

**Quantifying the Impact of Climate Change on Water Availability and Water Quality in
the Chesapeake Bay Watershed**

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ABSTRACT

Climate change impacts hydrology, nutrient cycling, agricultural conservation practices, and greenhouse gas (GHG) emissions. The Chesapeake Bay and its watershed are subject to the largest and most expensive Total Maximum Daily Load (TMDL) ever developed. It is unclear if the TMDL can be met given climate change and variability (e.g., extreme weather events). The objective of this dissertation is to quantify the impact of climate change and climate on water resources, nutrient cycling and export in agroecosystems, and agricultural conservation practices in the Chesapeake Bay watershed. This is accomplished by developing and employing a suite of modelling tools.

GHG emissions from agroecosystems, particularly nitrous oxide (N_2O), are an increasing concern. To quantify N_2O emissions a routine was developed for the Soil and Water Assessment Tool (SWAT) model. The new routine predicts N_2O and di-nitrogen (N_2) emissions by coupling the C and N cycles with soil moisture, temperature, and pH in SWAT. The model uses reduction functions to predict total denitrification ($N_2 + N_2O$ production) and partitions N_2 from N_2O using a ratio method. The SWAT nitrification routine was modified to predict N_2O emissions using reduction functions. The new model was tested using GRACEnet data at University Park, Pennsylvania, and West Lafayette, Indiana. Results showed strong correlations between plot measurements of N_2O flux and the model predictions for both test sites and suggest that N_2O emissions are particularly sensitive to soil pH and soil N, and moderately sensitive to soil temperature/moisture and total soil C levels.

The new GHG model was then used to analyze the impact of climate change and extreme weather conditions on the denitrification rate, N_2O emissions, and nutrient cycling/export in the 7.4 km² WE38 watershed in Pennsylvania. Climate change impacts hydrology and nutrient cycling by changing soil moisture, stoichiometric nutrient ratios, and soil temperature, potentially complicating mitigation measures. To quantify the impact of climate change we

forced the new GHG model with downscaled and bias-corrected regional climate model output and derived climate anomalies to assess their impact on hydrology, nitrate (NO₃-), phosphorus (P), and sediment export, and on emissions of N₂O and N₂. Model-average (\pm standard deviation) results indicate that climate change, through an increase in precipitation, will result in moderate increases in winter/spring flow ($2.7\pm 10.6\%$) and NO₃- export ($3.0\pm 7.3\%$), substantial increases in dissolved P (DP, $8.8\pm 19.8\%$), total P (TP, $4.5\pm 11.7\%$), and sediment ($17.9\pm 14.2\%$) export, and greater N₂O ($63.3\pm 50.8\%$) and N₂ ($17.6\pm 20.7\%$) emissions. Conversely, decreases in summer flow ($-12.4\pm 26.7\%$) and the export of P ($-11.4\pm 27.4\%$), TP ($-7.9\pm 24.5\%$), sediment ($-4.1\pm 21.4\%$), and NO₃- ($-12.2\pm 31.4\%$) are driven by greater evapotranspiration from increasing summer temperatures. Increases in N₂O ($20.1\pm 29.3\%$) and decreases in N₂ ($-13.0\pm 14.6\%$) are also predicted in the summer and driven by increases in soil moisture and temperature.

In an effort to assess the impact of climate change at a regional level, the model was then scaled-up to the entire Susquehanna River basin and was used to evaluate if agricultural best management practices (BMPs) can offset the impact of climate change. Agricultural BMPs are increasingly and widely employed to reduce diffuse nutrient pollution. Climate change can complicate the development, implementation, and efficiency of BMPs by altering hydrology, nutrient cycling, and erosion. We select and evaluate four common BMPs (buffer strips, strip crop, no-till, and tile drainage) to test their response to climate change. We force the calibrated model with six downscaled global climate models (GCMs) for a historic period (1990-2014) and two future scenario periods (2041-2065) and (2075-2099) and quantify the impact of climate change on hydrology, NO₃-, total N (TN), DP, TP, and sediment export with and without BMPs. We also tested prioritizing BMP installation on the 30% of agricultural lands that generate the most runoff (e.g., critical source areas-CSAs). Compared against the historical baseline and excluding the impact of BMPs, the ensemble model mean (\pm standard deviation?) predictions indicate that climate change results in annual increases in flow ($4.5\pm 7.3\%$), surface runoff ($3.5\pm 6.1\%$), sediment export ($28.5\pm 18.2\%$) and TN ($9.5\pm 5.1\%$), but decreases in NO₃- ($12\pm 12.8\%$), DP ($14\pm 11.5\%$), and TP ($2.5\pm 7.4\%$) export. When agricultural BMPs are simulated most do not appreciably change the overall water balance; however, tile drainage and strip crop decrease surface runoff generation and the export of sediment, DP, and TP, while buffer strips reduced N export substantially. Installing BMPs on critical source areas (CSAs) results in nearly the same level of performance for most practices and most pollutants. These results suggest that

climate change will influence the performance of BMPs and that targeting BMPs to CSAs can provide nearly the same level of water quality impact as more widespread adoption.

Finally, recognizing that all of these model applications have considerable uncertainty associated with their predictions, we develop and employ a Bayesian multi-model ensemble to evaluate structural model prediction uncertainty. The reliability of watershed models in a management context depends largely on associated uncertainties. Our Objective is to quantify structural uncertainty for predictions of flow, sediment, TN, and TP predictions using three models: the SWAT-Variable Source Area model (SWAT-VSA), the standard SWAT model (SWAT-ST), and the Chesapeake Bay watershed model (CBP-model). We initialize each of the models using weather, soil, and land use data and analyze outputs of flow, sediment, TN, and TP for the Susquehanna River basin at the Conowingo Dam in Conowingo, Maryland. Using these three models we fit Bayesian Generalized Non - Linear Multilevel Models (BGMM) for flow, sediment, TN, and TP and obtain estimated outputs with 95% confidence intervals. We compare the BGMM results against the individual model results and straight model averaging (SMA) results using a split time period analysis (training period and testing period) to assess the BGMM in a predictive fashion. The BGMM provided better predictions of flow, sediment, TN, and TP compared to individual models and the SMA during the training period. However, during the testing period the BGMM was not always the best predictor, in fact, there was no clear best model during the testing period. Perhaps more importantly, the BGMM provides estimates of prediction uncertainty, which can enhance decision making and improve watershed management by providing a risk-based assessment of outcomes.

**Quantifying the Impact of Climate Change on Water Availability and Water Quality in
the Chesapeake Bay Watershed**

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GENERAL AUDIENCE ABSTRACT

Climate change impacts hydrology, nutrient cycling, agricultural conservation practices, and greenhouse gas (GHG) emissions. The Chesapeake Bay and its watershed are subject to the largest and most expensive Total Maximum Daily Load (TMDL) ever developed. It is unclear if the TMDL can be met given climate change and variability. The objective of this dissertation is to quantify the impact of climate change and climate on water resources, nutrient cycling and export in agroecosystems, and agricultural conservation practices in the Chesapeake Bay watershed. This is accomplished by developing and employing different modeling tools.

First, GHG emissions model was developed to quantify nitrous oxide (N_2O) emissions from agroecosystems, which are an increasing concern. The new model was then tested using observed N_2O emissions data at University Park, Pennsylvania, and West Lafayette, Indiana. Results showed strong correlations between plot measurements of N_2O flux and the model predictions for both test sites.

Second, the new GHG model was then used to analyze the impact of climate change and extreme weather conditions on the N_2O emissions, and nutrient cycling/export in small and regional watershed scale. To quantify the impact of climate change we forced the new GHG model with downscaled and bias-corrected regional climate model data to assess their impact on hydrology, nitrate (NO_3^-), phosphorus (P), and sediment export, and on emissions of N_2O and N_2 . Finally, recognizing that all of these model applications have considerable uncertainty associated with their predictions, we developed and employed a Bayesian multi-model ensemble to evaluate structural model prediction uncertainty.

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CHAPTER 1

INTRODUCTION

Introduction

Climate change has the potential to impact hydrology and diffuse nutrient export from agricultural landscapes. The Chesapeake Bay and its watershed are subject to the largest and most expensive Total Maximum Daily Load (TMDL) ever developed. It is unclear if the TMDL can be met given climate change and variability (e.g., extreme weather events).

Greenhouse gas (GHG) emissions from agroecosystems, particularly nitrous oxide (N₂O), are of increasing importance and a major contributor to global climate change. N₂O is a potent GHG, with 310 times the radiative forcing as CO₂ on a molecule-by-molecule basis (Beheydt *et al.*, 2008; Jahangir *et al.*, 2013) and is an intermediate product of denitrification (Jahangir *et al.*, 2013) and nitrification (Parton *et al.*, 2001). Denitrification is the microbial process that converts reactive nitrate (NO₃⁻) to N₂O and unreactive dinitrogen (N₂), and is favored by anaerobic soil conditions, adequate soil NO₃⁻ and carbon (C) content, moderate to high soil temperature, neutral to basic soil pH, and the presence of denitrifying microorganisms (Knowles, 1982; Parton *et al.*, 1996). Nitrification is a microbial process that transforms ammonium (NH₄⁺) to NO₃⁻ and occurs under aerobic soil conditions in the presence of adequate NH₄⁺, high soil temperature, and high pH. These factors vary in space and time in agroecosystems and interact with each other in complicated ways (Henault & Germon, 2000). Consequently, N₂O emissions vary spatially across a landscape and temporarily over the course of a year (Groffman, Butterbach-Bahl, *et al.*, 2009a). Identifying when, where, and how these factors interact to form hotspots and hot moments of N₂O emissions (e.g., areas or times of large emissions) is a current area of research and a daunting challenge. Thus, there is a need to develop integrated models capable of incorporating these relevant controls to predict N₂O emissions across a range of scales to better inform the selection of landscape management practices to reduce N₂O emissions (Bruland *et al.*, 2006; Clement *et al.*, 2002; Mosier *et al.*, 2002).

Agricultural best management practices (BMPs) are increasingly and widely used to reduce impact of diffuse pollutant export from agricultural landscapes (Ullrich & Volk, 2009). For instance,

conservation tillage or no-till, enhances soil organic carbon, soil quality, and soil aggregation leading to less soil erosion in agricultural landscapes (Roldán et al., 2007). BMPs such as riparian vegetation, strip crop, and buffer strip can all help reduce diffuse pollutants, by reducing inputs to the crop, enhancing sequestration of nutrients in plant tissue, or reducing surface and subsurface losses due to hydrologic pathway alterations (Carpenter et al., 1998). However, it is not clear what impact a changing climate will have on the function of BMPs. For instance, increased precipitation volume and intensity may overwhelm many BMPs like riparian buffers, but higher temperatures, longer growing seasons, and more rainfall might cause that same buffer to mature more quickly, thus trapping more sediment and sequestering more nutrients. Thus, agricultural conservation practices need to be assessed for performance under a changing climate (Hatfield & Prueger, 2004).

All of these model applications have considerable uncertainty associated with their predictions. The reliability of watershed models in a management context depends largely on associated uncertainties. Numerous approaches have been proposed to quantify uncertainties in watershed models including Bayesian Model Averaging (Raftery et al., 1997; Vrugt et al., 2008), Generalized Likelihood Uncertainty Estimation (GLUE) (Blasone et al., 2008; Vrugt et al., 2005), multiple objective function criteria (Blasone et al., 2008), sequential data assimilation (Moradkhani et al., 2005), Bayesian Recursive Estimation (Thiemann et al., 2001), and Ensemble Kalman (Abaza et al., 2014). However, only a few methods such as multi-model ensembles (MME) (Duan et al., 2007; Stoica et al., 2004), are proposed for quantifying structural model uncertainties. This is due to the complexity and difficulty of separating structural uncertainties from model parameter or input data uncertainty (Zhang et al., 2011). Sharifi et al. (2017) evaluated the performance of different watershed models to assess water quality impacts on Queenstown drainage. Stow and Scavia (2009) demonstrate improved performance in estimating hypoxia in the Chesapeake Bay using a hierarchical Bayesian ensemble approach, but the study is limited to processes within the Bay and does not describe upland watershed processes. Boomer et al. (2013) and Exbrayat et al. (2010) also suggested use of multi model ensemble. However, research describing ensembles used to quantify structural uncertainty in watershed models is lacking, and no consensus on application of methods or evaluation guidelines has been reached

Thus, this dissertation focuses on quantifying the impact of climate change and hydrologic anomalies on water resources, water quality, and agricultural practices in the Chesapeake Bay watershed. This is accomplished by coupling process-based modeling with downscaled climate models. The results of the study are presented as four separate, but related chapters, prefaced by an introduction reviewing the relevant literature. The introduction chapter contains the literature related to climate change, greenhouse gas (GHG) production/emissions, agricultural conservation practices, and model uncertainty. Chapter 2 describes the development of a nitrous oxide (N₂O) emissions routine for the soil waters assessment tool (SWAT) model to assess GHG and di-nitrogen (N₂) emissions from agroecosystems. This chapter details model development, sensitivity analyses, and test application to predict GHG emissions at both the field and watershed scales as well as the implications of agricultural GHG emissions. The impact of climate change and climate anomalies on hydrologic and biogeochemical processes in the Chesapeake Bay watershed is described in chapter 3. Chapter 4 assess how agricultural conservation practices can help to mitigate the impact of climate change on water quality and discusses the most promising agricultural conservation practices to mitigate climate change. This chapter details downscaling and bias correction of the most recent climate change models from the World Climate Research Programme's Coupled Model Intercomparison Project Phase 5 (CMIP5). Finally, chapter 5 details a new method to quantify structural model predictions uncertainty in watershed models. This chapter employs a Bayesian Multi Level Model ensemble, which incorporates three separate, but complimentary watershed models into the ensemble, and provides estimates of ensemble model prediction uncertainty at each prediction interval.

Context

The gross production value of agricultural products in the United States (US) was an estimated \$252 billion in 2014, accounting for over one percent of the gross domestic product (GDP) (CIA factbook, 2017; FAO stat, 2017). The US is the world's largest agricultural exporter and provides over half of the total exported corn in the world (CIA factbook, 2017). Over 85% percent of households in the US were considered food secure in 2014, and the US received a top score in the Global Food Security Index in 2016 (Coleman-Jensen et al., 2014; The Economist Intelligence Unit, 2016). The success of agriculture in the US is very important to food and energy security, and economic development in the US (Joint Economic Committee, 2013);

however, industrialized agriculture can cause many negative environmental consequences, including habitat destruction, greenhouse gas emissions, and perhaps most critically, water quality degradation. The impact of climate change complicates water quality protection strategies, and threatens to reverse what progress has been made.

Climate Change

The land, water, and air of earth are linked to the atmosphere through gaseous exchange of the GHGs carbon dioxide (CO₂), nitrous oxide (N₂O), and methane (CH₄). These GHGs are critical atmospheric constituents, and largely determine the long-term climate trends of planet earth; and historically made the earth suitable to habitation and eventually agricultural production capable of supporting 9 billion people. While these GHGs are naturally occurring, and are a critical component of the atmosphere at certain levels, when the concentration increases above baseline levels more infrared radiation is trapped, which results in global warming (Clayton *et al.*, 1997), and ultimately climate change (Rosenzweig & Hillel, 1998). The Intergovernmental Panel on Climate Change (IPCC), drawing on a comprehensive review of published modeling results, forecasts an increase in world average temperature by 2100 within the range 1.4–5.8 °C (McMichael *et al.*, 2006), and an increase in the speed and intensity of the hydrologic cycle, which increases both flood and drought occurrence (Barnett *et al.*, 2005; Fowler & Hennessy, 1995), all of which threatens human and ecosystem health (Patz *et al.*, 2005). One area of climate change impact that has, as of yet, been little studied is the impact on diffuse nutrient export from agricultural landscapes (Howarth *et al.*, 2006). Excess nutrient export from the landscape to aquatic ecosystems accelerates eutrophication and harmful algal blooms (Burgin & Hamilton, 2007), leading to undesirable changes in ecosystem structure and function (Smith *et al.*, 1999), such as areas of low oxygen concentrations, known as dead zones, in coastal waters (Diaz & Rosenberg, 2008). However, understanding the processes that underlie these changes and their impact on water quality is highly uncertain and an area of research in need of significant work.

Climate change, through change of precipitation and temperature, can change the soil temperature and the soil moisture condition, which controls nutrient cycling in agroecosystems (Suseela *et al.*, 2012). For instance, increased soil temperature can accelerate the growth of soil microbes (Davidson & Janssens, 2006) that control nutrient processes such as nitrification,

denitrification, and P mineralization. These processes are primarily controlled by soil and environmental factors that are affected by a changing climate (Parton *et al.*, 1996). Thus, there is urgent need to quantify the impact of climate change on nutrient cycling, and enhance our understanding of the complex process in agroecosystems in order to protect water quality.

Impact of Climate Change on Nutrient Cycling

Climate change has the potential to impact hydrology and nutrient cycling in agroecosystems in the Mid-Atlantic (Huntington, 2003; Johnson *et al.*, 2012; Najjar *et al.*, 2009a; Najjar *et al.*, 2010; Neff *et al.*, 2000). Climate predictions for the Mid-Atlantic suggest that annual precipitation (especially during the winter/spring) quantity and intensity will increase, which could increase nitrogen (N), phosphorus (P), and sediment export from watersheds (Chang *et al.*, 2001; Cousino *et al.*, 2015). Drier conditions in the summer and fall also have been shown to increase the buildup of soil nutrients that can subsequently be flushed from the system when wet conditions return (Kaushal *et al.*, 2008; Wetz & Yoskowitz, 2013).

Nutrient export from the landscape to surface waters are controlled by a combination of key biogeochemical and hydrologic processes. Changes in precipitation and temperature alter the timing and magnitude of runoff, soil moisture, and biogeochemical cycles (Gleick, 1989). For instance, N mineralization, nitrification, and denitrification are, to a large extent, controlled by factors that climate change influences, such as soil temperature and soil moisture (Butterbach-Bahl & Dannenmann, 2011). Similarly, increased soil temperatures and moisture content can influence the sorption and desorption of P, as well as immobilization and mineralization rates, all factors affecting P export (Sheppard & Racz, 1984). It is also well established that sediment transport is affected by soil moisture (Wiggs *et al.*, 2004), by precipitation amount, and by precipitation intensity (Römken *et al.*, 2002).

A fundamental understanding of these coupled processes (hydrology and nutrient cycling) under a changing climate is critical to managing N, P, and sediment export from ecosystems to sensitive coastal zones. Development of effective landscape management strategies to improve water quality requires an understanding of how processes that regulate nutrient/sediment production on the landscape are coupled with hydrologic transport to water bodies. Of particular interest is the impact of climate change on hydrologically active areas of the landscape that

contribute disproportionately to watershed nutrient export (e.g., Critical Source Areas, CSAs), where active hydrologic transport and high nutrient availability coincide (Groffman, Butterbach-Bahl, *et al.*, 2009b). A better understanding of climate change and its potential influence on landscape biogeochemistry can be used to develop new strategies for protecting coastal waters and their contributing watersheds from pollution. For instance, it is entirely possible that climate change would enhance some natural ecosystem services that protect water quality. One example is through a potential change in denitrification, a natural process that transforms dissolved NO_3^- into nitrogen gases, and returns it to the atmosphere. Hydrologically active areas in the landscape prone to soil saturation are recognized as denitrification hotspots (McClain *et al.*, 2003; Vidon *et al.*, 2010) and understanding where these areas are, or will be, can help develop physical models that can predict GHG emissions in the agroecosystems.

Some recent effort has been made to develop physical models that are capable of assessing the impact of climate change on nutrient cycles in agroecosystems. Unfortunately, most existing models are of coarse spatial resolution, such as the Carnegie-Ames-Stanford (CASA) Biosphere model, a coupled ecosystem production and soil carbon-nitrogen model (Potter *et al.*, 1996), or do not model key processes, such as the IPCC N_2O emissions methodology (Nevison, 2000), or are empirically based models (Beheydt *et al.*, 2007) and thus difficult to use to develop mitigation or adaptation measures. If we can correctly model key processes at a fine spatial resolution (e.g., field level), we can attempt to develop mitigation and adaptation strategies that reduce the impact of climate change. Thus, there is a need to build and test new models of key hydrologic and nutrient cycling processes that enable the modeling of climate change impacts.

Greenhouse Gas (GHG) Emissions

Greenhouse gases are comprised of four compounds, CO_2 , N_2O , CH_4 , CFCs, ozone, and water vapor. These gases are known by their ability to absorb infrared radiation, warm the atmosphere, and increase the flux of infrared radiation to the earth's surface, increasing the surface temperature. Since the industrial revolution and the advent of industrial agriculture, the concentration of GHGs in the atmosphere has steadily increased (Meinshausen *et al.*, 2011). For instance, the atmospheric concentration of N_2O has increased by 46 ppb, or 17% since 1750 and is currently increasing at rate of $0.25\% \text{ yr}^{-1}$, globally (Helgason *et al.*, 2005). Of the GHGs, N_2O

is by far the most potent on a molecule-by-molecule basis, with 310 times the radiative forcing as CO₂ (Beheydt *et al.*, 2008; Jahangir *et al.*, 2013), and is an intermediate product of denitrification (Jahangir *et al.*, 2013), and nitrification (Parton *et al.*, 2001). Denitrification is the microbial process that converts reactive nitrate (NO₃⁻) to N₂O and unreactive di-nitrogen (N₂) while nitrification is the biological oxidation of ammonia (NH₃) or ammonium (NH₄⁺) to nitrite (NO₂⁻) followed by the oxidation of the NO₂⁻ to NO₃⁻.

Emissions of N₂O occur both naturally and as a result of human activities. Naturally, N₂O is produced during the circulation of nitrogen among the atmosphere, plants, animals, and microorganisms that live in soil and water (Seitzinger *et al.*, 2000), within the atmosphere (e.g., lightning, heterogeneous reaction) (Thomson *et al.*, 2012). Human activities produce N₂O during agricultural activities, transportation, and industry, including fossil fuel burning, biomass burning, sewage disposal, aquifer contamination, and land-use change (Khalil & Rasmussen, 1992). N₂O is also emitted from grazing animals on managed pastures and rangelands from both urine and manure (Oenema *et al.*, 1997). Among these sources, agricultural soil is the main contributor of N₂O to the atmosphere, emitting 70% of total emissions (Mosier, 1994). The N₂O emissions from agricultural soil result from N fertilizer applications, atmospheric deposition of N, crop residue breakdown, and biologically fixed N (Mosier, 1994).

The soil and environmental factors such as anaerobic soil conditions expressed as soil moisture, N and carbon (C) content in the soil, soil temperature, soil pH, and the presence of denitrifying microorganisms in soil (Knowles, 1982; Parton *et al.*, 1996) are controlling factors of N₂O emission in agricultural soils. These soil and environmental factors vary in space and time, and interact with each other in complicated ways (Henault *et al.*, 2000). Consequently, N₂O emissions vary spatially across a landscape (Folorunso & Rolston, 1984; Folorunso & Rolston, 1985) and temporally over the course of a year depending on the above-mentioned soil and environmental factors (Groffman, Butterbach-Bahl, *et al.*, 2009a; Parkin, 2008). High soil moisture (indicative of anaerobic conditions), high soil temperature, a low rate of oxygen diffusion, and the presence of organic C favors N₂O production during denitrification (Luo *et al.*, 1999), whereas low soil moisture (aerobic conditions), low soil ammonium concentrations, low soil temperature, and high soil pH favors N₂O production during nitrification (Parton *et al.*,

2001). Elevated N₂O emissions have also been observed in response to rainfall, fertilizer events and freeze-thaw cycles (Baggs *et al.*, 2003; Parkin, 2008).

Different techniques have been used to quantify denitrification and N₂O emissions both in terrestrial and aquatic environment: direct measurement, statistical methods or models. Most commonly used direct measurements include: micrometeorological techniques and automated chambers (Parkin, 2008; Smith *et al.*, 1994); ¹⁵N labelling and acetylene inhibition methods (Tiedje *et al.*, 1989); and N₂:Ar ratio quantification, mass balance approaches, stoichiometric approaches, and methods based on stable isotopes (Groffman *et al.*, 2006). Simple regression equations have been also used to relate N₂O emissions with soil and environmental factors (Hoben *et al.*, 2011). Since direct measurement of N₂O emission is costly, time expensive, and laborious (Groffman *et al.*, 2006), simulation models are commonly used to quantify N₂O emissions. Identifying when, where, and how these factors interact to form hotspots of N₂O emissions is a current area of research and a daunting challenge, particularly when scaling from the field to watershed or river basin scales. Thus, models capable of incorporating the relevant controls can be used to quantify N₂O emissions at watershed or field scales (Bruland *et al.*, 2006; Clement *et al.*, 2002; Mosier *et al.*, 2002), and direct management practices to reduce N₂O emissions.

