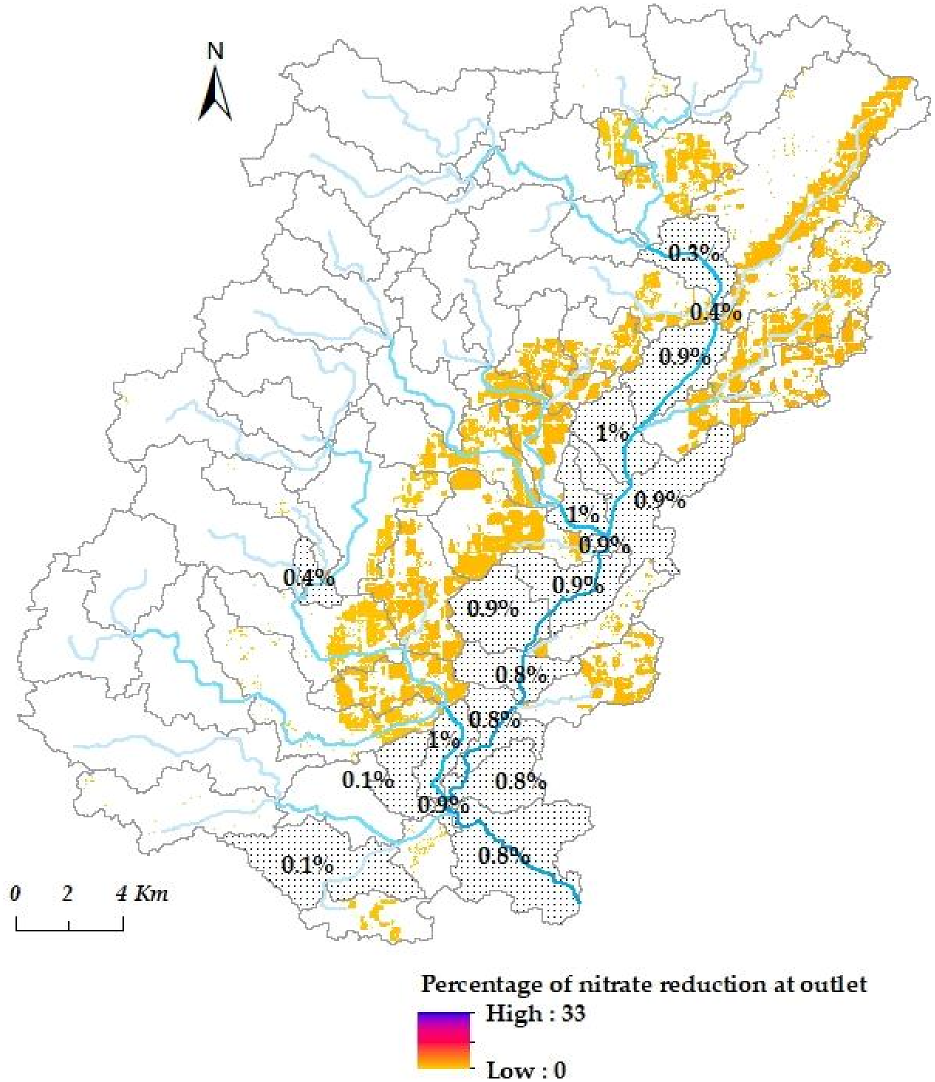

Figure A21. Subwatersheds and spring 10% fertiliser reduction for CFD

N

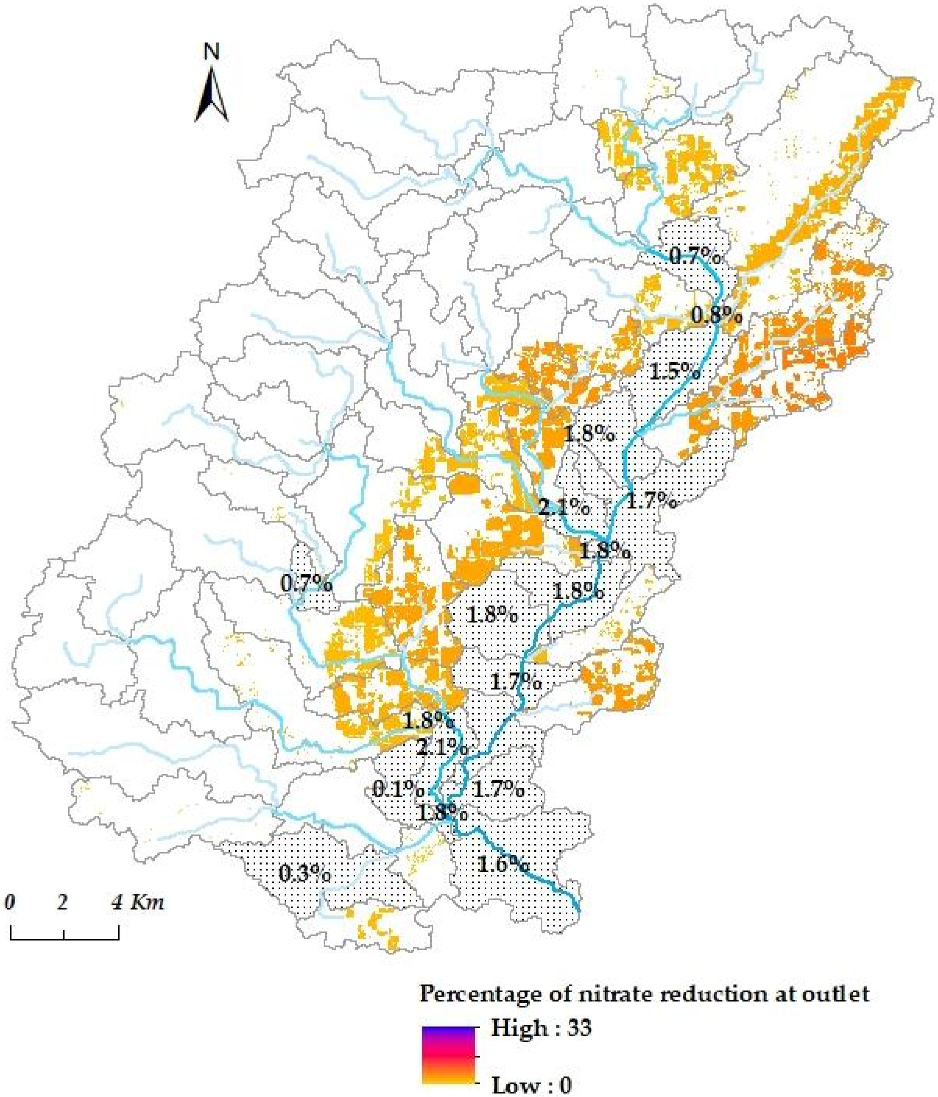