Numerous models have been proposed and developed to predict N₂O emissions during nitrification and denitrification; most, however, were developed to function in more natural systems where the N and C ratios are more closely aligned. Indeed, very few models exist for agroecosystems. These models widely vary in their conceptual design and structure, with some empirically based and some process based, some are plot level models while others are continental scale. Due to the complex nature of N₂O emissions and the limited understanding of the main processes that control it, many models rely on empirical relationships with exogenous factors like temperature and soil C to ‘predict’ emissions (Butterbach-Bahl *et al.*, 2011). Most of these models have historically focused on forested or natural systems [e.g., ECOSYS (Metivier *et al.*, 2009), GLEAMS (Leonard *et al.*, 1987), DAYCENT (Del Grosso *et al.*, 2002; Parton *et al.*, 1998) and DAISY (Hansen *et al.*, 1991)]. Generally, N₂O emission models can be classified based on their application (Shaffer, 2002): (1) relatively simple index or screening type models, (e.g., IPCC Tier 2 model), (2) empirically based models, and (3) process-based models.

Empirical models do not consider microbial processes or soil physics (gas diffusion) but rather the models depend on easily measurable parameters, such as soil moisture, soil pH, temperature, soil nutrients such as NO_3^- , and labile C availability in the soil, and then use regression equations to relate them to N_2O emissions (Heinen, 2006; Parton *et al.*, 1996). These models include WNMM (Li *et al.*, 2007), NLEAP (Shaffer *et al.*, 1991), EPIC (Sharpley & Williams, 1990), DLEM (Tian *et al.*, 2015), EXPERT-N (Priesack *et al.*, 2001), and NEMIS (Henault *et al.*, 2000). While these models are capable of predicting N_2O emissions under relatively controlled and known conditions, these models should not be applied outside of the range of conditions for which they were developed.

Most of the recent advances in N_2O emission models have been made in the 3rd class of models, process based models, which can be classified into three model types (Parton *et al.*, 1996): (1) microbial growth models, (2) soil structure models, and (3) physically based models.

Microbial growth models simulate N_2O emissions by representing the dynamics of microbes that are responsible for nitrification and denitrification processes (Heinen, 2006; Parton *et al.*, 1996). Examples of such models include DENLEFWAT (Leffelaar, 1988; Leffelaar & Wessel, 1988); DNDC (Frolking *et al.*, 1992; Li *et al.*, 1997), NLOSS (Riley & Matson, 2000); ECOSYS (Grant, 1991), and RZWQM (Ma *et al.*, 2001). Factors that affect the microbial growth rate in these models are the soil N and C content, soil temperature, soil pH, and soil moisture content. Microbial growth rates are assumed to be an estimate of the N_2O emission potential of a system; that is, higher microbial growth rates translate to higher N_2O emissions (they are an estimate of the system potential), which may or may not be the case in reality. The strength of these models is the representation of microbial growth and activity. This includes the number and type of microbes, the community structure and the death and growth of microbes over time. The models can be applied at field to regional scales. The weakness of these models is that environmental factors, particularly soil organic matter, are not characterized. Thus, it would be difficult to use such models to assess the impact of something like climate change. These models are good for assessing the upper bound N_2O emissions from a system, but may over estimate N_2O emissions when conditions approach boundary conditions.

Soil structural models are based on soil physics and primarily consider the diffusion of gases and solutes in soil aggregates and use it as a proxy for anaerobic state, a primary control on N₂O emissions (Heinen, 2006; Parton *et al.*, 1996). N₂O and nutrients such as NO₃⁻ and oxygen (O₂) are modeled moving into and out of soil aggregates. Soil structural models include: the Steady State Denitrification model (Arah & Smith, 1989a), which predicts steady state denitrification rates as a function of soil moisture characteristics, aggregate soil particle size, oxygen reduction potential and nitrate concentration; the SLIM solute leaching model (Vinten *et al.*, 1996), which simulates N₂O emissions by considering the interaction between soil aggregates, soil moisture and O₂ diffusion; and methods described by Grant (1991), which uses a Michaelis-Menten function of rate versus nitrate concentration. The strength of soil structural models is that the anaerobic and aerobic condition of soil can be determined, resulting in the identification of denitrification and nitrification stages and hotspots in a soil. These models are well suited to assessing fine-scale N₂O emissions (pore to plot scale), but require well-defined input data or calibration. Finally, soil structural models are only applicable for steady-state conditions.

The third type of process-based models of N₂O emissions are physically based models. These models attempt to incorporate the relevant physical controls on N₂O emissions by simulating interactions between soil factors and environmental factors, such as in the GLEAMS model (Leonard *et al.*, 1987), or use the denitrification potential as estimated by the interaction between the plant, soil and atmospheric environments to estimate N₂O emissions, such as in the DAYCENT (Del Grosso *et al.*, 2002; Parton *et al.*, 1998) and DAISY models (Hansen *et al.*, 1991). Physically based models incorporate soil parameters such as soil pH, soil temperature, moisture, and nutrients as driving forces controlling microbial growth and activity. Soil moisture is considered as proxy for O₂ diffusion; i.e., when the soil is saturated, O₂ diffusion in soil is limited and anaerobic condition will be created, which accelerates the denitrification process. Physically based models can be applied at fine or large scales with time steps of hourly to yearly and hot spots and hot moments on the landscape can be determined using these models. One weakness of these models is that they are not capable of modeling the response of the microbial community to external factors. The models also use different parameters to calculate the reduction functions of environmental factors such as soil pH, temperature, soil moisture and nutrients, and hence the model output is highly dependent on the accuracy of the input data. These models are generally considered the most robust and can be used outside of the range for

which they were developed, unlike empirical models. This makes them ideally suited for various scenario analyses, such as assessing the impact of climate or land use change.

Changes in temperature and precipitation are likely to affect denitrification rates and emissions of N₂O in agroecosystems (Butterbach-Bahl *et al.*, 2011), as well as the microorganisms responsible for denitrification (Singh *et al.*, 2010). Reliable prediction of climate change impacts on N cycling requires better understanding of the linkage between the controlling factors of N₂O emission and climate change. A better understanding of climate change and its potential impact on landscape biogeochemical processes and pathways can also be used to develop new strategies for protecting coastal waters and their contributing watersheds from pollution. Best management practice (BMPs) are commonly used to reduce the impact of pollutant export from agricultural land (Arabi *et al.*, 2008). Furthermore, nutrient management performed to reduce GHG emissions, precision conservation management and other management alternatives can help us mitigate and/or adapt to climate change (Lal *et al.*, 2011).

Agricultural Best Management Practices (BMPs)

Agricultural lands are the primary source of nutrients and sediment in the Chesapeake Bay region and cause numerous problems when they enter water bodies, such as eutrophication (Sharpley *et al.*, 2003), reduced dissolved oxygen, fish kills, loss of biodiversity, and human health threats (Carpenter *et al.*, 1998; Peterjohn & Correll, 1984). Agricultural best management practices (BMPs) are increasingly and widely used to reduce the impact of diffuse pollutant export from agricultural landscapes and improve water quality (Ullrich *et al.*, 2009). BMPs can be structural or management based. Structural BMPs include physical structures, such as manure storage, or altered landscape features, such as stream restoration, while management BMPs involve altering some sort of landscape management practice, such as nutrient management, or conservation tillage. For instance, conservation tillage or no-till, enhances soil organic carbon, soil quality, and soil aggregation, leading to less soil erosion in agricultural landscapes (Roldán *et al.*, 2007). BMPs such as riparian vegetation, strip crop, and buffer strip can all help reduce diffuse pollutants, by reducing inputs to the crop, enhancing sequestration of nutrients in plant tissue, or reducing surface and subsurface losses due to hydrologic pathway alterations (Carpenter *et al.*, 1998). However, it is not clear what impact a changing climate will have on the

function of BMPs. For instance, increased precipitation volume and intensity may overwhelm many BMPs like riparian buffers, but higher temperatures, longer growing seasons, and more rainfall might cause that same buffer to mature more quickly, thus trapping more sediment and sequestering more nutrients. Thus, agricultural conservation practices need to be assessed for performance under a changing climate (Hatfield *et al.*, 2004; Peterjohn *et al.*, 1984).

The Chesapeake Bay is already experiencing the impact of a changing climate (Najjar *et al.*, 2009b), with increasing temperatures reducing winter snowpack and increasing winter runoff, and more frequent high-intensity rainfall events mobilizing more sediment (Hayhoe *et al.*, 2007). The predicted changes to climate in the region include continued increases in temperature, anywhere between 1-5 °C by when?, dependent on emissions scenarios and season, more precipitation in the winter and spring, primarily as rainfall rather than snowfall, and less rainfall in the late summer and fall (Sheffield *et al.*, 2013a). These changes to precipitation and temperature are likely to alter the timing and magnitude of streamflow and nutrient/sediment production and transport in the watershed. For instance, increased spring nutrient export from the watershed and delivery to the estuary can set up conditions that cause particularly acute summer hypoxia (Boesch *et al.*, 2001b), and drier conditions in the summer and fall have been shown to increase the buildup of soil nutrients that can subsequently be flushed from the system when wet conditions return (Kaushal *et al.*, 2008; Wetz *et al.*, 2013). Temperature changes can alter nutrient cycling, plant growth, evapotranspiration, and soil water content, which all impact the availability and transport of nutrients from agricultural fields. Thus, BMPs designed and installed to handle historic weather conditions may not function as well under a changing climate, and new strategies or comprehensive study of the impact of climate change on BMPs is required. However, the design and performance of BMPs to account for climate change heavily depends on model outputs used to analyze different scenarios where there are no observations. These model outputs have considerable uncertainty associated with their predictions due to uncertainty in model input parameters, model process conceptualization, and computational methodology (Cressie *et al.*, 2009). Thus, efforts to address uncertainty are a critical next step for watershed modeling in the face of a changing environment.

Structural Model Uncertainty

Ecosystems operate under dynamic and complex physical, chemical, and biological interactions. The complexity of the interactions leads to difficulties in conceptualizing the processes mathematically, which in turn makes accurately modeling these systems challenging (Cressie *et al.*, 2009). Although complex and sophisticated physical models have been built to approximate real-world processes and to assist in effective decision-making, quantifying structural uncertainties in model process conceptualization, initial conditions, and input data remain challenging. Most previous research into model uncertainty has focused on model parameter or input data uncertainty (Renard *et al.*, 2010), and less on structural model uncertainty (e.g., the functional form of the model or whether the processes are correctly represented). Thus, structural model uncertainty can occur even if the true input values for all model parameters are known. Sources of structural model uncertainty include exclusion of important controlling variables, processes either missing or incorrectly represented, and improperly defined boundary conditions (Ascough *et al.*, 2008). All these uncertainties propagate to total model prediction uncertainty (Shen *et al.*, 2015; Vrugt *et al.*, 2005). Thus, quantifying uncertainties associated with watershed models cannot be neglected and should be explicitly considered to obtain credible model outputs with associated prediction uncertainty bounds to make effective management decisions.

Numerous approaches have been proposed to quantify uncertainties in watershed models including Bayesian Model Averaging (Raftery *et al.*, 1997; Vrugt *et al.*, 2008), Generalized Likelihood Uncertainty Estimation (GLUE) (Blasone *et al.*, 2008; Vrugt *et al.*, 2005), multiple objective function criteria (Blasone *et al.*, 2008), sequential data assimilation (Moradkhani *et al.*, 2005), Bayesian Recursive Estimation (Thiemann *et al.*, 2001), and the Ensemble Kalman Filter? (Abaza *et al.*, 2014). However, only a few methods such as multi-model ensembles (MME) (Duan *et al.*, 2007; Stoica *et al.*, 2004), are proposed for quantifying structural model uncertainties. This is due to the complexity and difficulty of separating structural uncertainties from model parameter or input data uncertainty (Zhang *et al.*, 2011). Sharifi *et al.* (2017) evaluated the performance of different watershed models to assess water quality impacts on Queenstown drainage. Stow *et al.* (2009) demonstrate improved performance in estimating hypoxia in the Chesapeake Bay using a hierarchical Bayesian ensemble approach, but the study is limited to processes within the Bay and does not describe upland watershed processes. Boomer

et al. (2013) and Exbrayat et al. (2010) also suggested use of multi-model ensembles. However, research describing ensembles used to quantify structural uncertainty in watershed models is lacking, and no consensus on application of methods or evaluation guidelines has been reached.

Multi-model ensembles combine two or more models in an effort to improve model prediction and objectively evaluate model uncertainty (Boomer *et al.*, 2013). Multi-model ensembles utilize the diversity of skillful predictions from different models and improve the estimation of structural uncertainties associated with model outputs (Duan *et al.*, 2007). Multi-model ensemble methods are commonly used in weather forecasting (Krishnamurti *et al.*, 2000) and climate change analysis (Christensen & Lettenmaier, 2006). For instance, climate forecasters used a multi-model approach to include the weaknesses and strengths of each model in the forecast (Wiley *et al.*, 2010). Flood forecasters also employ multi-model approaches to exploit the diversity of skillful predictions from different models (Cloke & Pappenberger, 2009; Duan *et al.*, 2007). There are different ways to implement multi-model approaches. Ensembles can be used to sample uncertainty in forcing assumptions, initial conditions, process conceptualization, input data, and training/calibration data. Generally, multi-model ensembles use multiple models to simulate responses to identical driving forces (e.g., climate inputs). Model projections are aggregated and compared to estimate uncertainty in system responses. For example, a multi-model ensemble could be used to evaluate management practices needed to achieve a water quality standard. Multiple solutions would be obtained from several models and then be aggregated to obtain an estimated mean nutrient reduction achieved and the probability that the target will achieve the desired water quality improvements. Average model projections have been found to reproduce historical observations more accurately than individual models in a number of fields (Najafi *et al.*, 2011; Reichler & Kim, 2008), and historically the variability in model projections has been used as a measure of uncertainty. Under these assumptions, solutions that generate smaller uncertainty ranges theoretically represent more conservative management approaches.

Little research has been carried out to quantify structural uncertainties of watershed models using the multi-model approach (Duan *et al.*, 2007), and the application and analysis of ensemble methods remains a challenge in this field. Raftery *et al.* (2005) proposed Bayesian model averaging (BMA) post-processing methods to ensemble weather prediction models; however, the

method requires accurate estimates of the weights and variances of the individual competing models in the ensemble (Vrugt et al., 2008) additionally the proposed algorithm cannot be guaranteed to arrive at a global optimum (Vrugt et al., 2006). The BMA approach requires accurate estimation of the weights and variances of each model and then averages over all possible models (Vrugt et al., 2008). In the BMA approach, model averaging is performed by obtaining a prediction for each model and then averaging the estimates using a weighting factor based on how likely each model predicts the observed data (Wasserman, 2000). The BMA approach sometimes underperformed compared to simple unweighted averages because the process does not consider two equally performing variables with the same weights. For instance, if two predictors perform equally well (i.e., have the same weights), BMA selects only one predictor (Graefe et al., 2015). The Ensemble Kalman Filter approach assumes all probability distributions are Gaussian in shape, which is suitable for large state variables, but problematic for constituents that are described by non-Gaussian distributions (Evensen, 2003; Mandel, 2009), such as sediment. Thus, new approaches are required that integrate different probability distributions and explicitly incorporate prior knowledge about parameter distributions to improve prediction skill.

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CHAPTER 2

DEVELOPMENT OF A NITROUS OXIDE ROUTINE FOR THE SWAT MODEL TO ASSESS GREENHOUSE GAS EMISSIONS FROM AGROECOSYSTEMS

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Abstract

Greenhouse gas emissions from agroecosystems, particularly nitrous oxide (N₂O), are an increasing concern. To quantify N₂O emissions from agroecosystems, a new physically based routine was developed for the Soil and Water Assessment Tool (SWAT) model during denitrification and an existing nitrification routine was modified. The new routines predict N₂O emissions by coupling the carbon (C), and nitrogen (N) cycles with soil moisture, temperature, and pH. The model uses reduction functions to predict total denitrification (N₂ + N₂O) and partitions N₂ from N₂O using a ratio method. The modified SWAT nitrification routine predicts N₂O emissions using reduction functions. The new routine was tested using GRACEnet data at University Park, Pennsylvania, and West Lafayette, Indiana. Results showed strong correlations between measurements of N₂O flux and model predictions for both sites and suggest that N₂O emissions are particularly sensitive to soil pH and soil N, and moderately sensitive to soil temperature, moisture and total soil C.

Software Availability

Model name: SWAT-GHG model. Developed by M. Berbero (bwmoges4@vt.edu) and Z.M. Easton (zeaston@vt.edu), Department of Biological Systems Engineering, Virginia Tech, Blacksburg, VA 24060. Year available: 2016. Availability: Contact developers. Cost: Free and open source. Language: FORTRAN.

Introduction

Greenhouse gas (GHG) emissions from agroecosystems, particularly nitrous oxide (N_2O), are of increasing importance and a major contributor to global climate change. N_2O is a potent GHG, with 310 times the radiative forcing as CO_2 on a molecule-by-molecule basis (Beheydt *et al.*, 2008; Jahangir *et al.*, 2013) and is an intermediate product of denitrification (Jahangir *et al.*, 2013) and nitrification (Parton *et al.*, 2001). Denitrification is the microbial process that converts reactive nitrate (NO_3^-) to N_2O and unreactive dinitrogen (N_2), and is favored by anaerobic soil conditions, adequate soil NO_3^- and carbon (C) content, moderate to high soil temperature, neutral to basic soil pH, and the presence of denitrifying microorganisms (Knowles, 1982; Parton *et al.*, 1996). Nitrification is a microbial process that transforms ammonium (NH_4^+) to NO_3^- and occurs under aerobic soil conditions in the presence of adequate NH_4^+ , high soil temperature, and high pH. These factors vary in space and time in agroecosystems and interact with each other in complicated ways (Henault *et al.*, 2000). Consequently, N_2O emissions vary spatially across a landscape and temporarily over the course of a year (Groffman, Butterbach-Bahl, *et al.*, 2009a). Identifying when, where, and how these factors interact to form hotspots and hot moments of N_2O emissions (e.g., areas or times of large emissions) is a current area of research and a daunting challenge. Thus, there is a need to develop integrated models capable of incorporating these relevant controls to predict N_2O emissions across a range of scales to better inform the selection of landscape management practices to reduce N_2O emissions (Bruland *et al.*, 2006; Clement *et al.*, 2002; Mosier *et al.*, 2002).

Numerous system dynamics models (Kelly *et al.*, 2013) have been developed to predict N_2O emissions. Most, however, were developed for more natural systems in the absence of anthropogenic N application, where the N and C cycles are more closely coupled and N is often limiting. Consequently, the need for new models that capture N_2O emissions in landscapes with an abundance of bioavailable N is driven by the inability of models developed for natural systems, without N enrichment, to capture N_2O emissions when the N and C cycles are decoupled as a result of this enrichment. Existing models widely vary in their concept and structure, with some empirically-based and some process-based, and range in scale from plot to global. Generally, N_2O emission models can be classified based on their application (Shaffer, 2002): (1) relatively simple index or screening type models, (e.g. Intergovernmental Panel on

Climate Change (IPPC) Tier 2 model), (2) empirically-based models, and (3) process-based models.

Empirical models rely on easily measurable parameters (e.g., soil moisture/temperature, pH, and soil nutrients) and then use regression equations to relate them to N₂O emissions (Heinen, 2006; Parton *et al.*, 1996). Empirical models include WNMM (Li *et al.*, 2007), NLEAP (Shaffer *et al.*, 1991), EPIC (Williams, 1990), DLEM (Tian *et al.*, 2015), EXPERT-N (Priesack *et al.*, 2001), and NEMIS (Henault *et al.*, 2000). While these models are capable of predicting N₂O emissions under relatively controlled and known conditions, these models can be challenging to apply outside of the range of conditions for which they were developed and thus have limited utility to drive landscape management or predict the effects of processes such as climate change.

Most of the recent advances in N₂O emission models have been made in process-based modeling, which can generally be classified in to three model types (Parton *et al.*, 1996): (1) microbial growth models, (2) soil structure models, and (3) physically-based models.

Microbial growth models simulate N₂O emissions by representing the dynamics of the microbial community (Heinen, 2006; Parton *et al.*, 1996). Examples of such models include the DENLEFWAT model (Leffelaar, 1988; Leffelaar *et al.*, 1988), DNDC model (Frolking *et al.*, 1992; Li *et al.*, 1997), NLOSS model (Riley *et al.*, 2000), ECOSYS model (Metivier *et al.*, 2009), and the RZWQM model (Shaffer *et al.*, 2001). Factors that affect the microbial growth rate in these models are the soil N and C content, soil temperature, soil pH and soil moisture content. Microbial growth rates are assumed to be an estimate of the N₂O emission potential of a system that is higher microbial growth rates translate to higher N₂O emissions. The strength of these models is the representation of microbial growth and activity in the model. This includes the number and type of microbes, the community structure and the death and growth of microbes over time.

Soil structural models are based on soil physics and primarily consider the diffusion of gases and solutes into and out of soil aggregates; these models use diffusion of gases and solutes as a proxy for the anaerobic state, a primary control on N₂O emissions (Heinen, 2006; Parton *et al.*, 1996). N₂O and nutrients such as NO₃⁻ and oxygen (O₂) are modeled moving into and out of soil aggregates. Soil structural models include: the Steady State Denitrification model (Arah &

Smith, 1989b), which predicts steady state denitrification rates as a function of soil moisture characteristics, aggregate soil particle size, oxygen reduction potential, and NO_3^- concentration; the SLIM solute leaching model (Vinten *et al.*, 1996), which simulates N_2O emissions by considering the interaction between soil aggregates, soil moisture and O_2 diffusion; and methods described by Grant (1991), which uses a Michaelis-Menten function to predict emissions based on the soil NO_3^- concentration. The strength of soil structural models is that the anaerobic and aerobic condition of soil can be determined, resulting in the identification of denitrification and nitrification stages and hotspots in a soil. These models are well suited to assessing fine scale N_2O emissions (pore to plot scale), but require well-defined input data and/or calibration.

Physically-based, or integrated models, incorporate the relevant physical controls on N_2O emissions by simulating interactions between plant, soil, hydrologic, management, and atmospheric factors to estimate N_2O emissions. Kragt *et al.* (2011) and Kelly *et al.* (2013) suggest that integrated modeling (or integrated models) improve information transfer and decision-making by providing the ability to capture complex biological, chemical, and physical processes. Several of these integrated models exist, for example the DAYCENT (Del Grosso *et al.*, 2002; Parton *et al.*, 1998), DAISY (Hansen *et al.*, 1991) and RZWQM2 models (Fang *et al.*, 2015). These models incorporate soil parameters such as soil pH, soil temperature, soil moisture, and nutrients as driving forces controlling emissions. These models can be applied at fine or large scales with time steps of hourly to yearly and hotspots/hot moments on the landscape can be determined using these models. This class of models is generally considered the most robust and can be used outside of the range for which they were developed, unlike empirical models. This makes them ideally suited for various scenario analyses, such as assessing the impact of climate or land use change. Unfortunately, these models also require large amounts of data, some of which can be difficult to find.

In order to provide the ability to predict N_2O emissions, we developed a new physically-based routine for the Soil and Water Assessment Tool model (SWAT), hereafter referred to as SWAT-GHG. Semi-distributed, process-based models such as SWAT offer a promising platform on which to build GHG emission models because of detailed plant/crop and nutrient routines, relatively flexible hydrologic underpinnings and open source code. Indeed, recent coupling of SWAT with the biogeochemical model DAYCENT highlights the flexibility of SWAT (Wu *et*

al., 2016). In addition, most of the parameters required to predict N₂O emissions already exist in SWAT (total soil C and N, pH, temperature and precipitation), and SWAT has built in databases for plant and soil factors, so general model initialization requires very little additional data. The development of SWAT-GHG involved a two-part addition to SWAT: first, a set of reduction functions was developed to model the total denitrification (N₂+ N₂O) and nitrification rates and second, a ratio method was applied to partition denitrification products N₂ and N₂O. The new N₂O routine was tested using plot data from the GRACEnet database in two locations: University Park, Pennsylvania, and West Lafayette, Indiana. A sensitivity analysis of total soil C and pH, N application, and climate forcing (temperature and precipitation) was performed to assess the sensitivity of the model to changes in input parameter values. We compared the predicted spatial distribution of N₂O emission at the two sites with the field level measurements to assess the ability of SWAT-GHG to elucidate where and when hotspots of N₂O production occur across agroecosystems.

Materials and Methods

Model Development: Here we describe the development of a new sub-model for SWAT, termed SWAT-GHG, to predict N₂O emissions from agroecosystems. SWAT-GHG was developed by defining a set of reduction functions based on soil and environmental factors. The soil conditions include nutrient content (NO₃⁻, NH₄⁺ and total soil C) and soil pH, while the environmental factors (precipitation and temperature) control the soil temperature and soil moisture conditions (Heinen, 2006; Morse *et al.*, 2012; Weier *et al.*, 1993). The reduction functions are based on work from Weier *et al.* (1993) and Parton *et al.* (2001) with adjustments made for the impact of soil pH and soil temperature.