Figure A22. Subwatersheds and summer 10% fertiliser reduction for CFD

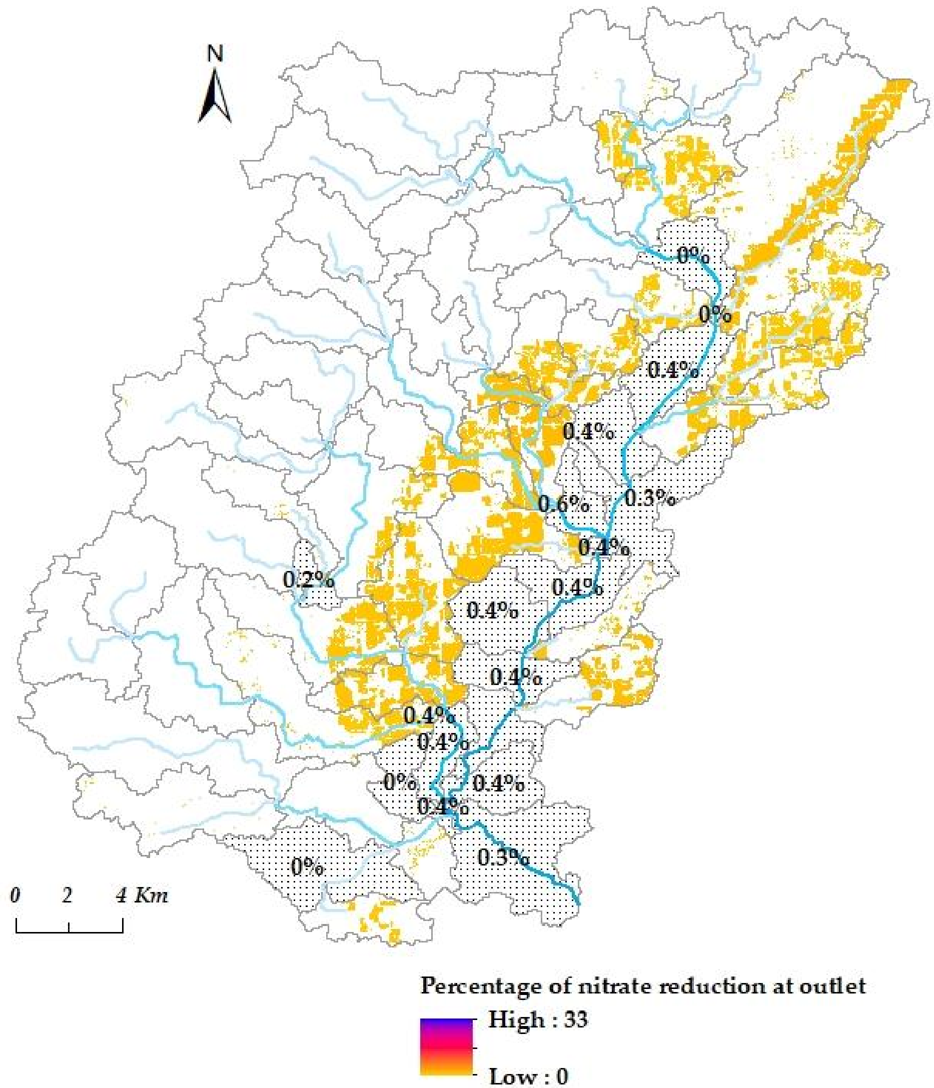