SWAT Model Description: The SWAT model is a process-based, semi-distributed watershed model developed to predict the impact of land management on water availability and water quality (Arnold *et al.*, 1998). SWAT requires weather, soil, land cover, and land management data to simulate surface and subsurface hydrology and various chemical, nutrient and sediment fluxes. SWAT-VSA re-conceptualizes SWAT to account for areas of the landscape subject to variable saturation dynamics (Easton *et al.*, 2008). In SWTA-VSA the area of each hydrologic response unit (HRU) is defined by the coincidence of land use and wetness index class

determined from a Topographic Index (TI) to differentiate areas of the landscape with respect to their moisture storage and saturation index (Easton *et al.*, 2008). SWAT-VSA has been shown to provide better predictions of soil moisture and runoff generation than the standard SWAT model in watersheds with similar physical characteristics and climate to the study watersheds (Easton *et al.*, 2008), and thus should provide a better platform to predict the spatial and temporal evolution of N₂O emission hotspots.

SWAT was selected as the model to build on for several reasons: it is well documented, it is supported and available as open-source code, it has robust crop/plant simulation abilities, it contains numerous potential code linkage points, and recent improvements capture the spatial and temporal evolution of saturated areas of the landscape, which are known N₂O emission hotspots (Groffman *et al.*, 2009). Denitrification and nitrification processes are currently modeled in SWAT with first order reaction constants (e.g., denitrification only occurs above a threshold soil moisture content input by the user), but SWAT does not model N₂O emissions from either process, predicting N₂ as the only denitrification product. We incorporated the ability to predict N₂O emissions by coupling the C and N cycles with soil moisture, pH, and soil temperature by developing a denitrification subroutine “ndent_V2.f” and by modifying the existing nitrification and volatilization subroutine “nitvol.f” in SWAT. All of the parameters required to develop the routines [soil temperature, pH, and nutrient content (NH₄⁺, NO₃⁻, C)] are already incorporated in SWAT in various subroutines. Both subroutines predict N₂O emission at the hydrologic HRU level (the smallest unit at which the model provides output and represents a unique combination land use and moisture index).

N₂O from denitrification was obtained by a two-part addition: (1) developing a set of equations to model the total denitrification rate (N₂+ N₂O) and (2) partitioning N₂ from N₂O. N₂O from nitrification was obtained by modifying the existing nitrification rate equation in SWAT and partitioning N₂O from NO₃.

The total denitrification flux from Parton *et al.* (1996) and Mosier *et al.* (2002) is:

$$D_{N_{total}} = \min[Fd(NO_3), Fd(C)] * Fd(\theta) * Fd(T) * Fd(pH) \quad (1)$$

where D_{Ntotal} is the denitrification rate per unit area (production of $N_2 + N_2O$, $g\ N\ ha^{-1}\ d^{-1}$); $Fd(NO_3)$ is the maximum total N gas flux per unit area for a given soil NO_3^- level in $g\ N\ ha^{-1}\ d^{-1}$ (assuming total soil C is not limiting); $Fd(C)$ is the maximum total N gas flux per unit area for a given total soil C level in $g\ N\ ha^{-1}\ d^{-1}$ (assuming soil N is not limiting); and $Fd(\theta)$, $Fd(T)$, and $Fd(pH)$ are functions that represent the effects of soil moisture, soil temperature, and pH on N gas flux, respectively. While the functional form of these relationships can differ to some extent, Parton *et al.* (1996) and Weier *et al.* (1993) have developed relatively robust functions for estimating $Fd(NO_3)$, $Fd(C)$, and $Fd(\theta)$:

$$Fd(NO_3) = 11,000 + \frac{40,000 + \text{atan}(\pi * 0.002 * (NO_3 - 180))}{\pi} \quad (2)$$

$$Fd(C) = \frac{24,000}{1 + \frac{200}{e^{0.35 * C}}} - 100 \quad (3)$$

$$Fd(\theta) = \frac{a}{b * \theta^{(d * \theta)}} \quad (4)$$

where $Fd(NO_3)$ and $Fd(C)$ have units of $g\ N\ ha^{-1}\ d^{-1}$, θ is water-filled pore space in units of $m^3\ m^{-3}$, C is the C content in $g\ N\ ha^{-1}\ d^{-1}$, and a, b, c and d are soil-specific fitting parameters (Table 2-1) to incorporate the effect of soil texture.

Table 2-1: Soil texture fitting parameters for denitrification rate model (Parton *et al.*, 1996).

Texture	a	b	c	d
Sand	1.56	12	16	2.01
Loam	4.82	14	16	1.39
Clay	60	18	22	1.06

The soil temperature effect function, $Fd(T)$, was derived from Seligman and Keulen (1981):

$$Fd(T) = \text{Max}\left[\left(0.9 * \frac{\text{Soil Temp}}{\text{Soil Temp} + \exp(9.93 - 0.312 * \text{Soil Temp})} + 0.1\right), 0.1\right] \quad (5)$$

The pH function, $Fd(pH)$, was developed from Simek and Cooper (2002):

$$Fd(pH) = \begin{cases} 0.001 & \text{for } pH \leq 3.5 \\ \frac{pH-3.5}{3} & \text{for } 3.5 < pH < 6.5 \\ 1 & \text{for } pH \geq 6.5 \end{cases} \quad (6)$$

We developed a ratio method to differentiate the N_2O from N_2 produced during denitrification:

$$R_{N_2/N_2O} = \min[Fr(NO_3), Fr(C)] * Fr(\theta) * Fr(pH) \quad (7)$$

where R_{N_2/N_2O} is ratio of N_2 to N_2O , and $Fr(NO_3)$, $Fr(C)$, $Fr(\theta)$ and $Fr(pH)$ represent the effects of soil NO_3^- -N, total soil C, soil moisture, and pH on the ratio of N_2 to N_2O , respectively. Note here that temperature is not included in the ratio prediction as increasing temperature increases both N_2 and N_2O production similarly (Parton *et al.* (1996). Again, functions from Parton *et al.* (1996) are adapted for $Fr(NO_3)$, $Fr(C)$, and $Fr(\theta)$, while $Fr(pH)$ was modified from Dannenmann *et al.* (2008) and Rochester (2003).

$$Fr(NO_3) = 1 - \left[0.5 + \frac{1 * \tan(\pi * 0.01 * (NO_3 - 190))}{\pi} \right] * 25 \quad (8)$$

$$Fr(C) = 13 + \frac{30.78 * \tan(\pi * 0.07 * (C - 13))}{\pi} \quad (9)$$

$$Fr(\theta) = \frac{14}{13^{13 \frac{17}{(2.2 * \theta)}}} \quad (10)$$

$$Fr(pH) = \frac{1}{1470 * e^{-11 * pH}} \quad (11)$$

Total N_2O production during denitrification is given by:

$$DN_{2O} = \frac{Dt}{1 + R_{N_2/N_2O}} \quad (12)$$

where DN_{2O} is total N_2O flux per unit area in $g\ N\ ha^{-1}\ d^{-1}$.

N_2O emissions from nitrification were obtained by modifying the existing nitrification routine in SWAT and developing a set of equations for partitioning N_2O from NO_3^- . To calculate the total N_2O flux from nitrification an equation from (Parton *et al.*, 1998; Parton *et al.*, 2001) is used:

$$F_{N_2O} = F_{NO_3} * K_2 * F_{\theta} * F_{Temp} * F_{pH} \quad (13)$$

Where F_{N_2O} is N₂O flux from nitrification (g N ha⁻¹ d⁻¹), K₂ is the fraction of nitrified N lost as N₂O (K₂=0.02). F_{NO_3} is the rate of nitrification, F_{θ} is the effect of soil water on nitrification, F_{Temp} is the effect of temperature, and F_{pH} is the effect of soil pH. Both F_{NO_3} and F_{θ} are taken directly from SWAT.

The F_{NO_3} factor is given by:

$$F_{NO_3} = \frac{f_{nit}}{f_{nit} + f_{vol}} * N_{nitvol} \quad (14)$$

Where f_{nit} is the fraction of N lost to nitrification, f_{vol} is the fraction of N lost to volatilization and N_{nitvol} (g N ha⁻¹ d⁻¹) is the amount of ammonium converted via nitrification and volatilization.

The F_{θ} factor is given by:

$$F_{\theta} = \frac{SW_{ly} - WP_{ly}}{0.25 * (FC_{ly} - WP_{ly})} \quad \text{if } SW_{ly} < 0.25 * FC_{ly} - 0.75 * WP_{ly} \quad (15)$$

$$F_{\theta} = 1.0 \quad \text{if } SW_{ly} \geq 0.25 * FC_{ly} - 0.75 * WP_{ly} \quad (16)$$

Where SW_{ly} is soil water content (mm), WP_{ly} is the amount of water held in the soil at wilting point water content (mm), and FC_{ly} is amount of water held in the soil layer at field capacity water content (mm).

The F_{Temp} factor is given by:

$$F_{Temp} = -0.06 + 0.13 * e^{(0.07 * SoilTemp)} \quad (17)$$

The F_{pH} factor is given by:

$$F_{pH} = 0.56 + \frac{\arctan(\pi * 0.45 * (-5 + soil\ pH))}{\pi} \quad (18)$$

The total N₂O production from both denitrification and nitrification is given by:

$$N_2O_{Total} = D_{N_2O} + F_{N_2O} \quad (19)$$

where N_2O_{Total} is total N_2O flux in $g\ ha^{-1}\ d^{-1}$.

Linking SWAT-GHG with SWAT Parameters: All of the variables described above are already defined in SWAT and used in various other subroutines except for θ . θ is calculated from the soil moisture characteristics for each soil layer as the fraction of pore space occupied by water. Soil pH is included but is inactive in SWAT code and is a user-defined input. Thus, for model development we used a constant soil pH over the user defined run time (note, however, that pH can be varied by the user during different model runs). In order to incorporate the impact of total soil C on N_2O emissions, the new N_2O routine utilizes one of two existing C routines in SWAT. In the basins.bsn file in SWAT, users can select the original routine from SWAT (nminrl.f) or a modified C routine (C-Farm) developed by Kremanian et al. (2010). Note, the application that follows utilized the C-Farm routine.

Study Area: SWAT-GHG was tested using plot level data from agricultural watersheds in West Lafayette, Indiana (Fig.2-1a), and University Park, Pennsylvania (Fig.2-1b). The watersheds have an area of $0.4\ km^2$ (Fig.2-1a) and $0.6\ km^2$ (Fig.2-1b), respectively. The crop types in University Park consist of corn, soybean, pasture and alfalfa, and West Lafayette crops consist of corn, soybean, sorghum and switchgrass. The soil type of the West Lafayette watershed is a loam, and the University Park watershed soil is a sandy clay loam.

Model Testing: SWAT-GHG was tested using data from the GRACEnet database (<http://nrrc.ars.usda.gov/arsdataportal/> - /Home) at two locations: (1) University Park, Pennsylvania, and (2) West Lafayette, Indiana. SWAT-VSA (SWAT-Variable Source Area, Easton et al., 2008) was used for model testing. SWAT-VSA was initialized for both locations based on field level input data from the GRACEnet database to force the model where available. SWAT-VSA provided the soil moisture and temperature time series for the new routine, and all other inputs were taken from the GRACEnet database if available (soil properties) or left as default if unavailable (pH). In order to better understand which parameters had the largest effect on N_2O emissions we conducted a sensitivity analysis on N application rate, total soil C, pH, θ and soil temperature.

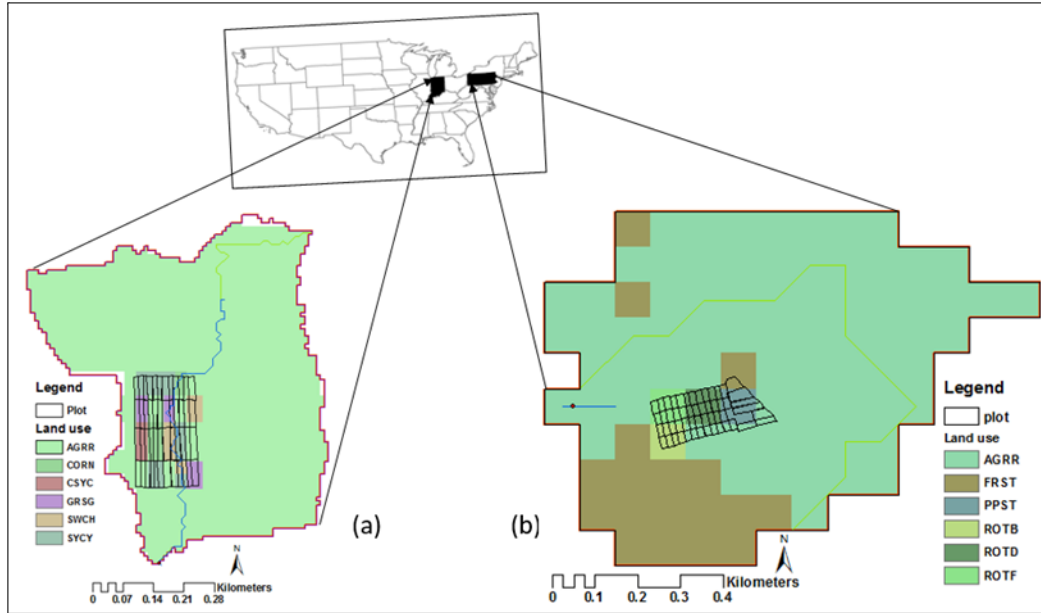


Figure 2-1: (a) West Lafayette, IN, watershed and GRACEnet site with land uses AGRR (Agriculture); Corn; CSYC (Corn-Soybean-Corn crop rotation); GRSG (Sorghum); SWCH (Switchgrass); SYCY (Soybean-Corn-Soybean crop rotation) and (b) University Park, PA, watershed and GRACEnet site with land uses AGRR (Agriculture); FRST (Forest); PPST (Pasture); ROTB (Soybean rotation); ROTD (Alfalfa rotation); ROTF (Corn rotation).

Model Initialization: SWAT-VSA was initialized for University Park and West Lafayette sites using ArcSWAT 2012 and TopoSWAT (available from <http://ww2.bse.vt.edu/eastonlab/>). TopoSWAT automates the SWAT-VSA initialization process by assimilating soil data, creating the TI map, overlaying the soil and TI maps, and developing the required database for model initialization (Fuka et al., 2016). Soils data included in TopoSWAT is based on Food and Agriculture Organization (FAO) soils database (FAO 2007). The FAO soils were used as the base map and parameters (total soil C and N, soil texture) were adjusted using data provided in the GRACEnet database for each site. The land use input for both watersheds was obtained by first digitizing plot level land use based on the crop rotation of plots in the GRACEnet database. Digitized plot level land use data was then cross-referenced with data from the National Land Cover database (NLCD 2011). The use of the NLDC was required because GRACEnet did not have all of the SWAT required soil, management, or plant growth and development parameters needed to run the model. A digital elevation model (DEM) with 10m resolution from the United

States Geologic Survey (USGS) National Elevation Dataset (NED) (Guenther & Maune, 2007) was used for both locations. The final initialization resulted in one subbasin with 58 HRUs for West Lafayette and one subbasin with 21 HRUs for University Park. Weather data from the GRACEnet database, including daily precipitation and temperature (min and max) from 2004 to 2013, was used to force the model. Soil properties such as organic C content (%), soil NO₃⁻ content (mg kg⁻¹) and a default pH value of 6.5 from the FAO database were used to initialize both models.

GRACEnet Database: GRACEnet (Greenhouse gas Reduction through Agricultural Carbon Enhancement network) is research program initiated by USDA Agricultural Research Service (ARS) to build high-quality data on trace gas fluxes in agroecosystems (Del Grosso *et al.*, 2013). GRACEnet provides a site description, measured greenhouse gas fluxes, soil carbon levels, biomass yield, soil nutrient content, planting date, and fertilizer application rate, type and amount. Emission data are provided at a daily scale when measured, but measurements are periodic (e.g., measurements are made weekly). Thus, we extract the model predicted fluxes on days that measurements are made for comparison. The spatial resolution is plot level, and measurements are made using the static chamber method where two chamber replicates are used per plot; detailed information about GRACEnet data can be found <http://nrrc.ars.usda.gov/arsdataportal/#/Home>.

Model Calibration: There are many different methods to calibrate the SWAT model including genetic approaches, directional searches and evolutionary optimization (Zhang *et al.*, 2016). However, given the complex crop rotations at the sites and the new variables introduced in SWAT-GHG both models were manually calibrated to the observed N₂O flux by changing the total soil C content in the first and second soil layers (as defined in the soils database), the amount and timing of N application⁻ in the management file, and the soil pH. Soil moisture and soil temperature were not used in the calibration since they were explicitly known and controlled by the measured precipitation and temperature.

Model Corroboration: After manual calibration of both models, model performance was verified using subsequent time series data from 2011 to 2012 for West Lafayette and 2008 for University Park for respective crop types. Since the GRACEnet plots were managed under specific

rotations, we corroborated both models by matching the crop rotation in the SWAT management files for those crop types that coincided between the calibration and corroboration time periods. Since there were multiple plots at each site managed under the same rotation (e.g., corn-soy) but at various stages in the rotation (e.g., one plot in the corn-soy rotation might be under corn in 2006 and another plot might be under soy), we extracted the modeled and observed N₂O fluxes that corresponded with each specific crop type by year and averaged the plot values together to create the time series of fluxes. As an example, in West Lafayette for the corn-soy rotation, the measured data started in 2008 and plot 1 was under soy, plot 2 was under corn and plot 3 was under soy, etc., so for 2008 soy fluxes consisted of measured and modeled data for plots 1 and 3 (averaged together), and corn for plot 2. In this manner, we iterated through each year sequentially extracting plot by crop fluxes to develop the time series of flux data. For each rotation year in the SWAT management file, where crop rotations are defined, we kept all calibrated parameters associated with each crop the same but changed the planting date and fertilizer application date according to the GRACEnet database and then reran the model.

There are many different model performance metrics available to test model skill (Bennett *et al.*, 2013). Among different quantitative methods, the coefficient of determination (r^2), Nash and Sutcliffe (1970) efficiency coefficient (NSE) are perhaps the most common (Moriassi *et al.*, 2015), but both tend to evaluate the model skill in capturing the mean response. Since the extreme N₂O fluxes are of greater environmental importance, we include a performance metric that describe model performance of the extremes, namely the absolute maximum error (AME) (Bennett *et al.*, 2013). The AME is a metric that indicates the maximum absolute deviation in the time series between measured and modeled data. Thus, the model skill was evaluated by comparing time series of simulated N₂O flux with observed N₂O flux data from the GRACEnet database and by comparing the predicted spatial distribution of emissions at the HRU level with the plot level N₂O emissions measured at each site.

Model Sensitivity Analysis (SA): A model sensitivity analysis was performed on each model by altering the initial conditions of the input parameters, including total soil C, N application rate, soil pH, air temperature (which subsequently alters soil temperature), and precipitation (which subsequently alters θ) by manually changing one variable at a time while keeping others unchanged (Norton, 2015; Pianosi *et al.*, 2016; Saltelli & Annoni, 2010). Manual SA was chosen

for several reasons 1) the relatively few number of HRUs and parameters of interest facilitated manual parameter adjustment and; 2) the most sensitive parameters can be easily identified. The SA was conducted by directly increasing or decreasing the C content by 10%, 20%, and 50% from the base model total soil C level, which resulted in a range of C contents typically found in agricultural soils for the two regions (0.6% - 1.7% total soil C). In contrast, the soil N content was changed by increasing or decreasing the applied N (fertilizer application rate) in the management file by 10%, 20%, and 50% relative to the base model, which in turn altered the soil N level (3-10%). The soil pH was varied from the default value of 6.5 to pH 4, 5, 7, and 8. The sensitivity of the model to soil temperature and θ was assessed by increasing or decreasing the air temperature and precipitation, respectively, by 10%, 20%, and 30%, as the +/-50% adjustment was deemed outside the range of plausible conditions. A joint SA was calculated for applied N and pH as the model was shown to be most sensitive to their input.

Results

Sensitivity Analysis: Model sensitivities were similar across all crop types; thus, we present SA results for the corn land use at both sites. Figure 2-2 shows the results of the SA on N₂O and N₂ emissions for the University Park and West Lafayette sites. Both models were very sensitive to pH and applied N, moderately sensitive to soil temperature and precipitation, and relatively insensitive to total soil C content. At University Park, N₂O emissions increased by 65 and 46% as the pH was lowered from the base condition of 6.5 to 5 and 4, respectively, while emissions declined by 34 and 74% when the pH was raised from 6.5 to 7 and 8, respectively. At West Lafayette, N₂O emissions increased by 11% at pH 5, but decreased by 11%, 38%, and 70% at pH 4, 7, and 8, respectively. The model was also sensitive to the N application rate; higher N application rates resulted in higher N₂O emissions, up to 130% at University Park and 94% at West Lafayette when N application was increased by 50%, while decreases in N application rates reduced N₂O emissions by as much as 76% at University Park and 77% at West Lafayette when N application was decreased by 50% (Fig. 2-2). At the University Park site increasing temperature by 10% and 20% resulted in small increases in emissions (1-6%), while a 30% temperature increase reduced emissions by 1%. At West Lafayette decreasing temperature increased emissions (3-27%) while increasing temperature decreased emissions (15-18%). At University Park increases in precipitation decreased N₂O emissions slightly, 2-9%, while

decreases in precipitation increased emissions 4-11% (Fig. 2-2). At West Lafayette both increase and decreases in precipitation tended to reduce emissions (1-15%). At both sites, increases in total soil C tended to increase N₂O emissions, while decreases in total soil C reduce N₂O emissions, although the magnitude of the changes was small ($\leq 7\%$).

N₂O to N₂ Comparison: Figures 2-2a and b show the breakdown of the modeled total daily denitrification products (N₂O and N₂) at University Park site and West Lafayette, respectively for each level of the parameters tested in the SA. Since the model results were found to be particularly sensitive to pH and applied N we present the results of a multi-level SA (Figs. 2-3a and b). In this analysis we varied applied N and pH together. Figures 2-3a and b illustrate that increasing the soil pH while simultaneously increasing the soil N content dramatically increases the total denitrification rate and decreases the N₂O:N₂ product ratio. These figures demonstrate that, like N₂O emissions, both total denitrification and the ratio of denitrification products are most sensitive to pH followed by N application rate, and highlight the importance of both total flux and the product ratio in driving the differences in N₂O emissions presented in Figure 2-2. For example, Figures 2-2a and b show that as pH increases total denitrification increases and the ratio N₂O:N₂ decreases. One exception to this is the lower level of denitrification observed at the University Park site at pH 7 compared to 8. While low pH is associated with higher N₂O emissions and higher ratio between N₂O:N₂ (Figs. 2-3a and b), the lower emissions predicted at pH 4 relative to pH 5 at both sites are driven by the decrease in total denitrification, which overwhelms the ratio effect, and limits N₂O flux at pH 4. After pH, N application rate has the greatest effect not only on N₂O emissions, but also on total denitrification flux. The relationship between pH and total denitrification and N₂O production is the same at both sites, as well as the effect of soil N content as expected. Both sites demonstrate the expected correlation, where total denitrification, N₂O:N₂, and N₂O emissions increase as soil N content increases. Temperature increases tended to reduce N₂O emissions at both sites but there was no clear impact on N₂ or the product ratio due to changing temperature. Increasing or decreasing total soil C or precipitation had little effect on denitrification emissions or the product ratio at either site.

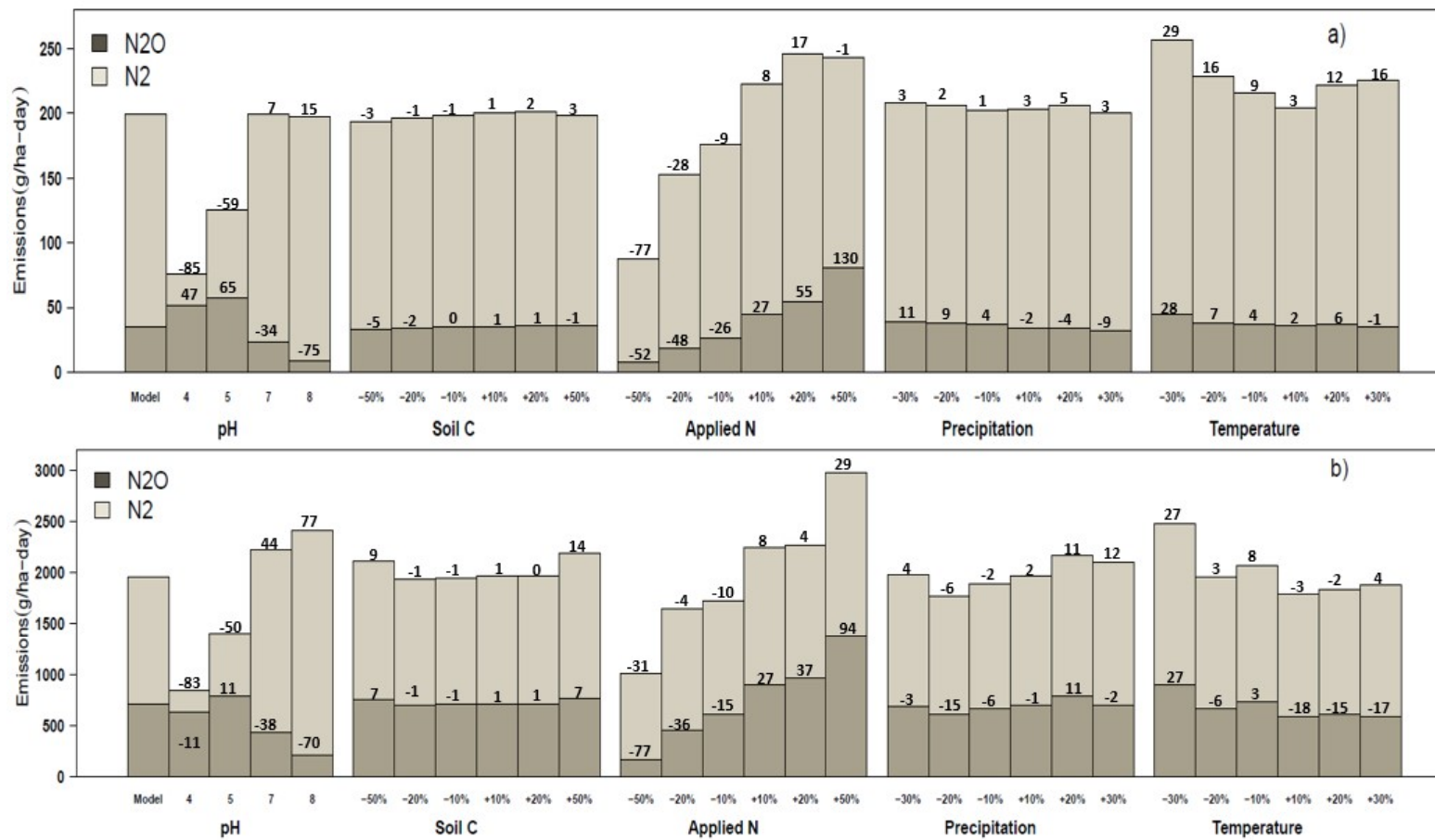


Figure 2-2: Comparison of model output N₂O and N₂ (from both nitrification and denitrification) for different soil and environmental factors and percent change (over each bar) from the base model1 at the University Park site (a) and the West Lafayette site (b) for the corn land use.