Figure A23. Subwatersheds and fall 10% fertiliser reduction for CFD

O

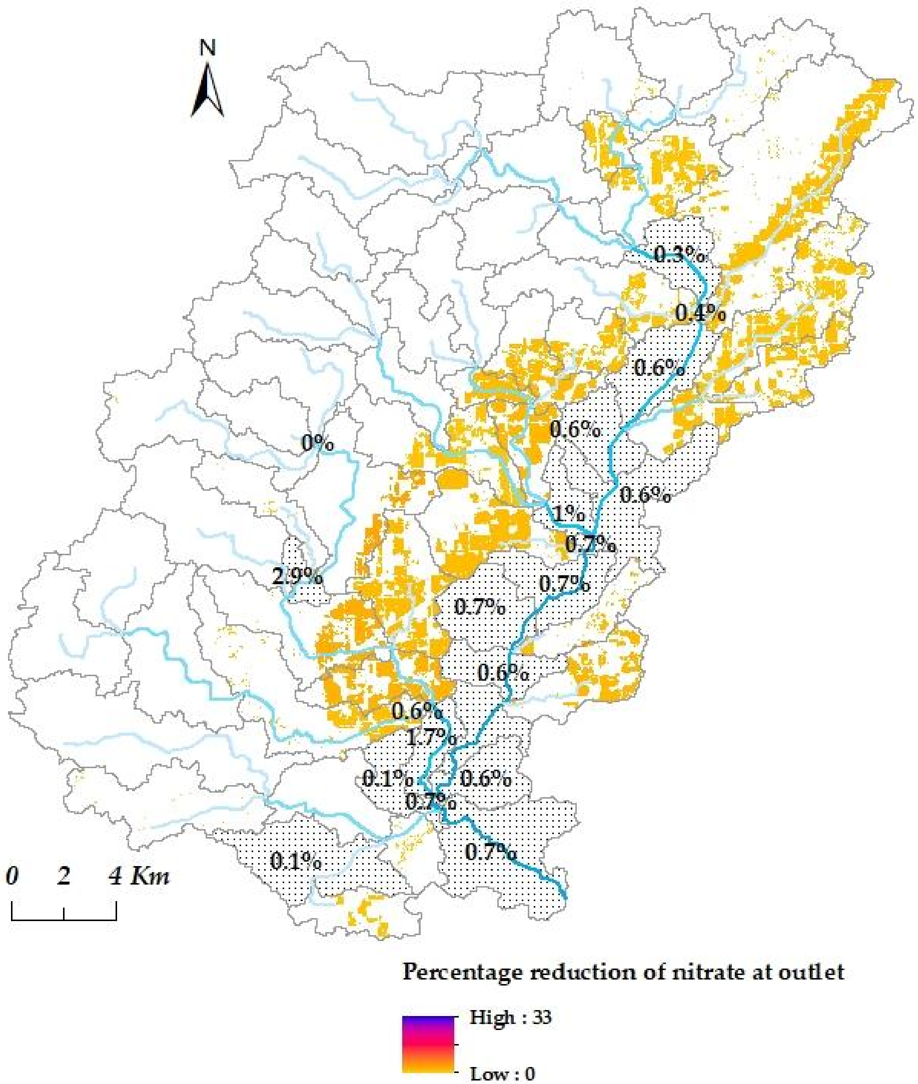

Figure A24. Subwatersheds and winter 20% fertiliser reduction for CFD

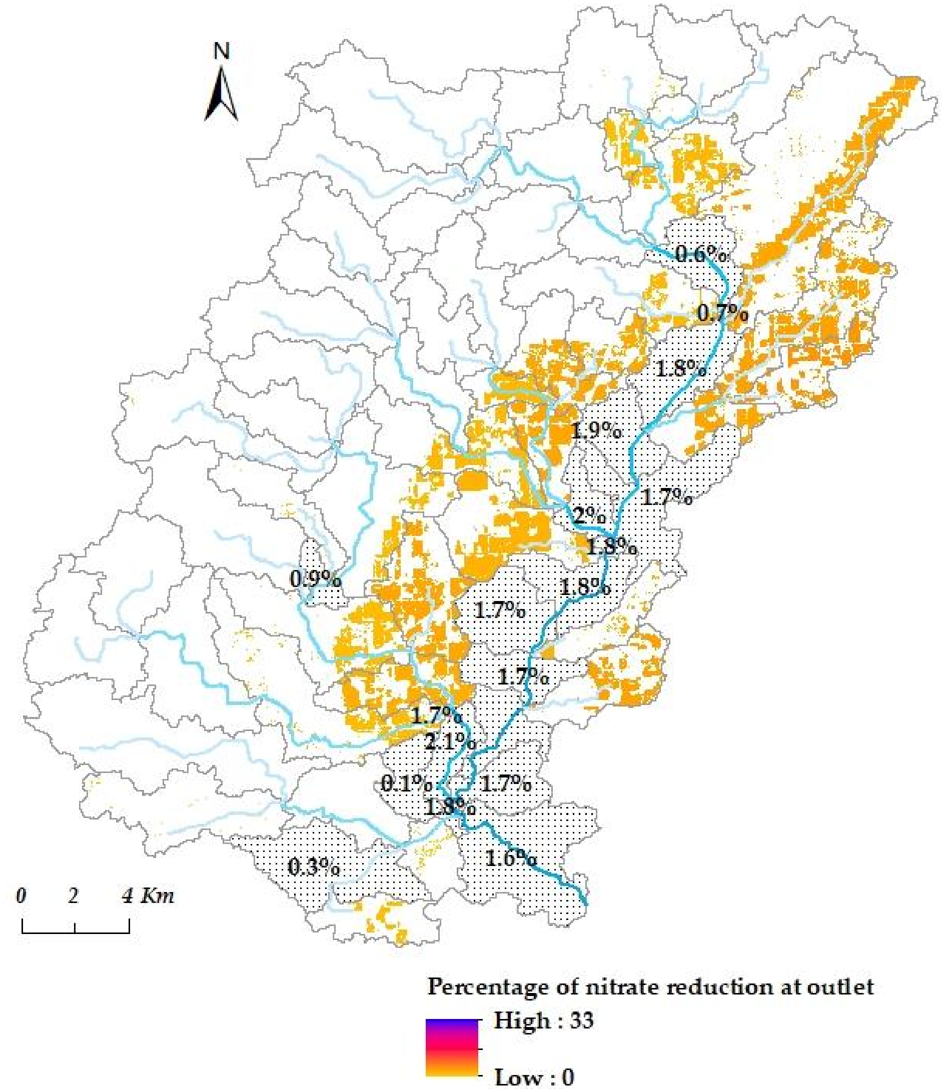

Figure A25. Subwatersheds and spring 20% fertiliser reduction for CFD