¹The base model parameter values for the University Park site are: pH =6.5, total soil C % = 1.7 for the first soil layer and 0.7 for the second soil layer; mean temperature = 10⁰ C, mean yearly precipitation =1035 mm, and soil N = 650 kg/ha. The initial model parameters for West Lafayette site are: pH= 6.5, total soil C % = 1.6 for the first soil layer and 0.7 for the second soil layer, mean daily temperature = 11.8⁰ C, mean yearly precipitation = 1174 mm, and soil N= 1800 kg/ha.

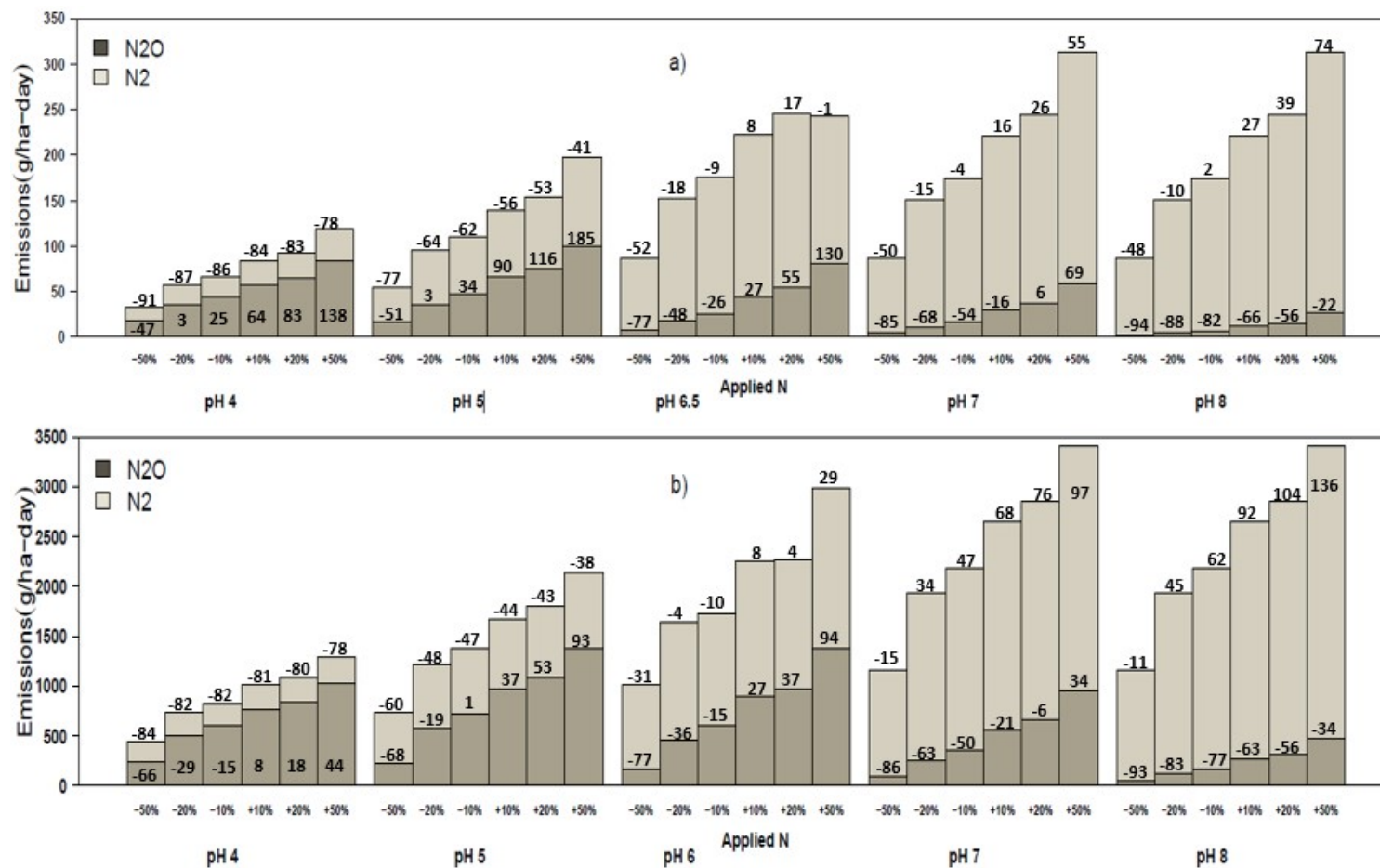


Figure 2-3: Comparison of model output N₂O and N₂ (from both nitrification and denitrification) and percent change (over each bar) against the base model in Figure 2 for simultaneous changes in applied N and pH at the University Park site (a) and the West Lafayette site (b) for the corn land use

Model Corroboration: Table 2-2 shows the NSE, R², and AME of the measured versus calibrated and corroborated model N₂O emissions for different crops at both test sites. The NSE values shows the model has good mean explanatory power for all crops at both test sites during the calibration period, with slightly lower, but still acceptable predictive power during the corroboration period. In terms of peak model prediction there is more variability; the model captures peak N₂O emissions generally well at both sites, but the AME indicated some peak error, some of which is due to mistimed peaks (e.g., corn at both sites) and some is due to under or over predicted peaks (e.g., soy at University Park, sorghum at West Lafayette, Figs. 2-4 and 2-6). Comparing each crop, the model predicted N₂O emissions best, as indicated by NSE value, for alfalfa followed by corn, soybean and pasture at University Park, and sorghum, followed by corn and soybean at West Lafayette. There was some reduced model performance during the corroboration periods at both sites, which is primarily due to averaging responses of different plots into one time series. Despite this, the models captured the timing and magnitude of N₂O emissions relatively well.

Table 2-2: R-squared values (R²), Nash-Sutcliffe coefficients (NSE), and absolute maximum error (AME) and for the calibrated model for all crop types at both test sites, University Park and West Lafayette. Note that the variables that were calibrated were the soil pH, N application rate, and total soil C level, and all others remained as defaults from the GRACEnet database or SWAT initialization.

Site	Crop	Calibration			Corroboration		
		R ²	NSE	AME	R ²	NSE	AME
University Park	Corn	0.67	0.65	95.0	0.51	0.44	45.2
	Alfalfa	0.95	0.86	9.0	0.48	0.42	26.0

	Soybean	0.81	0.56	39.2	0.42	0.24	95.7
	Pasture	0.52	0.51	51.6	0.60	0.51	39.3
West Lafayette	Corn	0.74	0.73	2953.7	0.70	0.41	2765.6
	Soybean	0.69	0.48	299.5	0.73	0.34	116.5
	Sorghum	0.80	0.78	426.8	0.48	0.44	309.7

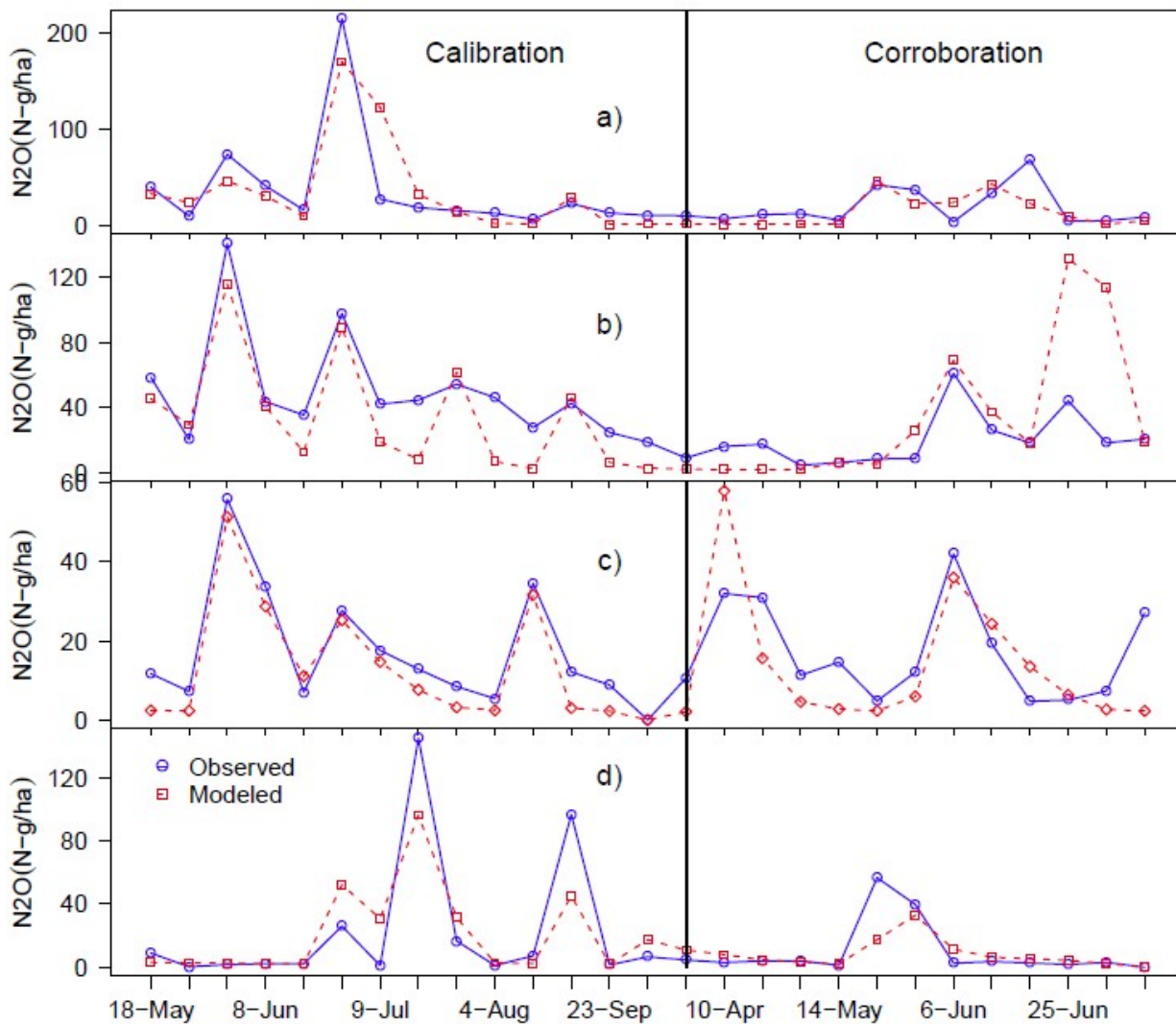


Figure 2-4: Comparison of observed and modeled N₂O emissions for the University Park site for 2006 during calibration and 2008 for corroboration; (a) Corn, (b) Soybean, (c) Alfalfa, and (d) Pasture

University Park, PA

Time Series Evaluation: The time series of measured and modeled N₂O emissions were compared for each crop type at the University Park site. The comparison between observed and simulated N₂O emissions for the corn crop (Fig. 2-4a) shows that the model captured both the magnitude and timing of emissions quite well in both the calibration and corroboration periods. For the soybean crop during the calibration period the model predicted the seasonal pattern of N₂O moderately well with a slight under estimation during July-September, although the peaks are well predicted (Fig. 2-4b). During the corroboration period the timing of emission peaks is well captured, but the June event is over predicted (Fig. 2-4b). For alfalfa, the model predicted both the timing and peak values well during the calibration period, particularly following the fertilizer applications in May, June, and August (Fig. 2-4c). During the corroboration period emission timing was well captured, but the event in April was over predicted (Fig. 2-4c). For pasture (Fig. 2-4d) in both the calibration and corroboration periods the model tended to underestimate the peaks but captured the timing and lower emissions well.

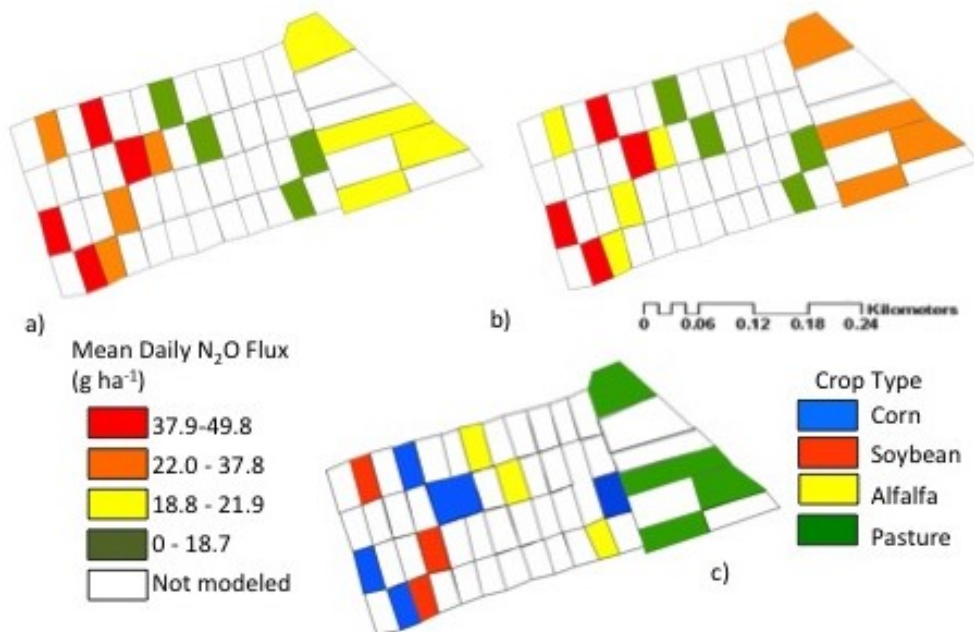


Figure 2-5: Spatial comparison of daily average N₂O emissions for the University Park site for 2008: (a) measured N₂O flux, (b) modeled N₂O flux, (c) crop types where measurements were made. The overlay polygon map shows the field layout for the site. Unpredicted plots are those for which GRACEnet N₂O measurements were unavailable, where we could not match the rotations or the crop type did not exist in the SWAT crop database.

Spatial Evaluation: Figure 2-5 shows the measured and predicted spatial distribution of N₂O emissions for the University Park site. In general, the model was able to predict the distribution of emission well, both spatially and in magnitude. The model tended to slightly over predict emissions from pasture (by about 15%), but corn, alfalfa, and soybean emissions were well predicted across the site, with less than a 10% difference (Fig. 2-5).

West Lafayette, IN

Time Series Evaluation: The time series evaluation between observed and simulated N₂O emissions for different crop types examines 2008 to 2010 for the calibration period and 2011 for the corroboration period. For corn, the model captured the magnitude of the peaks quite well during the calibration period, despite missing the timing of the peaks slightly in June 2008 and 2010 (Fig. 2-6a). During the corroboration period the event timing was well predicted but the magnitude was slightly under predicted (Fig. 2-6a). Emissions from the soybean crop (Fig. 2-6b) were well predicted during the calibration and corroboration periods. Figure 2-6c shows model predicted N₂O emissions for sorghum and that it was able capture the seasonal pattern of emissions, despite some underestimated peaks in both the calibration and corroboration periods.

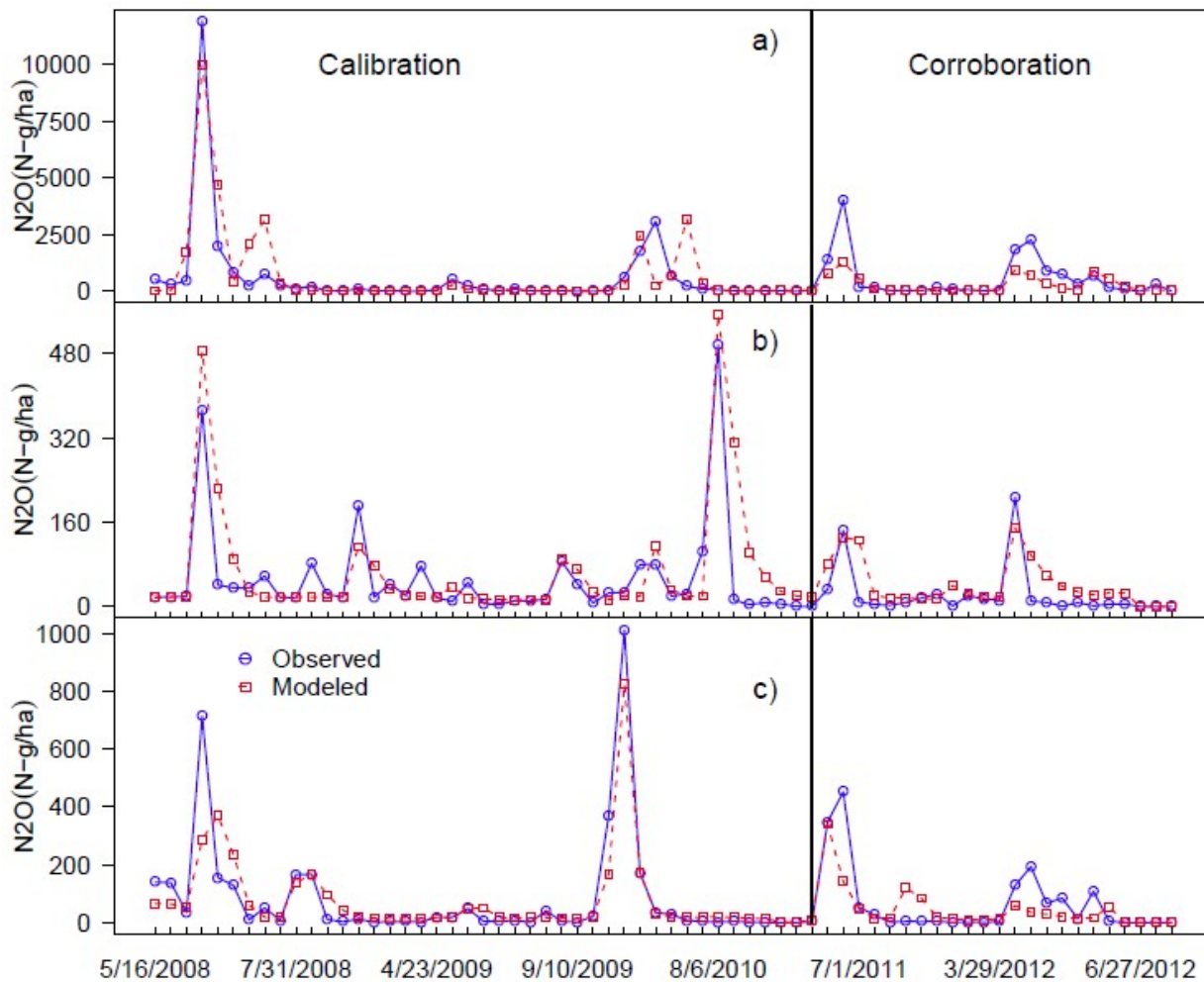


Figure 2-6: Comparison of observed and modeled N_2O emissions for West Lafayette, 2008 to 2010 for calibration and 2011 to 2012 for corroboration for (a) Corn, (b) Soybean, and (c) Sorghum.

Spatial Evaluation: Figure 2-7 shows the measured and predicted spatial distribution of N_2O emissions for the West Lafayette site. Similar to the University Park site the model generally predicted both the spatial distribution and magnitudes of emission well across the fields (Fig. 2-7). The corn and corn-soybean rotation were slightly more accurately predicted than the sorghum crop. The West Lafayette site exhibited variability between crop types and between plots than at University Park, which the model is able to capture. For instance, corn had measured emissions ranging from <5 to 50 g ha^{-1} at West Lafayette (Fig. 2-7) while the range at University Park was

22-50 g ha⁻¹ (Fig. 2-6). Clearly the model is able to capture the spatial distribution of N₂O hotspots quite well.

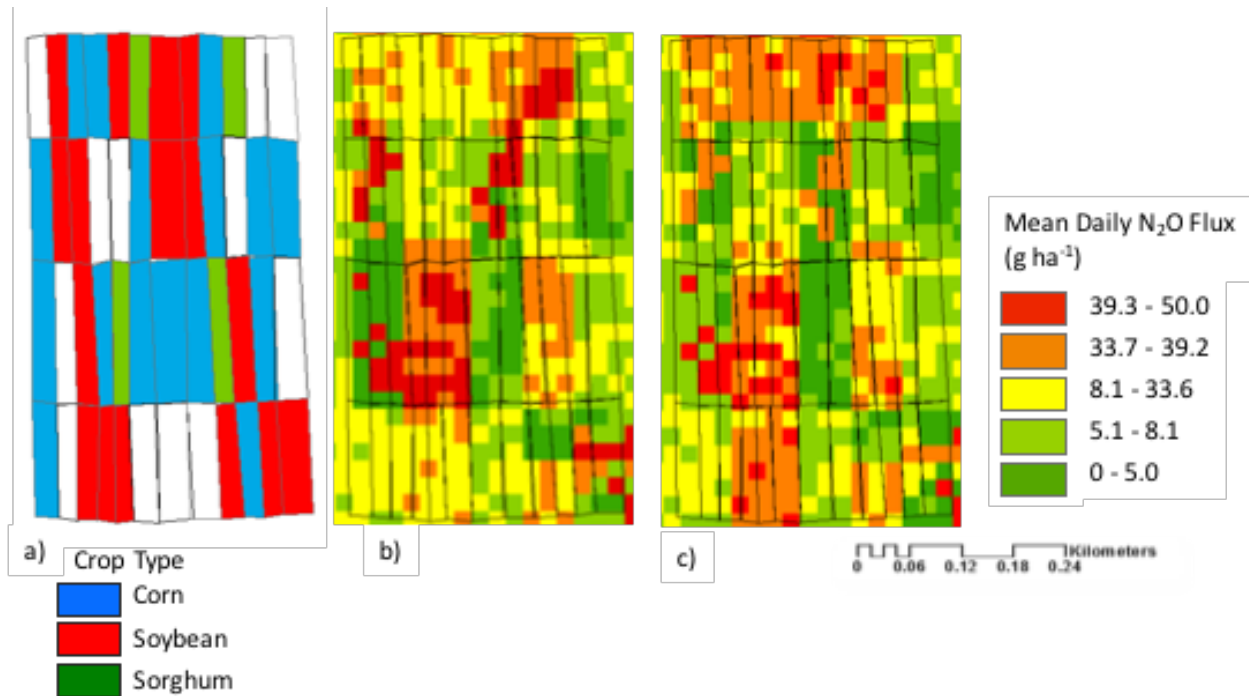


Figure 2-7: Spatial comparison of daily average N₂O emissions for West Lafayette test site for 2011, (a) measured N₂O flux, (b) modeled N₂O flux, (c) crop types where measurements were made. Unpredicted plots are those for which GRACEnet N₂O measurements were unavailable, rotations could not be matched or the crop type did not exist in SWAT. Note that multiple HRUs can occur in a single field due to differences in soil type and topography.

Discussion

Modeling the Environmental Controls on N₂O and N₂ Emissions

pH: N₂O emissions were by far the most sensitive to changes in pH (Figs. 2-2 and 2-3), and it is reassuring that the model was able to capture this effect because pH has long been known to exert both proximal and distal control on emissions (Mørkved *et al.*, 2007). Some of this effect is due to the proximal control (enzyme and substrate level effects) of pH on N₂O reducing enzymes, which are more sensitive to low pH than the enzymes that reduce NO₃⁻ and NO₂⁻; the

former being more active at $\text{pH} > 7$ and the latter more active at $\text{pH} < 7$ (Richardson et al., 2009). Thus, N_2O is produced at low pH but is not converted to N_2 and tends to build up in the system because the activity of nitrous oxide reductase is inhibited. In most soils N_2O emissions are smallest at neutral to basic pH (Liu et al., 2010), and our model predicts this; at a pH of 8 emissions were between 70% and 74% lower than at pH 6.5, although total denitrification was greater (Figs. 2-2 and 2-3), and decreasing pH generally increased the $\text{N}_2\text{O}:\text{N}_2$ ratio (Figs. 2-2 and 2-3). These results reflect the importance of pH not only as a dominant control on total denitrification, but also on the composition of the products; at pH values between 4 and 8, the ratio $\text{N}_2\text{O}:\text{N}_2$ increases as pH decreases, and below pH 4 denitrification is largely inhibited due to negative impacts on denitrifying enzyme synthesis (Liu et al., 2010). Interestingly, at both sites the highest emissions N_2O were predicted to occur at a pH of 5 (University Park, $58 \text{ gha}^{-1} \text{ d}^{-1}$ and West Lafayette, $787 \text{ gha}^{-1} \text{ d}^{-1}$) rather than at pH 4 (University Park, $51 \text{ gha}^{-1} \text{ d}^{-1}$ and West Lafayette, $630 \text{ gha}^{-1} \text{ d}^{-1}$), as might be expected. This is because total denitrification ($\text{N}_2 + \text{N}_2\text{O}$) was higher at pH 5 than pH 4, so despite the higher $\text{N}_2\text{O}:\text{N}_2$ at pH 4, the quantity of N_2O emitted at pH 4 was less than at pH 5 (Figs. 2 and 3). While total denitrification and $\text{N}_2\text{O}:\text{N}_2$ were significantly higher at the West Lafayette site for the corn land use in the base model and all conditions tested in the SA compared to University Park, the effect of pH on denitrification gas flux is consistent between research sites and with the literature (e.g. Morkved et al., 2007; Liu et al., 2010; Richardson et al., 2009).

Soil C:N Ratio: Altering total soil C levels by +/- 10%, 20%, and 50% had little impact on N_2O emissions, which is somewhat surprising given that both systems were C-limited under all of the scenarios tested (e.g., initial C:N ratios 2.6:1 for PA and 1:0.8 for IN). Generally C:N ratios <20:1 are considered C-limited (Richardson *et al.*, 2009), so an increase in the C content would be expected to increase the denitrification rate. However, changing C levels resulted in very little change in emissions at either site (-5% to 3% in PA, and 5% to 7% in IN). With such low soil C:N ratios at the study sites, N_2O emissions may have been overwhelmed by the effect of the relatively high N content of the soil; high NO_3^- concentrations can inhibit N_2O reduction as NO_3^- serves as an electron acceptor energetically preferable to N_2O . Indeed, emission were much more sensitive to the N application rate imparting a -76% to 130% change on emissions at University Park and -77% to 94% change at West Lafayette (Fig. 2-2). With respect to denitrification, the importance of the N application rate and by extension the soil N content is well established (Hai

et al., 2009; Saggar *et al.*, 2013) and the clear correlation between the N application rate and both total denitrification and N₂O emissions was as expected under C-limited conditions.

Temperature: Generally, increases in microbial activity are predicted as temperatures increase, but complex interactions among microbial processes that may be competing for soil nutrients make the net results difficult to predict. For example, some research has shown that increasing temperatures promote complete denitrification (reduction to N₂ rather than halting at N₂O), which could reduce N₂O emissions (Stres *et al.*, 2008), but increasing temperatures also increase overall microbial activity, which could increase emissions of both products. Indeed, the results of our simulations with respect to increased temperature (Fig. 2-2) suggest complex interactions, where moderate increases in temperature (+10% and 20%) at University Park slightly increased emissions (1-6%) but the 30% temperature increase actually decreased emissions 1%. At West Lafayette increases in temperatures decreased emissions (15-18%). Decreases in temperature at both sites increased N₂O emissions 3-28% (Fig. 2-2). N₂ and total denitrification (Fig. 2-2) are similarly affected, the highest total denitrification and N₂ emissions occur at a 30% decrease in temperature. The responses to temperature at the two sites may be reflective of differences in the soil types (sandy clay loam at University Park and loam at West Lafayette) and soil moisture status (precipitation quantity and timing differing between the sites) that affect how changes in air temperature translate to changes in the soil temperature (e.g., there is a dampened lag).

Soil Moisture, θ : Changes in θ do not produce a linear nor directionally consistent response in N₂O emissions. Changes in θ can cause rapid shifts between nitrification and denitrification (Bergsma *et al.*, 2002; Webster & Hopkins, 1996). As θ decreases pore space oxygen concentrations increase, most denitrification ceases, and nitrification rapidly becomes the dominant N transformation process. Return to anaerobic conditions causes a similar reversal to denitrification. These periods of transition often coincide with peak periods of N₂O flux, especially in agricultural soils (Butterbach-Bahl *et al.*, 2011). Indeed, the effect of soil moisture on N₂O emissions in Fig. 2-2 could be partially explained by the temporal dynamics of soil wetting/drying. However, while more frequent wetting and drying at University Park (data not shown) might lead us to expect higher N₂O emissions, the N₂O:N₂ ratio is higher at West Lafayette, presumably due to the greater soil N levels at West Lafayette (1800 kg/ha compared to

650 hg/ha at University Park), the higher levels of total denitrification, about ten times greater than University Park, are expected.

All of these factors interact in complex ways, which limits the value of conclusions drawn from assessing their individual impact. For instance, temperature affects C: N ratio by changing the rate of C decomposition and N cycling. Temperature also alters θ by changing evapotranspiration and plant moisture uptake. Increasing total soil C can also increase the water holding capacity of the soil and in turn increase θ as well. An integrated model capable of capturing these complex interactions is one of the only ways to assess how N₂O emissions change under altered environmental conditions. SWAT-GHG was able to reliably predict how these factors affect N₂O emission and is thus useful for assessing the impact of targeted landscape management on N₂O emissions.

Implications for Modeling: Accurate prediction of the spatial and temporal extent of GHG emissions is critical for managing agricultural nutrients. Despite some discrepancies in the timing or magnitude of peak N₂O emissions (e.g., Figs. 2-4 and 2-6), SWAT-GHG simulated N₂O emissions well at both sites. The reason for discrepancies might be due to the several factors; 1) the dynamic nature of N₂O emissions that can vary dramatically over the course of a day [e.g., the model integrates over a 24 hr period, while the measurements integrate over a 1 hr period (Parkin and Venterea, 2010)]; 2) the uncertainty in the input data (e.g., amount and time of application of fertilizer, soil pH, missed precipitation event); or 3) process conceptualization in the model itself. However, compared to other denitrification/N₂O models SWAT-GHG simulated the spatial and temporal N₂O emissions from agroecosystems as well or better than most other models in the literature. For instance, Parton *et al.* (2001) who developed DAYCENT were able to simulate annual and monthly N₂O emissions well but daily emissions were poorly predicted; the authors speculate that this is due to the effect of topography redistributing soil moisture, which DAYCENT was not developed to capture. Morse *et al.* (2012) suggest that finer temporal (and spatial) scale models that can capture the variability of N₂O emission are critical to better managing landscape scale GHG emissions. SWAT-GHG provides these enhanced simulation capabilities for agroecosystems by linking the effect of topography (SWAT-GHG is based on the SWAT-VSA model which incorporates the impact of topography) and the processes controlling GHG emissions. Indeed, the incorporation of more mechanistic soil moisture

predictions represents an improvement on previous modeling efforts. Although the model generally simulates N₂O emissions well, there are some areas where the model could be improved, such as including dynamic soil pH calculation (e.g. currently pH in is a user defined, static input). Addition of dynamic pH would allow the quantification of the impact of management practices, such as liming and/or use of acidifying fertilizers, on N₂O emissions over time.

SWAT-GHG can be used and applied to agroecosystems at a range of scales, crop types and management regimes and used to test scenarios related to crop production, agricultural best management practices and climate change. This would allow managers to identify areas of the landscape that have high emissions and a high potential for management practices to reduce emissions. For instance, the model can be used to assess the impacts of management practices such as tillage, drainage water management, nutrient management, and soil amendments on GHG emissions or for assessing the impact of climate change on N₂O emissions.

Conclusions

This paper describes SWAT-GHG, a new routine for the SWAT model to predict N₂O emissions in agroecosystems using soil and environmental factors such as soil N and C content, soil temperature, soil pH, and soil θ as the controlling factors. The base model upon which SWAT-GHG was developed incorporates the impact of topography on the redistribution on soil water. The model was tested for different crop types and compared with measured N₂O values at two test sites: University Park, PA and West Lafayette, IN. The model simulated N₂O well in both time and space as verified by comparison to measured N₂O flux from different crop types. Perhaps more importantly, the model was sensitive to changes in soil and environmental factors such as soil pH, soil nutrient content and precipitation. This new model represents an advance over many existing GHG emission models in several respects; 1) it incorporates the physical processes controlling N₂O emissions; 2) it uses easily available input parameters to initialize; 3) it provides predictions at the subfield scale; and 4) it is able to capture emission at a high temporal frequency.

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CHAPTER 3

IMPACT OF CLIMATE CHANGE AND CLIMATE ANOMALIES ON HYDROLOGIC AND BIOGEOCHEMICAL PROCESSES IN THE CHESAPEAKE BAY WATERSHED, USA

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Abstract

Nutrient export from agricultural landscapes is a water quality concern and the cause of mitigation activities worldwide. Climate change impacts hydrology and nutrient cycling by changing soil moisture, stoichiometric nutrient ratios, and soil temperature, potentially complicating mitigation measures. This research quantifies the impact of climate change and climate anomalies on hydrology, nutrient cycling, and greenhouse gas emissions in an agricultural catchment of the Chesapeake Bay watershed. We force a calibrated model with seven downscaled and bias-corrected regional climate models and derived climate anomalies to assess their impact on hydrology and the export of nitrate (NO_3^-), phosphorus (P), and sediment, and emissions of nitrous oxide (N_2O) and di-nitrogen (N_2). Model-average (\pm standard deviation) results indicate that climate change, through an increase in precipitation and temperature, will result in moderate increases in winter/spring flow ($2.7 \pm 10.6\%$) and NO_3^- export ($3.0 \pm 7.3\%$), substantial increases in dissolved P ($8.8 \pm 19.8\%$), total P ($4.5 \pm 11.7\%$), and sediment ($17.9 \pm 14.2\%$) export, and greater N_2O ($63.3 \pm 50.8\%$) and N_2 ($17.6 \pm 20.7\%$) emissions. Conversely, decreases in summer flow ($-12.4 \pm 26.7\%$) and the export of dissolved P ($-11.4 \pm 27.4\%$), total P ($-7.9 \pm 24.5\%$), sediment ($-4.1 \pm 21.4\%$), and NO_3^- ($-12.2 \pm 31.4\%$) are driven by greater evapotranspiration from increasing summer temperatures. Increases in N_2O ($20.1 \pm 29.3\%$) and decreases in N_2 ($-13.0 \pm 14.6\%$) are predicted in the summer and driven by increases in soil temperature. While the changes in flow are related directly to changes in precipitation and temperature, the changes in nutrient and sediment export are, to some extent, driven by changes

in agricultural management that climate change induces, such as earlier spring tillage and altered nutrient application timing and by alterations to nutrient cycling in the soil.

Introduction

Climate change has the potential to impact hydrology, nutrient cycling, and greenhouse gas (GHG) emissions from agroecosystems in the Mid-Atlantic region of United States (Huntington, 2003; Johnson *et al.*, 2012; Najjar *et al.*, 2009a; Najjar *et al.*, 2010; Neff *et al.*, 2000). Climate predictions for the Mid-Atlantic suggest that precipitation (especially during winter and spring) quantity and intensity will increase, which could increase nitrogen (N), phosphorus (P) and sediment export from watersheds (Chang *et al.*, 2001; Cousino *et al.*, 2015). Changes in soil moisture, temperature, and nutrient cycling rates also influence GHG emissions (Maag & Vinther, 1996). Excess nutrient export from the landscape to aquatic ecosystems accelerates eutrophication and harmful algal blooms (Burgin *et al.*, 2007), leading to undesirable changes in ecosystem structure and function (Smith *et al.*, 1999), such as coastal dead zones (areas of low oxygen concentrations) (Diaz *et al.*, 2008). The Chesapeake Bay is a eutrophic estuary that has been the subject of precedent-setting regulations to limit point and non-point source pollution from its 166,000 km² watershed. Commitments have been made by all six Chesapeake Bay states to reduce contributions to Bay nutrient and sediment loadings over the next several decades, however, a major uncertainty with Chesapeake Bay watershed mitigation strategies is the complicating influence of climate change and climate variability. There is also uncertainty over the effects of climate change on GHG emissions, which are often tied to the same hydrologic and nutrient cycles that are vulnerable to climatic shifts.

Nitrogen, P, and sediment export from the landscape to surface waters and GHG emissions are controlled by a combination of key biogeochemical and hydrologic processes. Changes in precipitation and temperature alter the timing and magnitude of runoff, soil moisture, and biogeochemical cycles (Gleick, 1989). For instance, N mineralization, nitrification and denitrification, are to a large extent controlled by factors that climate change influences, such as soil temperature and soil moisture (Butterbach-Bahl *et al.*, 2011). Similarly, increased soil temperatures and moisture content can influence the sorption and desorption of P, as well as immobilization and mineralization rates, all factors affecting P export (Sheppard *et al.*, 1984). It

is also well established that sediment transport is affected by soil moisture (Wiggs *et al.*, 2004), by precipitation amount, and by precipitation intensity (Römkens *et al.*, 2002).

A fundamental understanding of these coupled processes under a changing climate is critical to managing N, P, and sediment export from ecosystems to sensitive coastal zones. Development of effective landscape management strategies to improve water quality requires an understanding of how processes that regulate nutrient/sediment production on the landscape are coupled with hydrologic transport to water bodies. Of particular interest is the impact of climate change on hydrologically active areas of the landscape that contribute disproportionately to watershed nutrient export (e.g., Critical Source Areas, CSAs), where active hydrologic transport and high nutrient availability coincide (Groffman, Butterbach-Bahl, *et al.*, 2009b). A better understanding of climate change and its potential influence on landscape biogeochemistry can be used to develop new strategies for protecting coastal waters and their contributing watersheds from pollution. For instance, it is entirely possible that climate change would enhance some natural ecosystem services that protect water quality. One example is through a potential change in denitrification, a natural process that transforms dissolved nitrate (NO_3^-) into nitrogen gases, and returns it to the atmosphere. Hydrologically active areas in the landscape prone to soil saturation are recognized as denitrification hotspots (McClain *et al.*, 2003; Vidon *et al.*, 2010) and understanding where these areas are, or will be, can help develop management approaches that utilize ecosystem services to protect water quality.

This study assesses the effects of climate change and weather anomalies on hydrology, nutrient and sediment export, and N_2O and N_2 emissions in an agricultural sub-catchment of the Chesapeake Bay watershed located in east-central Pennsylvania. Long-term watershed monitoring data are used along with outputs from seven downscaled and bias -corrected regional climate models (RCMs) to understand the implications of climate change on hydrology, water quality, nutrient cycling, and GHG emissions, using the Soil and Water Assessment Tool-Variable Source Area (SWAT-VSA) model (Easton *et al.*, 2008) modified to include GHG emissions (Wagena *et al.*, 2017), and improved P cycling (Collick *et al.*, 2016). We analyze the results of each climate model, as well as the ensemble model mean, for the impact on hydrology, water quality, N_2O and N_2 emissions and nutrient cycling. Results highlight processes, places,

and times that are vulnerable to climate impacts and point to watershed mitigation and adaptation strategies to address the long-term impacts of climate change.

Materials and Methods

Watershed Description

The WE-38 Experimental Watershed is a sub-watershed of Mahantango Creek in east-central Pennsylvania, which drains to the Susquehanna River (Fig. 3-1). The watershed has an area of 7.3 km² and has been extensively studied as a USDA-ARS experimental watershed beginning in 1966 and monitored through the Sustaining the Earth's Watersheds Agricultural Research Data System (STEWARDS) project (Bryant *et al.*, 2011). The climate of WE-38 is temperate humid, with a mean temperature of 10.1°C, mean precipitation of 1080 mm yr⁻¹, and mean streamflow equal to 46% of precipitation (Buda *et al.*, 2011; Lu *et al.*, 2015). Elevation ranges from 220 to 510 m and the land use of the watershed consists of agriculture (44.5%), forest (33.8%), and pasture (3.5%) (Collick *et al.*, 2015). As part of the Appalachian Valley and Ridge Province, the watershed is underlain by fine sand- and silt-stones, supporting soils prone to variable source area (VSA) hydrology. Specifically, uplands feature well-drained soils with high infiltration rates while the lower landscape positions are occupied by poorly drained soil with features that seasonally perch water and result in runoff generation by saturation excess processes (Lu *et al.*, 2015).

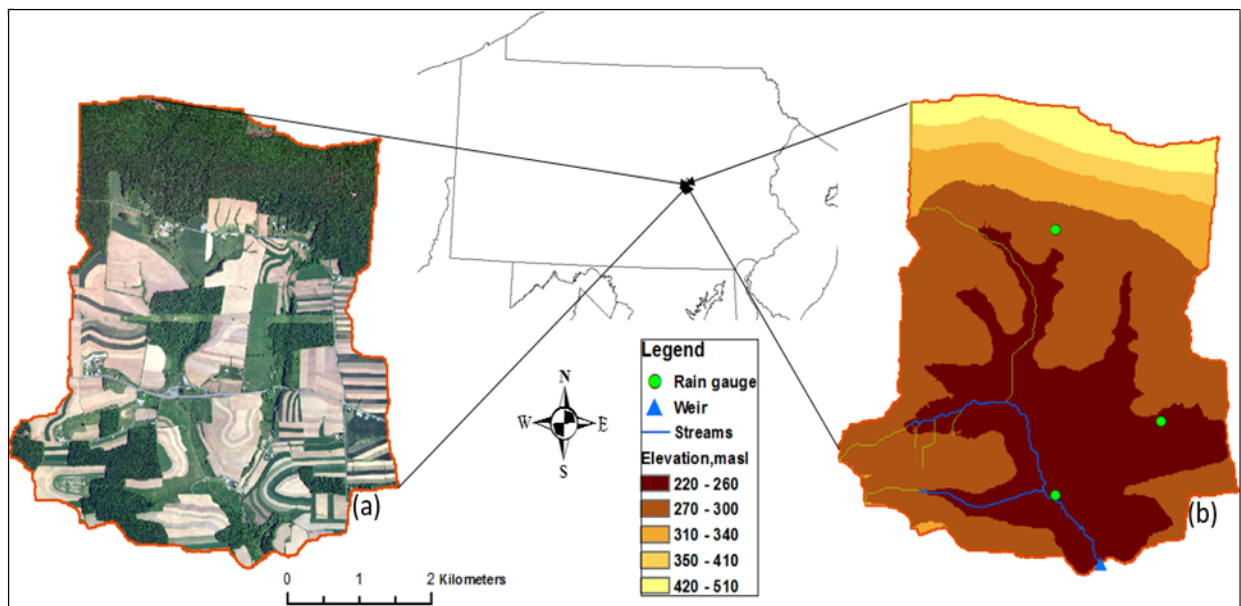


Figure 3-1: Location of WE-38 watershed in Pennsylvania, USA, and land cover ortho-imagery for 2015 (a) and digital elevation model (b) showing the location of the weir location and precipitation gauges.

SWAT Model Description

The SWAT model is a process based, semi-distributed watershed model developed to assess the impact of land management practices on water availability and water quality (Arnold *et al.*, 1998). SWAT requires meteorological (precipitation, min and max temperature, solar radiation, wind speed, and humidity), soil, land cover, and land management data to simulate surface and subsurface hydrology and various chemical, nutrient, and sediment fluxes. SWAT-VSA re-conceptualizes SWAT to account for areas of the landscape subject to variable saturation dynamics (Easton *et al.*, 2008). In SWAT-VSA the area of each hydrological Response Unit (HRU) is defined by the coincidence of land use and wetness index class determined from a Topographic Index (TI) to differentiate areas of the landscape with respect to their moisture storage and saturation/runoff potential (Easton *et al.*, 2008). SWAT-VSA has been shown to provide better predictions of soil moisture, runoff generation, and nutrient export than the standard SWAT model in WE-38 and similar watersheds (Easton *et al.*, 2008).

Wagena *et al.* (2017) further modified SWAT-VSA to predict N₂O and N₂ emissions from agroecosystems based on soil physical and chemical processes and environmental drivers. The model uses reduction functions to model the total denitrification (N₂ + N₂O) and nitrification rates, and then applies a ratio method to partition N₂ from N₂O. Greater detail can be found in Wagena *et al.* (2017). Collick *et al.* (2016) modified the P cycling routines in SWAT to better predict the fate and cycling of surface applied P (fertilizers and manures).

Watershed Model Initialization and Input Data

SWAT-VSA was initialized with a 10-m resolution digital elevation model resampled from 0.5 m LiDAR data obtained from Canaan Valley Institute (2007) using ArcSWAT 2012 and TopoSWAT (available from <https://dx.doi.org/10.6084/m9.figshare.1342823>) developed by Fuka, Collick, *et al.* (2016). TopoSWAT automates the SWAT-VSA initialization process by creating the TI data and then overlaying the soil and TI data to develop the required database for model initialization. Soils data utilized by Topo SWAT are based on the Food and Agriculture

Organization (FAO) soils database (FAO, 2007). This methodology downscales the FAO soils data, distributes the soil properties across TI classes, and has been shown to provide more accurate representation of soil properties than SSURGO (Fuka, Collick, *et al.* (2016). The land use characterization of WE-38 were derived from previous studies (Buda *et al.*, 2013; Buda *et al.*, 2009; Gburek *et al.*, 2002; Gburek *et al.*, 2006; Needelman *et al.*, 2004; Veith *et al.*, 2008) and used to parameterize the model at the field scale. There are two options to incorporate agricultural management practices in SWAT; they can be triggered by thresholds in the model (e.g. growing degree day, heat units), or they can be input into the management file as individual practices, should sufficient data exist. For this study, the later was utilized. Multi-year agricultural field management schedules of individual fields were built into the model by Collick *et al.* (2015). The management information has been consistently collected for each farm in WE-38, and includes annual farmer interviews, informal updates throughout the year, and regular field observations. In order to incorporate this management information into SWAT-VSA, georeferenced field boundaries are obtained annually by GPS, reconciled against publically available aerial satellite photos, and combined to represent the changing shape and size of the fields over the 12 years of the study (Collick *et al.*, 2015). The model was initialized by weather including precipitation, temperature (min and max), relative humidity, wind speed and solar radiation from 1987 to 2010 from land based stations in WE-38.

Model Calibration and Evaluation

The WE-38 SWAT-VSA model was calibrated and then evaluated using SWAT-CUP (SWAT Calibration and Uncertainty Procedure) (Arnold *et al.*, 2012) using the SUFI2 (Sequential Uncertainty Fitting) optimization algorithms with the objective function set to percent bias (PBIAS) method. The model was then evaluated by employing a jackknifing method, also referred to as leave one out cross validation (McCuen, 2005). In jackknifing, after calibration of n years of data, the model predictive power was evaluated based on holding out one year of the sample data and then the model was re-calibrated for $n-1$ years data to obtain predicted values of the withheld data. The process was iterated until all n sample years of data have been used to make predictions for all n sample data and statistics of n observed and predicted values were calculated (McCuen, 2005). This method was required because the standard split sample calibration/evaluation technique initially employed revealed significant differences in watershed

response for all constituents between the calibration and evaluation periods (data not shown), a result of non-stationarity in the observed climate over the period 1987-2010.

The SWAT-VSA model performance was evaluated based on three metrics, PBIAS, the normalized mean error (NME, eq. 1), and the normalized mean absolute error (NMAE, eq. 2), against the historical measured data from 1989 to 1999 for model calibration and 2000-2010 for model evaluation. The NME is an index of relative bias providing an estimate of over prediction (NME > 0) or under prediction (NME < 0) of the model. The NMAE (which is scaled relative to the observed mean) indicates discrepancy between model predictions and measured values; the smaller the NMAE the closer model simulations are to observed values (Pourmokhtarian *et al.*, 2012).

$$NME = \frac{\bar{P} - \bar{O}}{\bar{O}} \quad (1)$$

$$NMAE = \frac{\sum_{i=1}^n |P_i - O_i|}{n\bar{O}} \quad (2)$$

Where P_i is the predicted value and O_i is the observed value at time i . \bar{P} and \bar{O} are means of the individual observations of P_i and O_i , respectively, and n is the number of observations.