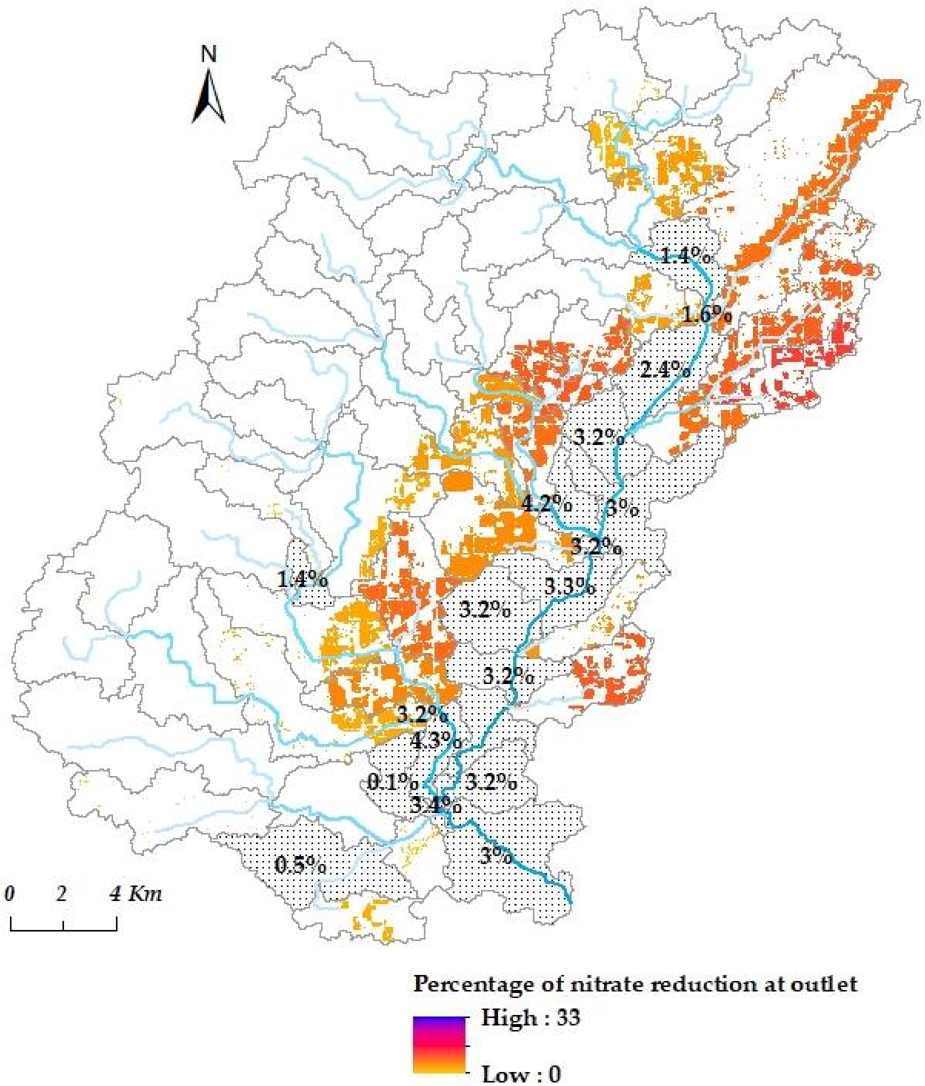

Figure A26. Subwatersheds and summer 20% fertiliser reduction for CFD

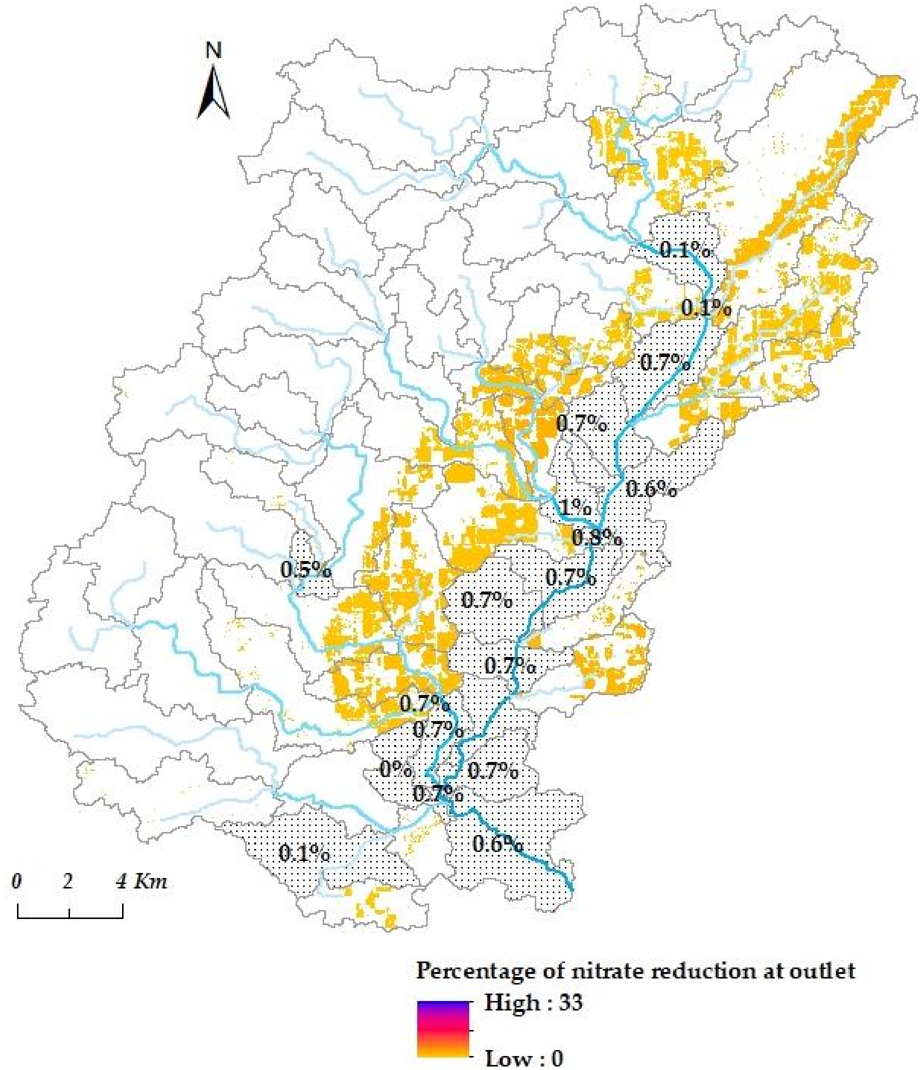