The use of PBIAS as the calibration objective function was employed to ensure that the mass balance was maintained, as the interest in this work was to assess the relative effect of climate change, not on the absolute daily predictions. The model was calibrated for flow, mineral phosphorus (PO₄-P), and NO₃-N from 1989 to 2010 and model predictive power was evaluated from 1989 to 2010 on a daily basis against measurements made at the WE38 watershed outlet based on the above method. Measured flow data consist of 15-min frequency measurements converted to a time weighted daily average. Nitrate and DP measurements are made less frequently and include both baseflow and stormflow samples, converted to a time-weighted daily average (Bryant *et al.*, 2011). Since the observed sediment data were only collected under baseflow conditions, and thus fail to capture storm events, calibration was not possible. The predicted N₂O emissions were evaluated (the parameters affecting N₂O were not calibrated) against measurements made in the watershed from May 2012 to Oct 2013 (Benjamin Rau, personnel comm). The frequency of measurements varied from every four days to less than once per month depending on precipitation and fertilization events. Soil N₂O flux was measured using vented static chambers (Parkin *et al.*, 2003). Gas samples were analyzed for N₂O concentration

using a Varian CP3800 gas chromatograph equipped with a ^{63}Ni electron capture detector (Varian, Walnut Creek, CA, USA).

Climate Scenario Incorporation

Results from seven climate models were obtained from the North American Climate Change Assessment Program (NARCCAP) model dataset (Mearns *et al.*, 2009). The models use dynamical downscaling—nesting a regional climate model (RCM) within a global climate model (GCM)—and provide data at high temporal (3-hourly) and spatial (50-km) resolutions, better capturing local processes (Rummukainen, 2010). Greenhouse gas concentrations in the NARCCAP future simulations are obtained from the medium-high SRES A2 emissions scenario (Nakicenovic *et al.*, 2000). The models used include the CRCM-CCSM (Canadian Regional Climate Model, Community Climate System Model), CRCM-CGCM3 (Canadian Regional Climate Model, Third Generation Coupled Global Climate Model), ECP2-GFDL (Experimental Climate Prediction Center, Geophysical Fluid Dynamics Laboratory GCM), HRM3-GFDL (Hadley Regional Model 3, Geophysical Fluid Dynamics Laboratory GCM), MM5I-CCSM (The PSU/NCAR Mesoscale Model, Community Climate System Model), RCM3-GFDL (Regional Climate Model version 3, Geophysical Fluid Dynamics Laboratory GCM), and WRF3-CGCM3 (Weather Research & Forecasting Model, Third Generation Coupled GCM).

Dynamical downscaling provides some advantages over the main alternative, statistical downscaling, which uses transfer functions based on historical observations in order to relate climate model output to the climate variables of interest (e.g., Abatzoglou & Brown, 2012). Dynamical downscaling is based on the same general physical principles that underlie GCMs, such as the conservation of mass, momentum, and energy. Thus, dynamical downscaling is not tied to the historical climate parameter space that statistical downscaling approaches are tuned to. This is of particular importance for large projected changes in climate, which may be out of the range of the historical record. However, statistical downscaling has the advantage of higher resolution (due to being less computationally expensive than dynamical downscaling) and, in general, a lack of bias in simulations of the historical record as a result of the aforementioned tuning. We solve the bias problem in the NARCCAP product by using a cumulative distribution function matching method (Dixon *et al.*, 2016; Li *et al.*, 2010; Teutschbein & Seibert, 2013;

Wang & Chen, 2014) with data from Phase 2 of the North American Land Data Assimilation System (NLDAS-2) (Xia *et al.*, 2012). In total, three separate data sets are needed to complete the procedure: historical data as a downscaling reference, historical data from the climate model source, and future (i.e., predicted) data from the climate model source. The matching functions defined by each quantile of historical observed reference data and historical modeled climate data are applied to the future modeled climate data. The accuracy of the historical, bias corrected NARCCAP data from each of the models was verified by employing the Equiratio Cumulative Distribution Function (ECDF) matching method (Li *et al.*, 2010; Wang *et al.*, 2014) against the historical climate dataset. After verifying that the bias corrected climate models statistically reproduced the observed historical climate, the calibrated SWAT-VSA model then was forced by output of the RCMs, including precipitation, minimum and maximum temperature, solar radiation, relative humidity, and wind speed for historical model runs (1975-1998) and future scenarios (2045-2068).

One shortcoming of the NARCCAP product is that its RCMs are not forced by the most recent set of GCMs. NARCCAP uses GCM output from Phase 3 of the Couple Model Intercomparison Project (CMIP3), whereas recent statistical downscaling products (e.g., Brekke *et al.*, 2013) use GCMs that participated in CMIP3 and CMIP5 (note that there was not CMIP4). However, despite the inevitable improvements expected in GCM performance with time (Reichler *et al.*, 2008) it turns out that the CMIP3 and CMIP5 projections are remarkably similar after accounting for the differences in GHG emissions scenarios (Knutti & Sedláček, 2013).

Using this climate model framework, we evaluate the hydrologic (watershed discharge, surface runoff, snow melt/accumulation), water quality (NO₃-N, dissolved P, sediment-bound P, total P, sediment export/yield), and N₂ and N₂O emissions implications of a changing climate. Results are presented at the aggregate watershed level for each individual climate model on an annual basis, for the ensemble model mean (each model run through SWAT-VSA and averaged) and range (minimum and maximum result derived from each climate model run through SWAT-VSA), and on a seasonal basis). Results are further broken down by developing quantile metrics to determine deviations from historic values. To do this we employ Q₁₀ and Q₉₀ metrics for all watershed outlet responses analyzed (e.g., flow, NO₃-N, dissolved P, total P, sediment export/yield). The Q₁₀ metric is the response value exceeded 90% of the time; a measure of low flows, and the Q₉₀ metric is the response value exceeded 10% of the time, a measure of high

flows. We then assess the responses of agricultural HRUs, or fields to better explain the finer scale responses observed at the watershed level.

Selection of Extreme Wet/Dry Events

Extreme weather anomalies (wet and dry periods) from the bias-corrected NARCCAP data were selected to test the effect of changes in soil moisture on nutrient cycling and the production of N₂ and N₂O. Years with wet and dry periods were selected by developing indices of climate anomalies (Karl *et al.*, 1999). To select years with dry periods, the maximum length of a dry spell, defined as the maximum number of consecutive days where daily precipitation is less than 1 mm, was counted for each year of both the historical and future climate periods. The average number of consecutive dry days across all climate models was 14 days with a standard deviation of 4 days.

Wet events were defined as the maximum number of consecutive days with daily precipitation depths greater than 1 mm, these were counted for both the historical and future climate periods. However, since there were a high number of wet events (according to our definition above) compared to the number of dry events, we reselected the top three wettest events in the time series. Model output corresponding to these events were extracted from the model runs analyzed for the change in the rate of N₂ and N₂O production, and soil moisture relative to the historical climate data. This analysis focuses on field scale responses and on specific times (and not representative of the long term responses discussed above).

Results

Watershed Model Performance Assessment

According to performance criteria recommended by Daniel *et al.* (2015) and Daniel *et al.* (2007), the results indicate that the model predicted the observed flow, NO₃-N, and DP export well in both the calibration and evaluation periods (Table 1), with a low PBIAS and acceptable NME and NAME metrics. Sediment was predicted well during the calibration period but displayed slightly more bias during the evaluation period. The model slightly under predicted streamflow, NO₃-N, DP, and sediment during the calibration period while slightly over predicted flow and NO₃-N and under predicted DP and sediment during the evaluation period (Table 3-1). N₂O

emissions were over predicted during the evaluation period, although there was not enough measured data to perform a full split-sample evaluation, but still fall within the acceptable range proposed by Daniel *et al.* (2015) particularly for daily model results.

Table 3-1: Percent bias (PBIAS), Normalized Mean Error (NME) and Normalized Mean Absolute Error (NMAE) values for daily model calibration and evaluation periods for WE38 watershed.

Response	Calibration	Evaluation	Calibration	Evaluation	Calibration	Evaluation
	PBIAS		NME		NMAE	
Flow	-7.2	3.0	0.07	0.03	0.94	0.99
Nitrate (NO ₃ -N)	-8.8	3.4	0.09	0.03	1.16	1.15
Phosphorus (DP)	-3.9	-4.0	0.04	-0.04	1.20	1.14
Sediment	-9.4	-30.0	0.09	-0.30	1.74	0.86
N ₂ O emissions	NA	42.2	NA	0.73	NA	1.47

Summary of Future Climatic Projections

Precipitation projections from the seven climate models ranged from slight decreases in mean annual precipitation for two of the models (CRCM-CCSM and WRF-GCM3 models) to increases predicted by the remaining models (Table 3-2). Averaged across the seven models, mean annual precipitation increases by 3.7% compared to the historical period. All climate models predict an increase in precipitation intensity with the exception of HRM3-GFDL model with the model mean intensity increasing by 5.1%. All models also predicted an increase in both the maximum and minimum temperature of 2.5°C. This increase in air temperature results in an average increase in the soil temperature of 1.9°C.

Table 3-2: Change in the mean precipitation, precipitation intensity, temperature (daily maximum and minimum), and soil temperature from 1987-2010 to 2045-2068 for the WE38 watershed.

Model	Change in Precipitation (%)	Change in Precipitation Intensity (%) ^a	Change in Temperature (°C)		Change in Soil Temperature (°C) ^b
			Maximum	Minimum	
	Mean	Mean	Mean	Mean	Mean
CRCM-CCSM	-1.4	0.7	2.8	2.7	2.1
CRCM-CGCM3	6.3	9.2	2.7	2.7	2.2
ECP2-GFDL	12.5	11.4	2.3	2.4	1.7
HRM3-GFDL	3.0	-3.8	3.4	3.0	2.3
MM5I-CCSM	5.8	8.7	2.3	2.4	1.7
RCM3-GFDL	1.9	6.5	2.0	2.5	1.9
WRFG-CGCM3	-1.5	2.6	2.0	2.0	1.5
Model Mean	3.7	5.1	2.5	2.5	1.9

^a The change in the precipitation intensity is calculated by summing the precipitation in time series divided by the total number of days with precipitation in time series.

^b The change in soil temperature is taken directly from the SWAT model output.

Climate Change Effects on Hydrology

Climate change is predicted to cause small changes in the magnitude, and substantial changes in the timing of streamflow in the WE38 watershed. Ensemble model results suggest a small decrease of 1.2% in mean annual flow (Fig. 3-2a), but there is considerable variability among individual climate model predictions (-12.6% to + 22.0%). Despite an increase in December–January flows, a result of the increase in surface runoff (Fig. 3-4a) and the reduction in the ratio of snow to rain during the winter (Fig. 3-4b), winter and spring flows generally decrease (Fig. 3-3a). Flow reductions in late spring and early summer (Fig. 3-3a) are primarily due to greater evapotranspiration (Fig. 3-4c).

The CRCM-CGCM3 and ECP2-GFDL models predict the greatest increase in annual flow (9.5% and 22.0%, respectively, Fig. 3-2a), while the CRCM-CCSM, HRM3-GFDL, RCM3-GFDL, and WRF3-CGCM3 models predict the greatest decrease in annual flow (7.4 to 12.6%, Fig. 3-2a). However, these changes appear to be driven by changes at extreme flows (e.g., four of seven models suggest increases in Q₁₀ flows, five of seven models suggest decreases in Q₉₀ flows, Fig. 3-2a). The CRCM-CCSM, HRM3-GFDL, MM5I-CCSM, RCM3-GFDL, and WRF3-CGCM3 models all predict a decrease in Q₉₀ flows (1.2 to 25.7%, Fig. 3-2a), while CRCM-CGCM3 and ECP2-GFDL models predict an increase in Q₉₀ flows (7.5 and 13.5%, respectively, Fig. 3-2a). The CRCM-CCSM, HRM3-GFDL, and RCM3-GFDL models predict a decrease in Q₁₀ flows (8.9 to 22.2%) while CRCM-CGCM3, ECP2-GFDL, MM5I-CCSM and WRF3-CGCM3 models predict an increase in Q₁₀ flows (3.2 to 43.1%).

Climate Change Effects on Water Quality

The ensemble model mean predicts a small decrease in mean annual NO₃⁻ watershed level export of approximately 0.5% (Fig.3-2b). Similar to streamflow, there is considerable variability among annual model predictions (-9.4% to +19.8%). Most models suggest a substantial increase in Q₉₀ NO₃⁻ export and a decrease in Q₁₀ NO₃⁻ export (Fig. 3-2b), indicating less variability than the historic record displayed. Peak NO₃⁻ export timing does not change considerably, historically occurring in late March, during snowmelt, late May, following fertilizer application and again in December following crop harvest (Fig. 3-3b), but decreases substantially from a peak of 293 kg d⁻¹ occurring in December to 153 kg d⁻¹ occurring in May. The historic late winter (February -

March) NO_3^- export peak is substantially reduced under future conditions, primarily a result of decreased streamflow from reduced snowpack (Fig. 3-4b).

Model mean results indicate that mean annual DP export from the watershed will increase approximately 2.7% (Fig. 3-2c). Similar to streamflow, there is considerable variability among the mean annual change predicted by the models for DP export (-10.2% to +26.0%). Most models suggest substantial decreases in Q_{90} (five of seven models) and increases in Q_{10} (five of seven models) DP export (Fig. 3-2c). Peak DP watershed level export shifts in both timing and magnitude, historically occurring in late May (reflective of spring tillage in the watershed) and December (Fig. 3-3c), and shifting to late April and October with the peak export increased from 0.5 kg d^{-1} to 0.8 kg d^{-1} .

Dissolved P yield from agricultural fields declines slightly on an annual basis (-1.9%, Fig. 3-4f), despite significant increases in surface runoff (Fig. 3-4a). This appears to be due to a decrease in soil P mineralization (Fig. 3-4h), the conversion of insoluble organic P to soluble inorganic P. These results suggest that other, nonagricultural land uses in the watershed are contributing proportionally greater DP loads to the watershed level export.

The mean annual TP watershed level export (sum of DP, sediment bound P, and organic P) is predicted to increase slightly (0.3%), however there is a wide range of predicted responses (-9.2% to +20.5%, Figs. 2d and 3d). Most model predictions (five of seven) result in a decrease in both the Q_{10} and Q_{90} TP export (Fig. 3-2d), suggesting a decrease in both the high and low flows compared to the historic record. Peak TP export, historically occurring in February-March, coinciding with the spring snowmelt flush, shifts to late October, when fields in the watershed are harvested or often fallow (Fig. 3-3d). Peak TP export also increases from a mean of 6.7 kg d^{-1} to 7.7 kg d^{-1} , although the maximum predicted by individual models was far greater, up to 34.1 kg d^{-1} .

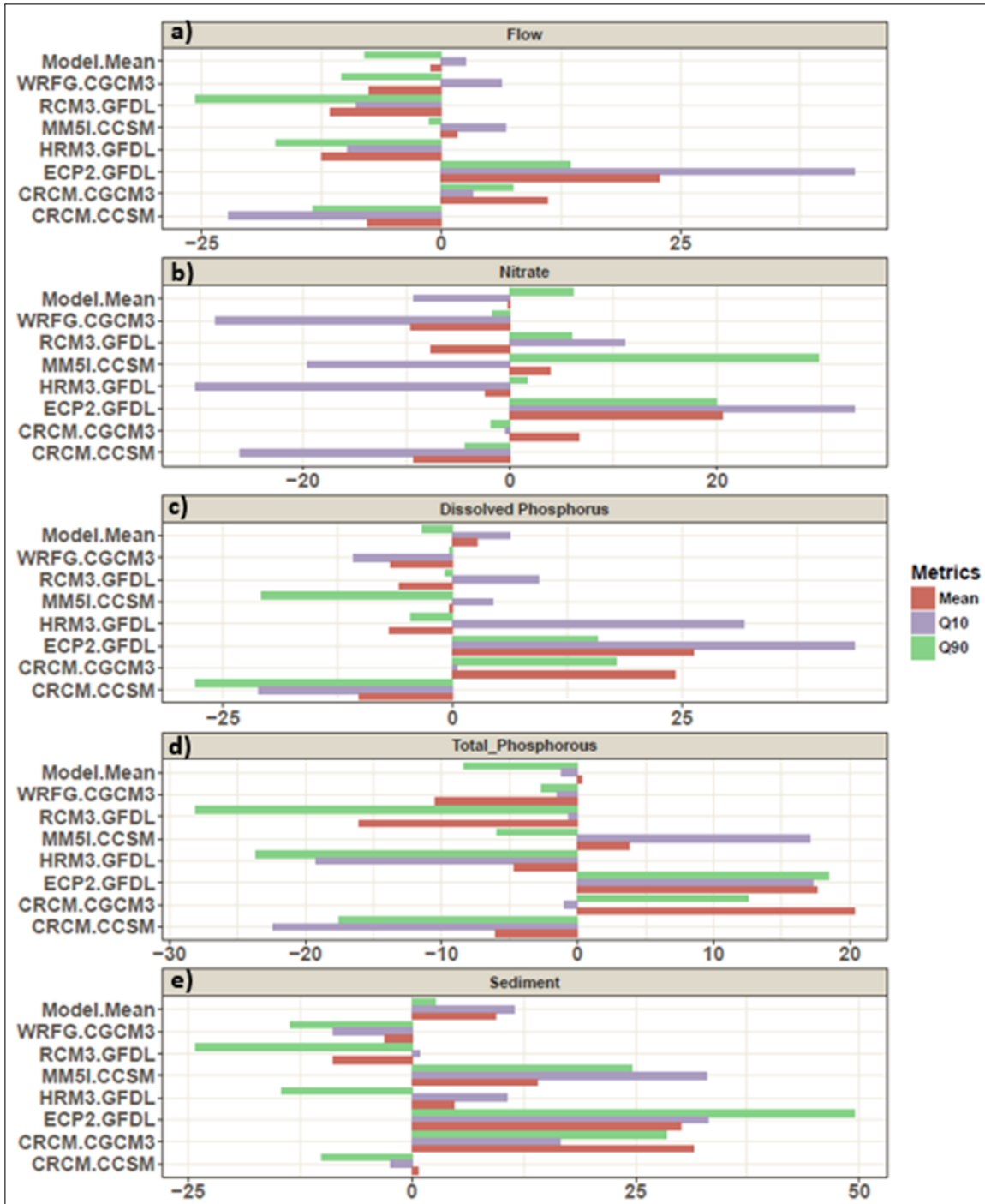


Figure 3-2: Percent change in the mean watershed outlet, Q₁₀, and Q₉₀ for annual flow (a), nitrate (b), dissolved P (c), total P (d), and sediment (e) export for seven climate models relative to the historical scenario (1975-1998) for the future time period (2045-2068).

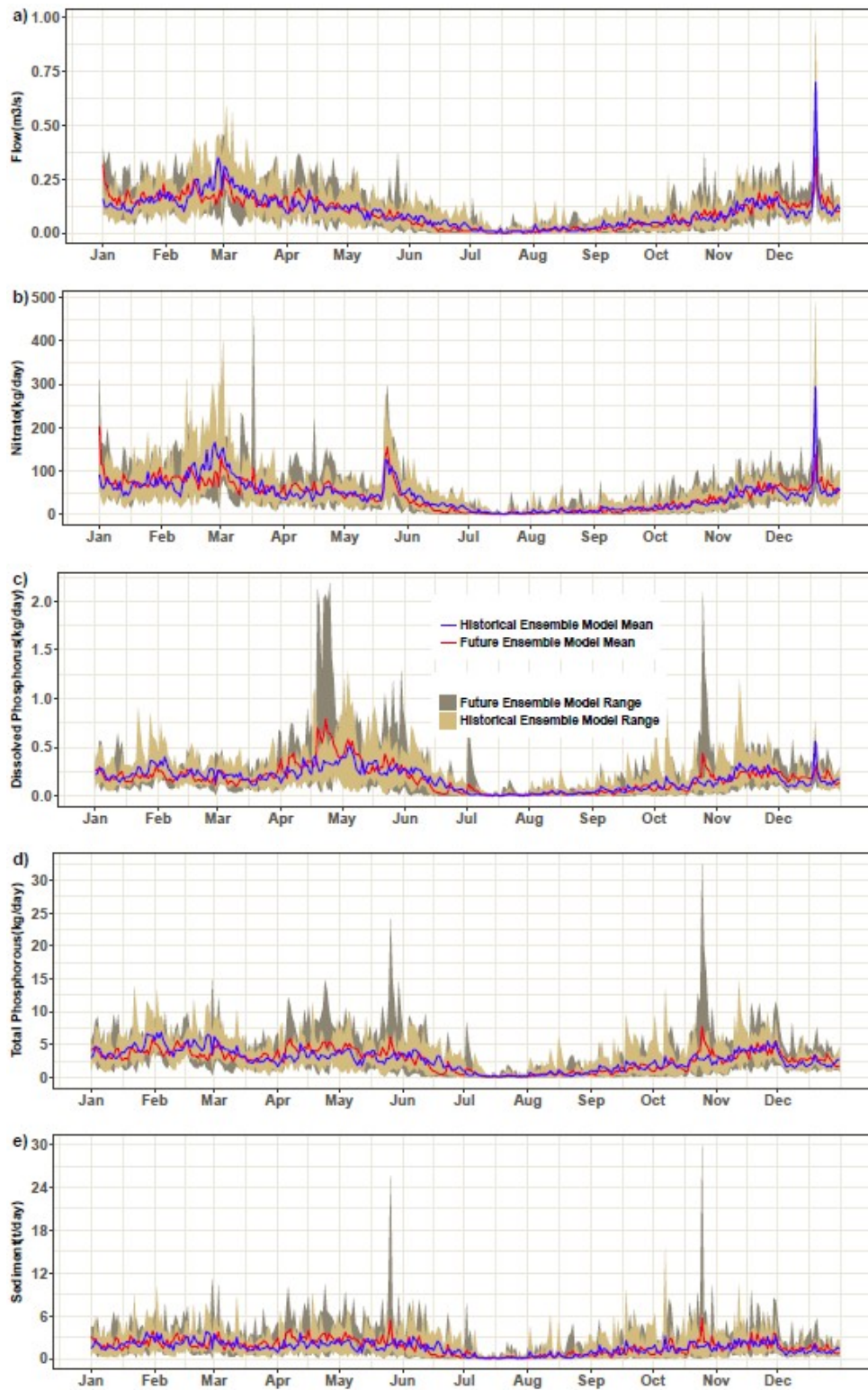


Figure 3-3: Historical (1975 -1998) and future (2045-2068) average-by-day from the ensemble model mean and the ensemble model range for streamflow (a), and the export of nitrate (b), dissolved P (c), total P (d), and sediment (e) for the seven regional climate models.

At the agricultural field scale, almost all models agree that sediment-bound P yield will increase substantially, across all seasons (Fig. 3-4e). Mean annual increases range from 2.1% to 23.8% (Fig. 3-4e), with a model mean increase of 16.1%. Increases in the winter/spring range from 3.6% to 40.6% (Fig. 3-4e), while summer/fall increases, though not as large in magnitude, are still relatively large (-11.8% to 16.5%, note only one model predicts a decrease). The increase in peak export, particularly in the winter/spring is due to the combined effect of increased surface runoff (Fig. 3-4a) and rainfall intensity (Table 3-2), coupled with reduced snow cover (Fig. 3-4b).

Mean annual watershed level sediment export increases 9.6% during the future period, again, with considerable variability among models (-7.4 to +31%, Fig. 3-2e). There are also substantial changes in the Q_{10} and Q_{90} sediment export with mean annual Q_{10} and Q_{90} increasing, 11.5% and 4.2%, respectively (Fig. 3-2e). Much of the annual increase is due to increased sediment export in the winter/spring; there is very little change in summer sediment export (Fig. 3-3e). Peak sediment export increases from 3.1 tons d^{-1} , historically occurring in late February- early March, to 5.9 tons d^{-1} in October, again, coinciding with harvest of the agricultural fields and reduced ground cover (Fig. 3-3e).

Mean annual sediment yield from agricultural fields in the watershed increases by 16.6% (Fig. 3-4d). All models predicted substantial increases in sediment yield in both the winter/spring (1.8 to 36.7%) and most models predicted increases in the summer/fall (five of seven models, Fig. 3-4d). This is consistent with and of similar magnitude as the increase in surface runoff predicted for both periods (Fig. 3-4a). Note that the increase in sediment-bound P (Fig. 3-4e) is almost directly proportional to the increase in sediment yield (Fig. 3-4d).

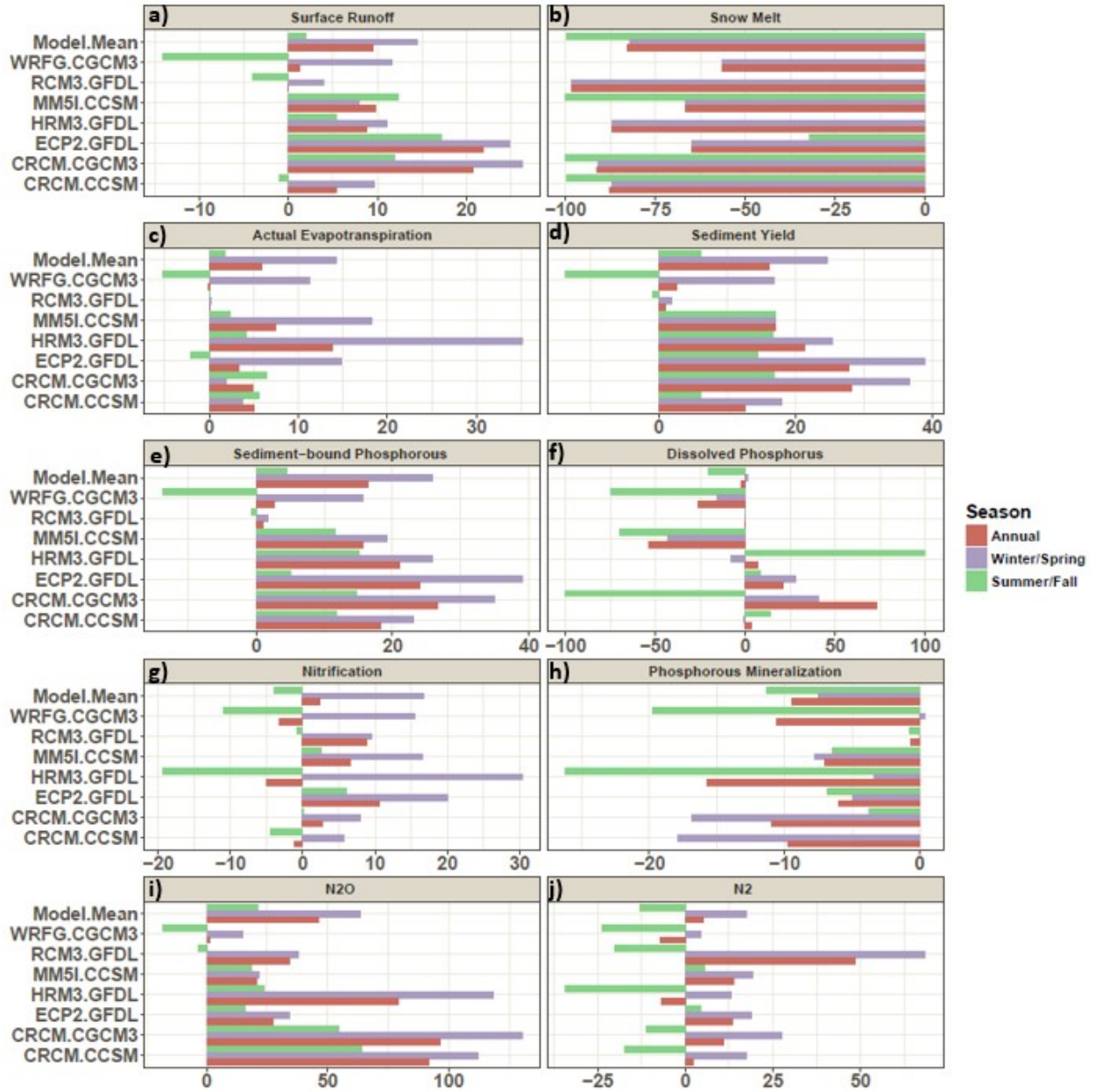


Figure 3-4: Annual and seasonal changes (%) for surface runoff (a), snowmelt (b), actual evapotranspiration (c), sediment yield (d), sediment bound P export (e), dissolved P export (f), nitrification rate (g), phosphorus mineralization rate (h), N₂O emission rate (i), and N₂ (j) emission rate averaged across agricultural HRUs for seven climate models relative to historical scenario (1975 -1998) for the future time period (2045-2068).

Emissions of N₂O and N₂

Figure 3-4i shows mean annual increases in the emission of N₂O of 46.3 %, driven primarily by winter/spring increases (65.4%); summer N₂O emissions also increase by 18.6%. N₂ emissions increase on an annual basis (5.0%, Fig. 3-4j), again, driven by substantial increases in winter/spring emissions (12.9%); a slight decrease is predicted for summer/fall (-9.4%). The increase in winter/spring N₂ and N₂O emissions is driven by increased soil nitrification (Fig. 3-4g), which provides more labile NO₃⁻ (the reactant for denitrification) coupled with increased soil temperatures (Table 3-2), which speeds up microbial denitrification.

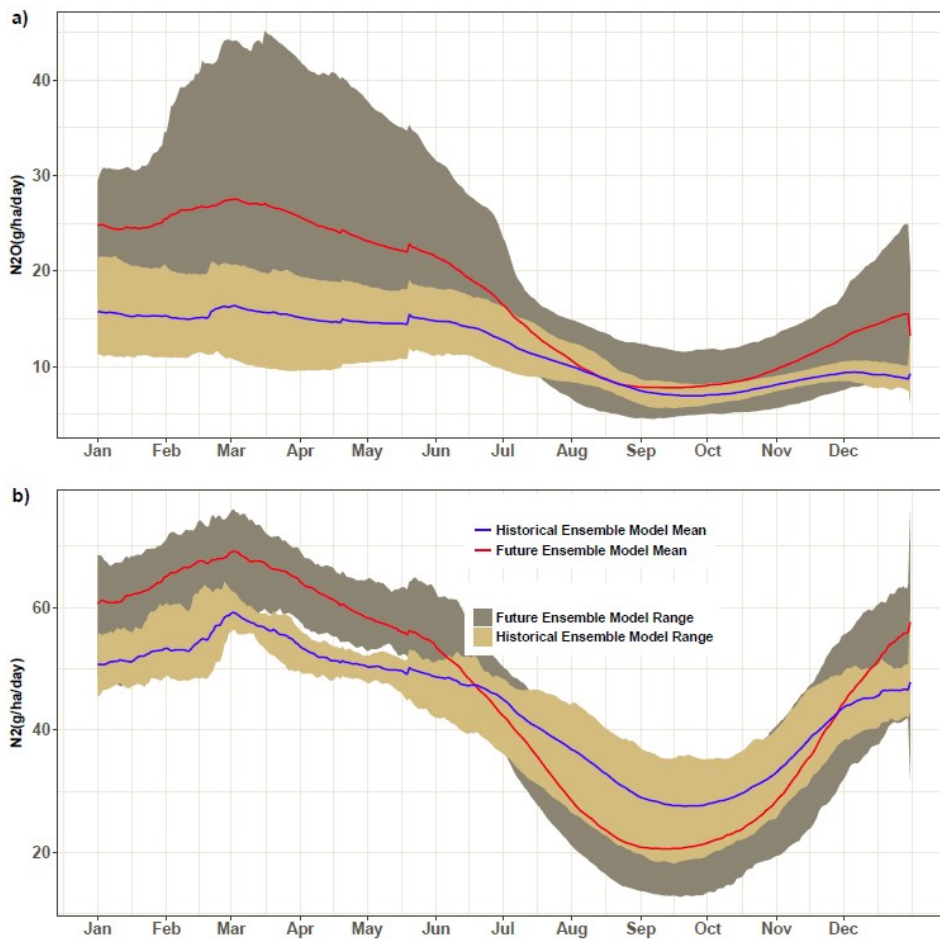


Figure 3-5: Model predicted average-by-day N₂O (a) and N₂ (b) emission rates for the seven climate models for the 24-year future time period and the historical period.

The ensemble model mean predicts substantial increases in N₂O emissions across almost the entire year compared to the historical baseline (Fig. 3-5a), except for a brief period in late August

where the historical and future emissions are equivalent. The greatest increase in N_2O emissions occurs in March-April, nearly doubling the historical emissions, and coincides with a period of high watershed discharge (Fig. 3-3a), indicative of saturated soils. Similar to N_2O , the ensemble model mean predicts large increases in emissions of N_2 from December to late June but then predicts decreases from July through late November (Fig. 3-5b). Increased emissions of both N_2O and N_2 are driven by higher winter soil temperatures (Table 3-2), which increase the nitrification rate in the soil (Fig. 3-4g), making more N available for denitrification (Figs. 3-4i and j, and 3-5). Increased soil temperatures (Table 3-2) similarly increase the microbial respiration rates, which fosters denitrification. Thus, despite the increase in soluble N available in the soil, less is exported from the watershed (Fig. 3-3b) because denitrification balances this increase.

Figure 3-6 shows the N_2O and N_2 emission under wet (Fig. 3-6a) and dry (Fig. 3-6b) conditions. The high emissions areas of both N_2O and N_2 in the watershed tend to coincide with areas of high soil moisture irrespective of whether the average watershed condition is wet or drier. That is, hotspots of N_2 and N_2O emissions are generally found in areas of higher soil moisture. The management influence is also clear in Fig. 3-6, where high soil moisture areas do not always result in areas of high emissions; high emission areas are also found on landuses that receive substantial fertilizer or manure additions, such as corn, increasing the N available to drive denitrification.

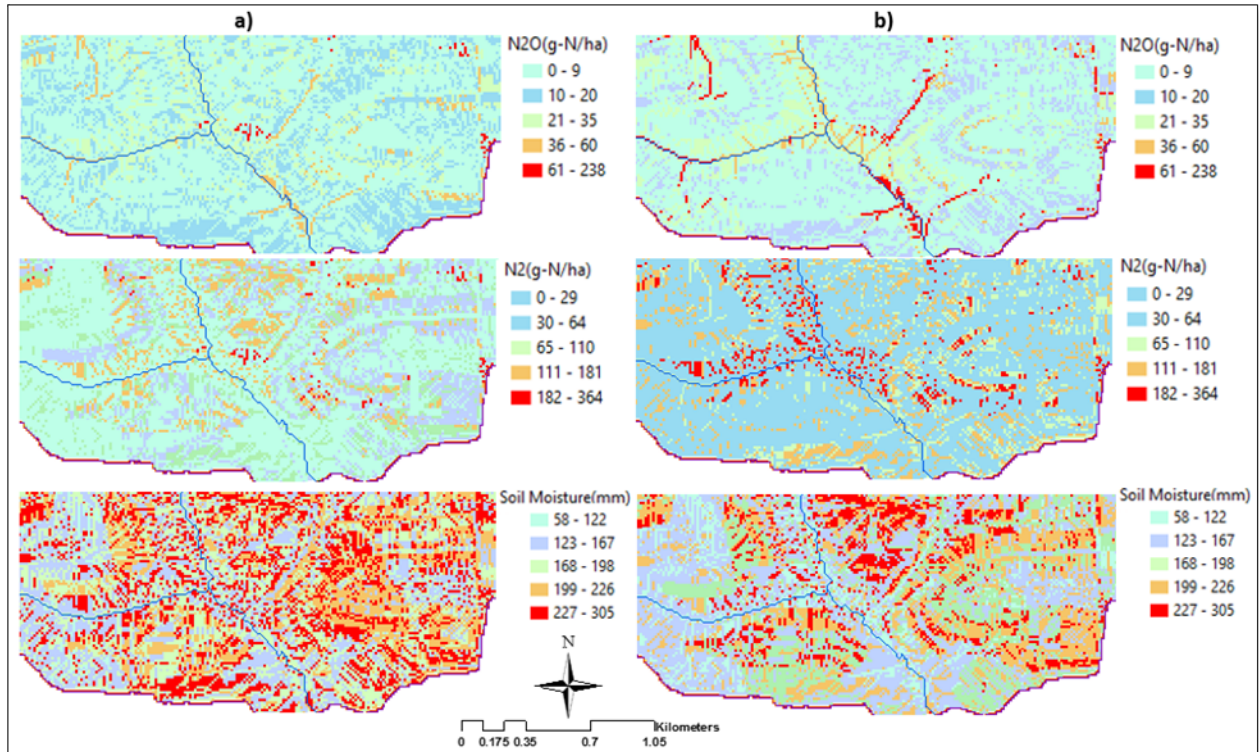


Figure 3-6: Spatial comparison of wet (a) and dry (b) weather periods on mean daily N₂O and N₂ flux, and soil moisture conditions for the future ensemble model mean.

Discussion

Ensemble modeling highlights how climate change and climate anomalies are likely to affect water availability and water quality in the Chesapeake Bay region and the level of uncertainty in those predictions. The results from this analysis indicate the region is likely to experience a slight decrease in mean annual flow although the magnitude of the change differs among the climate models (Fig. 3-2a). However, a slight increase in flow is predicted during the winter/spring (2.7%) while a significant decrease in flow is predicted during the summer/fall (-12.7%, Figs. 3-2a and 3-3a). These results corroborate findings by others in the region. For instance, Hayhoe *et al.* (2007), Rob *et al.* (2000), Lu *et al.* (2015), and Najjar *et al.* (2010) all predicted increases in seasonal streamflow variability with decreased flow during the summer due to increased evapotranspiration (driven by higher temperatures) and increased flow in the winter and spring due to increased winter precipitation.

The predicted decline in flow during summer from watersheds such as WE-38 could affect the ecology of the Chesapeake Bay estuary; in particular reducing dissolved oxygen, instream habitat, and increasing the potential for harmful algae blooms (Meyer *et al.*, 1999; Neff *et al.*, 2000). The increase in flow during winter/spring occurring on fields that have been harvested and thus have less plant cover, could result in increased sediment delivery to both reservoirs in the watershed and to the estuary (Cerco, 2016). Furthermore, the increase in winter flow is indicative of higher soil temperatures (Table 3-2), and reduced snowpack (Fig. 3-4b) in the watershed. These changes could result in producers in the regions shifting planting, field tillage, and fertilizer operations to earlier in the year to take advantage of warmer temperatures (Sims & Coale, 2002), which could change the timing of nutrient and sediment export from the watersheds.

Sediment export tends to be a function of streamflow; mean annual sediment export increased across all models (Fig. 3-4d). This increase in sediment export from landscape is due to increased runoff and precipitation intensity during winter and spring when there is reduced groundcover following harvest (Fig. 3-4d). The increased future sediment export is primarily derived from landscape sources (as opposed to channel sources). This is determined by subtraction: the HRU sediment yield was subtracted from the sediment yield at the outlet of the watershed. The ratio of channel-originated sediment to the HRU-originated sediment is 0.18 for the historic period and 0.20 for the future period. However, over time increased deposition of landscape sediment in channels could increase the contribution of the channel to overall export. Increased sediment deposition in the channels could also alter stream geomorphology, increase flooding and stream water temperature (Rehg *et al.*, 2005), reduce light penetration, and affect submerged aquatic vegetation (Bilotta & Brazier, 2008).

Phosphorus export exhibited substantial variability across models; with some climate models predicting slight increases in mean annual P export while others predict decreases (Figs. 3-2c and 3-2d and 3-4e and 3-4f). The ensemble model mean predicted an increase in mean annual P export; which is counter to predictions made by Roberts *et al.* (2009) for the Chesapeake Bay, who predicted a 19% reduction in P using the Spatially Referenced Regression On Watershed Attributes (SPARROW) model, but similar to results by Chang (2004) for southeastern Pennsylvania, who predicted increased P export. Our results suggest that the increase is largely

driven by increases in sediment-bound P export during the winter/spring (Fig. 3-4e), and increased precipitation intensity (Table 3- 2) and not from increased soil P mineralization (Fig. 3-4h). The increase in P export could result in eutrophication and depletion of dissolved oxygen in the stream (Boesch *et al.*, 2001a). Furthermore, the increase in spring DP and TP export is particularly troubling for the estuary as P delivered in the spring flush tends to set up more aggressive summer eutrophication conditions (Boesch *et al.*, 2001).

Most models used in this analysis predicted a slight decrease in mean annual NO₃⁻ export, but slight increases during the winter/spring season (3.0%), similar to results by Chang (2004) for southeastern Pennsylvania while significant decreases are predicted during the summer/fall season (-12.0%). The annual decrease in NO₃⁻ export is due to substantial increases in N₂O and N₂ emissions from denitrification (Fig.3-4i and 3-4j), although there is slight increase in nitrification (Fig. 3-4g). Increased nitrification creates a greater pool of N available for transport as NO₃⁻ is more mobile in the soil than organic N or NH₄⁻, (the reactants in N mineralization and nitrification, respectively). During the winter/spring, the increase in nitrification (Fig. 3-4g) provides more NO₃⁻ to the system than can be utilized by denitrification because this system is C limited (<5:1 C:N ratio). This process is driven by increased temperatures, soil moisture levels, and soil N levels (Agehara & Warncke, 2005; Guntiñas *et al.*, 2012). These results are indicative of an increase in the speed of the N-cycle, via mineralization, nitrification, and denitrification. While processes such as denitrification can counter the impact of increased soil N availability, it could ultimately result in producers needing to apply more N fertilizer to ensure adequate nutrition for crops, which could further increase export. In terms of spatial variability, these results corroborate the hot moment/hot spot theory of N emissions. Indeed, Fig. 3-6 shows those areas of the landscape with greater soil moisture levels are the primary sources of elevated N₂O emissions. However, the spatial heterogeneity also depends on soil NO₃⁻ and C availability, soil temperature, and management practices (Wagena *et al.*, 2017).

Finally, these results indicate that agricultural soils could continue to serve as a source of N₂O emissions even without fertilization for a long period of time (average soil total N is 16,667 kg/ha). However, there are practices that could reduce both N₂O emission and NO₃⁻ export. For example, Beheydt *et al.* (2008) and Six *et al.* (2004) recommended less intensive cultivation practices (e.g., no till, injected manure) which increases C sequestration and reduces N₂O

emissions. Alternatively, agriculture in the region may adapt to the new conditions, for instance by planting earlier to take advantage of increased soil temperatures or by introducing new crop varieties that may be adapted to the higher temperatures, altered soil moisture and nutrient cycling rates.

Conclusions

Climate change will likely alter water availability and quality. Results indicate that the future climate projected by most of the climate models used in this study will result in increased flow, sediment, P, and NO₃⁻ export during the winter and spring, while decreases are expected during the summer and fall, although there is considerable variability among models. The increase in N₂O and N₂ emissions coupled with the increased nitrification and N mineralization suggests that the N-cycle is speeding up; thus, denitrification balances the increased nitrification and potentially mitigates water quality degradation. Increased P export is driven primarily by increased sediment bound P export from the watershed, driven by increased surface runoff and rainfall intensity coinciding with periods of reduced soil plant cover. These results suggest biogeochemical cycles could be substantially altered, which may ultimately result in changes to agricultural management practices. The results of this effort will also help managers to develop strategies to maintain crop productivity, and water quality. Sustainable intensification should focus on the timing of planting and fertilizer applications so that crops are actively growing when fertilizers are applied. Precision agriculture and critical source area models can be utilized to determine where and how much fertilizer should be applied. With proper planning, agricultural management could increase crop yields, reduce greenhouse gas emissions, and improve water quality.

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CHAPTER 4

AGRICULTURAL CONSERVATION PRACTICES CAN HELP MITIGATE THE IMPACT OF CLIMATE CHANGE

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Abstract

Agricultural best management practices (BMPs) are increasingly and widely employed to reduce diffuse nutrient pollution. Climate change can complicate the development, implementation, and efficiency of BMPs by altering hydrology, nutrient cycling, and erosion. This research quantifies the impact of climate change on hydrology, nutrient cycling, erosion, and agricultural conservation practices in the Susquehanna River Basin (northeastern United States). We initialize the Soil and Water Assessment Tool-Variable Source Area model using weather, soil, and land use data and test four BMPs (buffer strips, strip crop, no-till, and tile drainage) for their response to climate change. We force the calibrated model with six downscaled global climate models (GCMs) for a historic period (1990-2014) and two future scenario periods (2041-2065) and (2075-2099) and quantify the impact of climate change on hydrology, nitrate-N (NO_3^-), total N (TN), dissolved phosphorus (DP), total phosphorus (TP), and sediment export with and without BMPs. We also tested prioritizing BMP installation on the 30% of agricultural lands that generate the most runoff (e.g., critical source areas-CSAs). Compared against the historical baseline and excluding the impact of BMPs, the ensemble model mean (\pm standard deviation) predictions indicate that climate change results in annual increases in flow ($4.5 \pm 7.3\%$), surface runoff ($3.5 \pm 6.1\%$), sediment export ($28.5 \pm 18.2\%$), and TN export ($9.5 \pm 5.1\%$), but decreases in the export of NO_3^- ($12 \pm 12.8\%$), DP ($14 \pm 11.5\%$), and TP ($2.5 \pm 7.4\%$). When agricultural BMPs are simulated, most do not appreciably change the overall water balance; however, tile drainage and strip crops decreased surface runoff generation and the export of sediment and DP and TP, while buffer strips reduced N export substantially. Installing BMPs on CSAs results in nearly the same level of performance for most practices and most pollutants. These results suggest that climate change will influence the performance of BMPs and that targeting BMPs to CSAs can provide nearly the same level of water quality impact as more widespread adoption.

Introduction

Climate change has the potential to impact hydrology and diffuse nutrient export from agricultural landscapes (Howarth *et al.*, 2006). In the humid temperate Eastern United States (US), climate predictions suggest that precipitation quantity and intensity will continue to increase (especially during the winter and spring), resulting in greater diffuse nutrient and sediment export from agricultural landscapes (Chang *et al.*, 2001; Cousino *et al.*, 2015). This increased export has a number of deleterious consequences for receiving water bodies: accelerated eutrophication and harmful algal blooms (Burgin *et al.*, 2007), undesirable changes in the river structure and function, and decreasing storage capacity or flood control of reservoirs (Cerco, 2016; DePhilip & Moberg, 2010). In addition, the loss of valuable nutrients and topsoil from agricultural fields decreases productivity or increases management intensity (Lal, 1998) .

Agricultural best management practices (BMPs) are increasingly and widely used to reduce the impact of diffuse pollutant export from agricultural landscapes (Ullrich *et al.*, 2009). For instance, conservation tillage, or no-till, enhances soil organic carbon, soil quality, and soil aggregation, leading to less soil erosion in agricultural landscapes (Roldán *et al.*, 2007). BMPs such as riparian vegetation, strip crops, and buffer strips can all help reduce diffuse pollutants by reducing inputs to the crop, enhancing sequestration of nutrients in plant tissue, or reducing surface and subsurface losses due to hydrologic pathway alterations (Carpenter *et al.*, 1998). However, it is not clear what impact a changing climate will have on the function of BMPs. For instance, increased precipitation volume and intensity may overwhelm many BMPs like riparian buffers, but higher temperatures, longer growing seasons, and more rainfall might cause that same buffer to mature more quickly, thus trapping more sediment and sequestering more nutrients. Thus, agricultural conservation practices need to be assessed for performance under a changing climate (Hatfield *et al.*, 2004).

In this study, we assess the effects of climate change on hydrology, water quality, and agricultural conservation practices in Susquehanna River Basin. The Susquehanna River watershed is the largest source of nutrients and sediment to the Chesapeake Bay, and has been the focus of intensive BMP implementation to reduce nutrient and sediment export from agricultural lands. The installation of BMPs is largely driven by the US Environmental

Protection Agency (USEPA) Total Maximum Daily Load (TMDL) to reduce nutrient and sediment to the Bay by approximately 25%. However, a major uncertainty with respect to BMPs in the watershed is the complicating influence of climate change on their function and efficacy. The Susquehanna River Basin is already experiencing the impact of a changing climate, with increasing temperatures reducing winter snowpack and increasing winter runoff, and more frequent high intensity rainfall events mobilizing more sediment (Hayhoe *et al.*, 2007). The predicted changes to climate in the region include continued increases in temperature, anywhere between 1-5°C dependent on emissions scenarios and season, more precipitation in the winter and spring, primarily as rainfall rather than snowfall, and less rainfall in the late summer and fall (Sheffield *et al.*, 2013a).

These changes to precipitation and temperature are likely to alter the timing and magnitude of streamflow and nutrient/sediment production and transport in the watershed. For instance, increased spring nutrient export from the watershed the estuary can set up conditions that cause particularly acute summer hypoxia (Boesch *et al.*, 2001b), and drier conditions in the summer and fall have been shown to increase the buildup of soil nutrients that can subsequently be flushed from the system when wet conditions return (Kaushal *et al.*, 2008; Wetz *et al.*, 2013). Temperature changes can alter nutrient cycling, plant growth, evapotranspiration, and soil water content, which all impact the availability and transport of nutrients from agricultural fields. Thus, BMPs designed and installed to handle historic weather conditions may not function as well under a changing climate.

In order to quantify the impact of climate change on agricultural BMP effectiveness, we use the Soil and Water Assessment Tool-Variable Source Area (SWAT-VSA) model (Easton *et al.*, 2008). SWAT-VSA is used because it represents agricultural conservation practices, can simulate hydrologic and biogeochemical processes that are affected by climate change, and can easily incorporate many common agricultural BMPs (Arabi *et al.*, 2008). The calibrated SWAT-VSA model was forced with six downscaled regional climate models derived from the Intergovernmental Panel on Climate Change Coupled Model Intercomparison Project 5 (CMIP5) dataset to analyze the impact of future climate change on four selected agricultural BMPs. We analyze the results of each climate model, as well as the ensemble model mean, for their impact on hydrology and water quality with and without the four BMPs on agricultural lands in the

Susquehanna River Basin. In an effort to define optimal BMP placement in the watershed, we leverage the ability of SWAT-VSA to represent the VSA hydrology that dominates the region and prioritize BMP placement on the 30% of the agricultural lands that cause the greatest nutrient and sediment loss. Results highlight processes, conservation practices, and time frames that are vulnerable to climate impacts and point to watershed mitigation and adaptation strategies to address the long-term impacts of climate change in the basin.