Figure A27. Subwatersheds and fall 20% fertiliser reduction for CFD

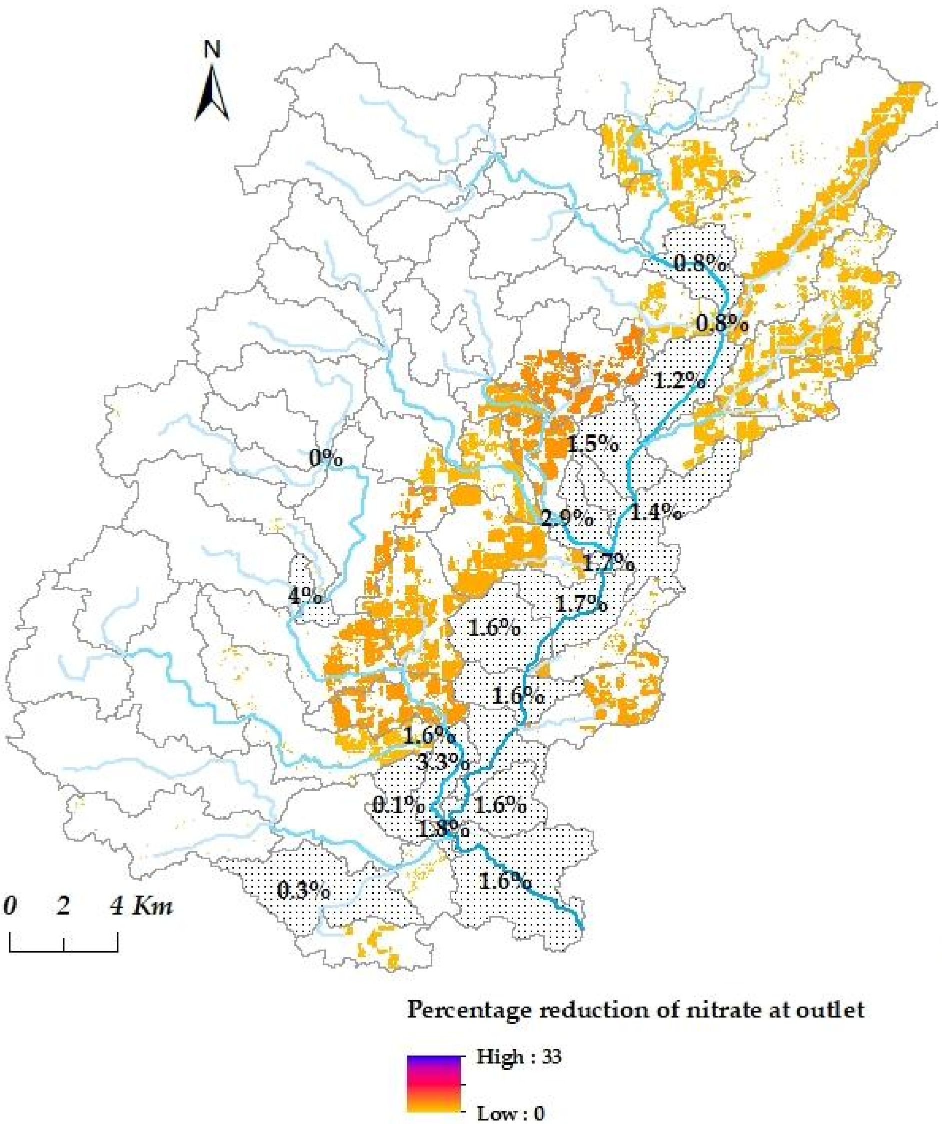

Figure A28. Subwatersheds and winter 50% fertiliser reduction for CFD

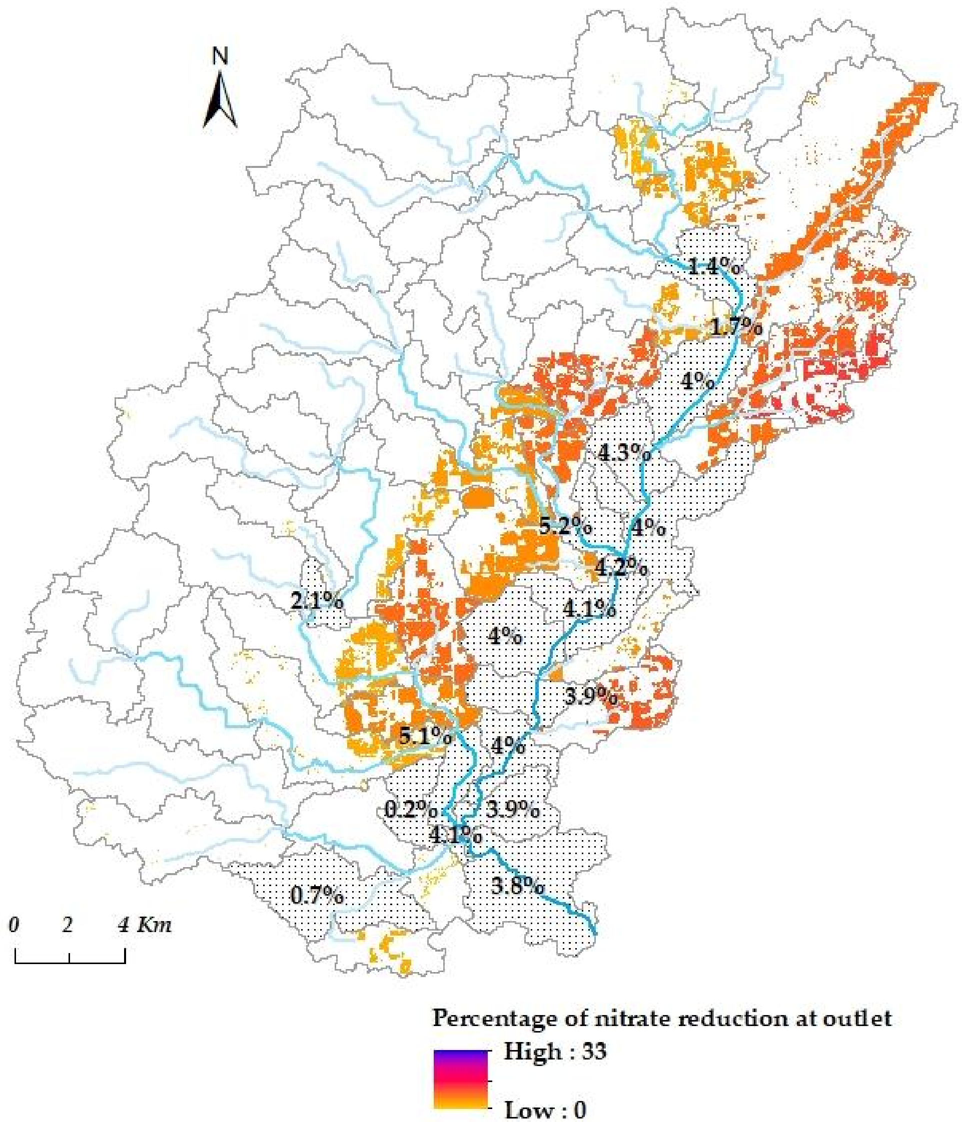

Figure A29. Subwatersheds and spring 50% fertilizer reduction for CFD

R

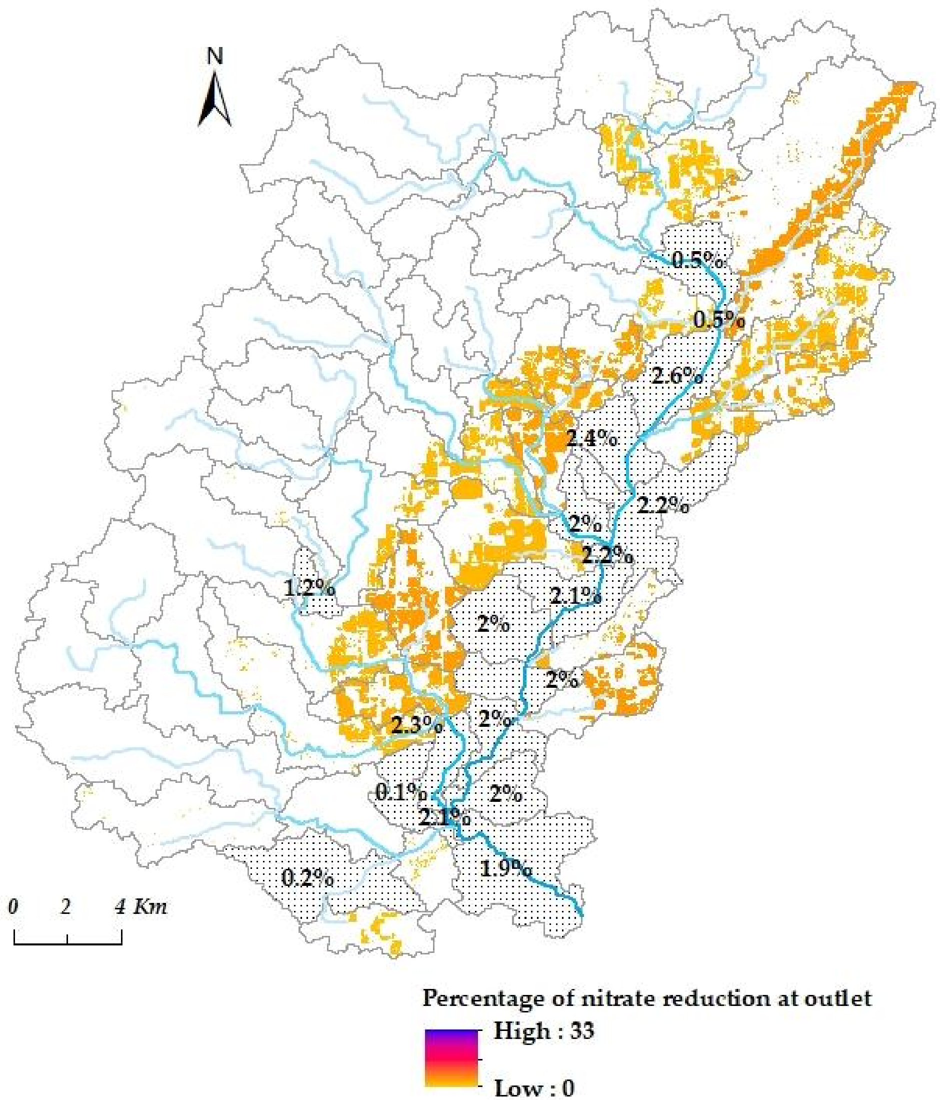

Figure A30. Subwatersheds and fall 50% fertilizer reduction for CFD