Materials and Methods

Study Area Description

The Susquehanna River Basin contributes more than 50% of the freshwater input to the Chesapeake Bay, drains approximately 71,000 km², or 42% of the Bay watershed (Ko & Baker, 2004) and largely controls salinity in the Bay (Gibson & Najjar, 2000). The Susquehanna River Basin drains areas in the states of New York, Pennsylvania, and Maryland, has six major sub basins (Upper, Chemung, Middle, West Branch, Juniata, and Lower subbasins, Fig. 4-1), and its elevation ranges from -10 to 960 m. The climate varies along a north-south gradient, with the northern portion of the basin receiving more precipitation (1240 mm) than the lower basin (838 mm) (DePhilip *et al.*, 2010). The land use of the basin consists of forest (70%), agriculture (22%), developed (7%), and water (1%). Soils are mainly silt loam or silty clay loam (Ray *et al.*, 2016) with soil hydrologic group C ratings dominating (NRCS, 1998). The northern region of the basin is typified by steep to moderate hillslopes of glacial origins with shallow permeable soils, underlain by a restrictive layer that causes perched water tables to form. Soils have depths ranging from <50 cm to >1 m and are underlain by a fragipan restricting layer (e.g., coarse-loamy, mixed, active, mesic, to frigid Typic Fragiudepts, Lytic or Typic Dystrudepts common to glacial tills). The southern region of the basin was never glaciated.

SWAT Model Description

The Soil and Water Assessment Tool (SWAT) model is a process-based, semi-distributed watershed model developed to simulate landscape processes and predict the impact of land management practices on water availability and water quality (Arnold *et al.*, 1998). SWAT requires weather, soil, land cover, and land management data to simulate surface and subsurface

hydrology and various chemical, nutrient, and sediment fluxes. In SWAT, the watershed is divided into sub-watersheds and then further into hydrologic response units (HRUs), which are unique combinations of soil type and land use. SWAT-VSA re-conceptualizes the standard SWAT to account for areas of the landscape subject to variable saturation dynamics (Easton *et al.*, 2008). In SWAT-VSA the area of each HRU is defined by the coincidence of land use and wetness index class determined from a Topographic Index (TI) to differentiate areas of the landscape with respect to their moisture storage and saturation index (Easton *et al.*, 2008). SWAT-VSA has been shown to provide better predictions of soil moisture and runoff generation than the standard SWAT model in watersheds with similar physical characteristics and climate to the study watershed (Easton *et al.*, 2008). The version of SWAT-VSA used here also includes modifications to the P routines of Collick *et al.* (2016), which improves the simulations of surface applied P, particularly from manures.

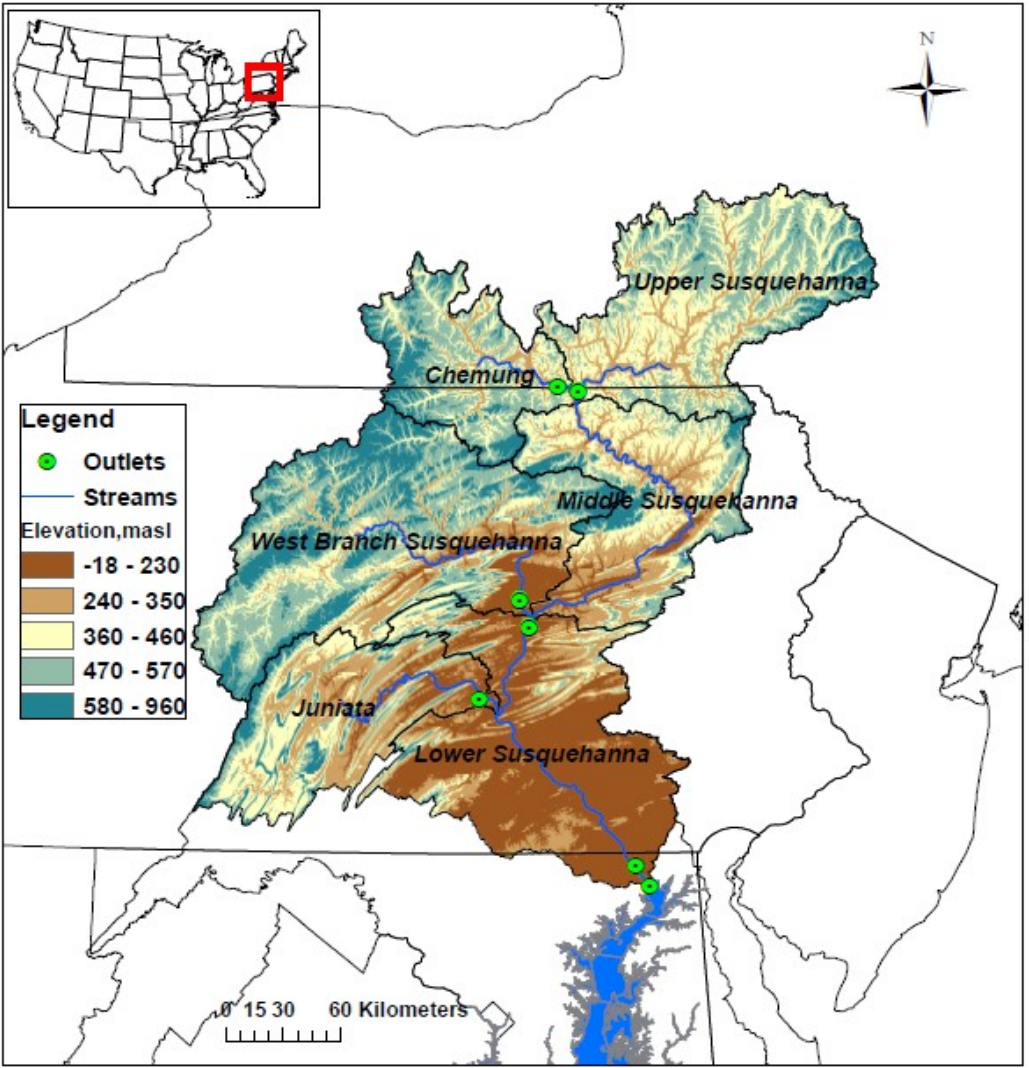


Figure 4-1: Map of the Susquehanna River basin, major subbasins, and elevation.

Model Inputs

The Susquehanna River Basin SWAT-VSA model was initialized with 10 m digital elevation model (DEM) obtained from the United States Geologic Survey (USGS) National Elevation Dataset (NED) (Guenther *et al.*, 2007) using ArcSWAT 2012 and TopoSWAT (Fuka & Easton, 2016). TopoSWAT automates the SWAT-VSA initialization process by assimilating soil data, creating the TI map, overlaying the soil and TI maps, and developing the required database for model initialization. Soils data included in TopoSWAT are based on the Food and Agriculture Organization (FAO) soils database (FAO, 2007). TopoSWAT downscales the FAO soils data

using the TI class as a proxy to distribute sand, silt and clay content, available soil water, hydraulic conductivity, bulk density, and soil depth, and has been shown to provide more accurate estimates of these parameters than finer resolution soils data such as SSURGO (Fuka et al., 2016). The land use of watershed was obtained from National Land Cover Database 2011, the most recent national land cover product created by the Multi-Resolution Land Characteristics (MRLC) Consortium (Homer *et al.*, 2015). The model was forced with daily historic weather data from the Climate Forecast System Reanalysis (CFSR) (Fuka *et al.*, 2014), including precipitation, temperature (min and max), relative humidity, wind speed, and solar radiation from 1979 to 2014. Weather data were interpolated to the centroids of the six subbasins using an inverse distance weighting squared procedure.

Model calibration and evaluation

Model calibration followed a cascading procedure, first calibrating all headwater basins (Upper Susquehanna, Chemung, West Branch, and Juanita subbasins) to observed USGS gage data. Next, the second order basin, the Middle Susquehanna was calibrated, leaving all parameter values for the headwater basins unchanged. Finally, the Lower Susquehanna subbasin was calibrated, leaving all parameter values for the headwater and second order basins unchanged. The model was calibrated and evaluated using the SWAT Calibration and Uncertainty Procedure (SWAT-CUP) (Arnold *et al.*, 2012) and the SUFI2 (Sequential Uncertainty Fitting) optimization algorithm with the objective function set to percent bias (PBIAS) method. The percent bias was used to ensure the model captured the mass balance, since the main focus of this work was quantifying the relative impact of climate change on BMPs rather than absolute daily prediction accuracy. The SWAT-VSA model performance was evaluated based on three metrics, PBIAS, the normalized mean error (NME), and the normalized mean absolute error (NMAE), against the historical measured data for flow, sediment, NO₃-N, and, TP from 1985 to 1994 for calibration and 2002 to 2011 for model evaluation. The NME is an index of relative bias providing an estimate of overprediction (NME > 0) or underprediction (NME < 0) of the model. The NMAE (which is scaled relative to the observed mean) indicates discrepancies between model predictions and measured values, with smaller NMAE corresponding to model simulations closer to observed values (Pourmokhtarian *et al.*, 2012). The daily flow in the six subbasins was obtained from the USGS waterdata website (<https://waterdata.usgs.gov/nwis/sw>). Monthly

sediment, NO₃-N, and TP data for the six subbasins were obtained from Hirsch *et al.* (2010) from (<https://cbrim.er.usgs.gov/methods.html>).

Incorporation of Climate Data

The most recent climate change models from the World Climate Research Programme's (WCRP's) Coupled Model Intercomparison Project Phase 5 (CMIP5) were obtained from the Earth System Grid Federation (ESGF): <https://esgf-data.dkrz.de/projects/esgf-dkrz/> and include two scenarios: RCP2.6 (peak in radiative forcing at 2.6 W m⁻² before 2100 and decline thereafter); RCP8.5 (increasing radiative forcing to 8.5 Wm⁻² by 2100). We initially elected to use two RCPs, RCP2.6 and RCP8.5, to represent the extremes of climate change potential on BMP performance. Six global climate models (GCMs) were selected based on Maloney *et al.* (2014) and Sheffield *et al.* (2013a and 2013b), who analyzed and ranked GCMs based on performance metrics to quantify the biases relative to observed seasonal precipitation, seasonal surface air temperature, and hydroclimate extremes in the Northeast and Mid-Atlantic US. The GCMs incorporated include the BCC-CSM1.1 (Beijing Climate Center, China Meteorological Administration), the CCSM4 (National Center for Atmospheric Research), the CSIRO-Mk3.6.0 (Commonwealth Scientific and Industrial Research Organization in collaboration with the Queensland Climate Change Centre of Excellence), the IPSL-CM5A-LR (Institut Pierre-Simon Laplace), the MIROC5 (Atmosphere and Ocean Research Institute The University of Tokyo, National Institute for Environmental Studies, and Japan Agency for Marine-Earth Science and Technology), and the MPI-ESM-LR (Max Planck Institute for Meteorology).

Each of the six CMIP5 GCMs was downscaled and bias corrected using a cumulative distribution function matching method, and the historical data from the GCMs were checked for bias/error correction against observed historical data (Li *et al.*, 2010; Wang *et al.*, 2014). This downscaling and bias correction was performed using the QMAP R package (Gudmundsson *et al.*, 2012) and requires three separate data sets to complete the procedure: historical data as a downscaling reference, historical data from the climate model source, and future, or predicted data from the climate model source. The matching functions defined by each quantile of historical reference and historical modeled data are applied to the future modeled data. The accuracy of the historical, bias-corrected GCM data from each of the models was verified by

employing the Equiratio Cumulative Distribution Function (ECDF) matching method (Li *et al.*, 2010) against the historical climate dataset. Detailed description of downscaling and bias correction can be found in Wagena *et al.* (2016). The calibrated SWAT-VSA model then was forced by the downscaled output of the six GCMs, including precipitation and minimum and maximum temperature for historical model runs (1990-2014) and two future periods (2041-2065) and (2075-2099).

Incorporation of Agricultural Conservation Practices

The impact of climate change on agricultural BMPs in the Susquehanna River Basin was evaluated by simulating four BMPs in the model, which was then forced by the downscaled CMIP5 GCM data. We evaluated each of the BMPs individually as well as the combined effect of all BMPs together. We evaluated these BMPs by simulating their effect on all of the agricultural HRUs in the watershed, representing a best-case scenario, and on the three highest agricultural TI classes, representing 30% of the agricultural land most susceptible to runoff, and nutrient/sediment export. Evaluating the BMPs' performance on the most critical source areas in the watershed highlights the impact that targeting can have. The model was also run with no BMPs for each future time period to serve as a baseline against which to compare BMP implementation. Based on the work of Arabi *et al.* (2008), BMPs and the parameters controlling BMP inclusion in the model were identified, and four agricultural conservation practices that are common in the region were simulated: buffer strips, strip crops, no-till, and tile drainage.

Buffer Strips

Field buffer strips consist of areas along stream channels or the edge of fields that are permanent unharvested vegetation intended to reduce sediment and nutrient delivery from farm fields to surface water bodies. Buffer strips are modeled in SWAT by changing the FILTERW parameter (width of the buffer strip) and is then used to calculate trapping efficiency. Based on the work of Bracmort *et al.* (2006), a 5 m buffer width was simulated.

Strip Crops

Strip crops consists of narrow rows of alternating crop types. The practicing is commonly implemented in upland areas to reduce the surface runoff volume, the peak runoff rate, and rill

and sheet erosion (Arabi *et al.*, 2008). Based on the work of Arabi *et al.* (2008), strip crops were represented in SWAT by lowering the curve number (CN) by three units to reduce surface runoff and peak flow rate, changing the USLE support practice factor (USLE_P) to 0.02 to reduce sediment export, and increasing the Manning's roughness coefficient for overland flow (OV_N) to 25 to reduce peak flow and slow surface runoff.

Tile Drainage

Tile drainage is implemented to drain excess water from the soil root zone to support crop growth. Tile drainage also reduces surface runoff from poorly drained soils. Tile drainage is represented in SWAT by setting the depth to subsurface tile drain (DDRAIN) to 1 m, the drain tile lag time (GDRAIN) to 48 hr, the drain spacing to 15 m, and effective radius of the tile drains to 50 mm.

No Till

No till is the agricultural practice of growing crops without disturbing the soil through tillage, thereby reducing erosion and sediment bound contaminants. No till was represented in the model by setting the tillage management operation to ZEROTILL in the management file, which means that there is no residue incorporation into the soil profile.

Results

Model Performance Evaluation

Table 4-1 shows the model performance for daily and monthly flow, and monthly sediment, NO₃-N, and TP export. According to criteria described by Daniel *et al.* (2015) SWAT-VSA predicted all constituents reasonably well. The PBIAS values during calibration and evaluation period of both daily and monthly flow show a slight under prediction by the model, but the PBIAS values are all in the acceptable range based on the recommendations of Daniel *et al.* (2007) and Daniel *et al.* (2015) The model slightly over predicted NO₃- and TP during calibration (NME = 0.04, 0.20) period, respectively while it under predicted NO₃- (NME=-0.37) and over predicted TP (NME=0.21) during the evaluation period. The NME of the calibration and evaluation periods for sediment indicates under predictions (NME=-0.52, -0.16), respectively.

The PBIAS values of sediment (PBIAS = 24.8, 16.4) shows the model under predicts sediment, NO₃⁻ (PBIAS= -4, 36.9) indicates over prediction of NO₃⁻, and TP (PBIAS = -19.9, -20.6) indicates the model over predicts TP during the calibration and evaluation periods respectively, and the PBIAS values are in range with recommended values by Daniel *et al.* (2015).

Table 4-1: Percent Bias (PBIAS), Normalized Mean Error (NME) and Normalized Mean Absolute Error (NMAE) values for model calibration and evaluation periods

	Daily						Monthly					
	Calibration			Evaluation			Calibration			Evaluation		
	PBIAS	NME	NMAE	PBIAS	NME	NMAE	PBIAS	NME	NMAE	PBIAS	NME	NMAE
¹ Lower Susquehanna Flow	-5.2	0.05	0.40	-3.3	0.03	0.34	-5.1	0.05	0.3	-6.0	0.06	0.25
¹ Lower Susquehanna Sediment	NA	NA	NA	NA	NA	NA	24.8	-0.25	0.74	16.4	-0.16	0.70
¹ Lower Susquehanna Nitrate	NA	NA	NA	NA	NA	NA	-4.0	0.04	0.55	36.9	-0.37	0.46
¹ Lower Susquehanna Total Phosphorus	NA	NA	NA	NA	NA	NA	-19.9	0.20	0.50	-20.6	0.21	0.84

¹Lower Susquehanna contains the watershed outlet

Summary of Climatic Projections

Precipitation is predicted to increase in the watershed by 2.5 to 5.1 % across all RCP levels (Table 4-2) by mid-century and 4.6 to 8.5 % by the end of the century. Higher emission scenario (RCP85) result in greater mean annual precipitation than lower emission scenario (RCP26) in both periods. On monthly basis, all scenarios predicted increases in mean monthly precipitation

in both scenario periods except for periods in the fall, although there is variability across the months (Table 4-2). By mid-century, the largest increase in mean monthly precipitation is predicted to occur in January by both RCP26 (12.9 %) and RCP85 (15.4 %) scenarios, while by the end-of-century greatest mean monthly precipitation is predicted in May by RCP26 (11.0 %) and in January by RCP85 (16.4 %). The largest decrease in mean monthly precipitation was predicted during mid-century in October by both RCP26 (-5.9%) and RCP85 (-4.4%), and by the end of the century in October by RCP26 (-6.1%) scenario.

Table 4-2: Percent precipitation change from historic period (1990 to 2014) for ensemble model mean for mid-century (2041 to 2065) and end- of -century (2075 to 2099).

Month	Mid Century		End of Century	
	RCP26	RCP85	RCP26	RCP85
Jan	12.9	15.4	5.0	16.4
Feb	0.4	11.1	4.8	16.0
Mar	1.0	7.3	3.6	13.3
Apr	2.6	0.0	0.8	2.6
May	2.5	2.3	11.0	9.2
Jun	0.8	5.6	5.5	2.0
Jul	9.7	4.0	7.7	11.6
Aug	0.9	3.3	5.5	7.0
Sep	1.9	8.1	10.5	10.3
Oct	-5.9	-4.4	-6.1	0.1
Nov	-2.0	3.7	0.4	3.7
Dec	3.8	5.5	4.3	11.1
Annual	2.5	5.1	4.6	8.5

Temperature

All RCP scenarios predicted increases in mean annual temperature (maximum and minimum) during both scenario periods (Table 4-3). The predicted maximum annual temperature change varies from 1.3^oC (RCP26) to 2.4^oC (RCP85) while minimum annual temperature change varies from 1.2^oC (RCP26) to 2.4^oC (RCP85) during mid-century. By the end-of-century, the annual maximum temperature increases vary from 1.1^oC (RCP26) to 4.5^oC (RCP85) while annual minimum temperature increases vary from 1.0^oC (RCP26) to 4.3^oC (RCP85).

Table 4-3: Change in monthly maximum and minimum temperature ($^{\circ}\text{C}$) compared to the historical period (1990 to 2014) for ensemble model mean for mid-century (2041 to 2065) and end-of-century (2075 to 2099).

Month	Mid Century				End of Century			
	RCP26		RCP85		RCP26		RCP85	
	Tmax	Tmin	Tmax	Tmin	Tmax	Tmin	Tmax	Tmin
Jan	1.4	1.4	2.0	2.3	1.0	1.2	3.8	4.2
Feb	1.3	1.4	2.3	2.4	1.2	1.3	4.0	4.2
Mar	1.4	1.2	2.5	2.2	1.1	0.9	3.6	3.4
Apr	1.8	1.6	2.8	2.5	1.4	1.2	4.7	4.4
May	1.2	1.1	2.4	2.2	0.9	0.9	4.8	4.5
Jun	1.2	1.1	2.4	2.3	0.9	0.9	4.7	4.3
Jul	1.2	1.2	2.7	2.5	1.1	1.1	5.0	4.8
Aug	1.1	1.0	2.6	2.5	1.1	1.0	5.2	4.9
Sep	1.4	1.2	2.5	2.4	1.1	1.0	5.1	5.0
Oct	1.2	0.9	2.3	1.8	0.8	0.4	4.6	4.5
Nov	1.1	1.0	2.3	2.1	1.1	1.0	4.0	4.0
Dec	1.3	1.2	2.3	2.3	1.3	1.3	4.0	4.1
Average	1.3	1.2	2.4	2.3	1.1	1.0	4.5	4.3

Climate Change Effects on Hydrology and Water Quality

The mean annual and winter/spring flow is predicted to increase across both scenarios and scenario periods (Table 4-4). The RCP26 climate data result in a larger increase in mean annual flow predicted (+5.9%) for the mid-century period, while RCP85 climate data result in a larger increase in winter/spring flow (+6.1%) for the end-of-century period. Across time periods, the RCP85 scenario data result in lower summer flow during 2041-2065 (-0.2%), and 2075-2099 (-2.3%). The increase in mean annual and winter/spring flow is primarily due to an increase in surface runoff (Table 4-4) as there was no discernable increase in the contribution of groundwater flow to overall discharge (not shown). Mean annual runoff increases by 1.2% in the 2041-2065 period and by 3.1% in the 2075-2099 period for RCP26 scenario data, and by 4.9% in the 2041-2065 period and by 8.0% in the 2075-2099 for RCP85 scenario data.

Mean annual sediment export is predicted to increase by 31.2% and 39.2% by the 2041-2065 and 2075-2099 scenario periods, respectively with the RCP26 scenario data (Table 4-4), which is attributed to large increases in runoff (Table 4-4) and rainfall intensity across all climate models.

For instance, the MPI-ESM-LR climate model, which predicted sediment increases ranging from 59.1% to 70.3%, predicted increases in rainfall intensity of 6.5% and 10.1% for the mid-century and end-of-century periods, respectively. The RCP85 scenario also resulted in an increase in annual and seasonal sediment export during both scenario periods (Table 4-4).

Relative to the historical climate record, both RCP scenarios produced both an annual and winter/spring NO₃⁻ export decrease, while export increases during the summer/fall period (Table 4-4). The ensemble model mean suggests a decrease in annual NO₃⁻ export of 13.7% for 2041-2065 and 14.5% for 2075-2099 (Fig. 4-2d) for RCP26 scenario data. Across time periods, the RCP85 scenario resulted in a decrease in winter/spring NO₃⁻ export of 10.2% and 24.0% during mid and end-of-century. Annual model mean TN export increases by 5.3% for mid-century and 6.4% for the end-of-century periods for RCP26 scenario while 10.8% and 14.1% during 2041-2065 and 2075-2099 scenario periods by RCP85 respectively. There was strong consensus among scenarios that seasonal TN export will increase in both periods (Table 4-4).

Both scenarios predicted a decrease in TP and DP during both scenario periods (Table 4-4). Annual model mean DP export decreases by 27.8% for mid-century and 26.3% for the end-of-century periods for RCP26 scenario data, while for RCP85 data the decreases are even greater, 29.8% and 30.4% during mid and end-of-century periods, respectively. On a seasonal basis, summer DP export is predicted to decrease by both scenarios during scenario periods 25.4% to 45.8%. Mean annual TP decreases by 8.6% for mid-century and 5.8% for the end-of century periods for RCP26 scenario data. The RCP85 resulted in a decrease in 8.6% and 7.5% mean annual TP export during mid and end-of-century, respectively. Like DP, the seasonal TP export is predicted to decrease for both RCP scenarios and during scenario periods.

Table 4-4 : Annual and seasonal percent change from the historical baseline for ensemble model mean, maximum, and minimum for two scenarios, and future climate periods.

Scenario	Season	Flow			Runoff			Sediment			NO ₃			TN			DP			TP		
		Mean	Min	Max	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max
RCP26	2041-2065																					
	Annual	1.9	-7.9	10.6	1.2	-8.9	9.4	18.7	3.4	49.0	-13.7	-35.0	8.6	5.3	-1.4	15.3	-27.8	-44.1	-0.6	-8.6	-19.8	3.4
	Winter	2.4	-8.9	11.9	0.5	-11.9	14.6	14.4	-9.2	53.7	-15.7	-38.2	11.0	5.0	-5.2	21.1	-25.4	-44.4	1.4	-8.5	-23.3	3.9
	Summer	0.9	-10.3	14.9	2.3	-6.4	15.6	38.1	18.1	100.7	1.7	-6.5	17.0	6.2	-7.6	26.1	-33.7	-60.4	1.3	-8.7	-23.8	5.7
	2075-2099																					
	Annual	5.9	-6.8	18.2	3.1	-6.9	16.7	18.9	0.9	39.9	-14.5	-32.6	2.8	6.4	-7.5	22.5	-26.3	-55.7	-10.0	-5.8	-20.9	8.3
	Winter	5.1	-7.5	15.3	0.7	-10.6	9.7	12.5	-2.9	26.7	-17.5	-37.5	-0.6	3.5	-9.4	16.0	-25.8	-54.9	-14.2	-7.1	-23.1	3.7
Summer	7.4	-5.6	28.7	7.4	-2.1	31.5	47.8	15.6	155.2	9.2	-8.1	38.9	14.0	-3.7	46.7	-27.4	-57.2	6.1	-3.5	-18.1	19.3	
RCP85	2041-2065																					
	Annual	3.0	-7.4	18.3	4.9	-3.0	11.6	31.2	18.5	72.8	-8.7	-26.6	21.3	10.8	9.4	12.6	-29.8	-54.1	8.3	-7.7	-27.7	10.7
	Winter	4.8	-6.2	20.8	3.8	-5.7	16.5	25.2	5.1	69.7	-10.2	-31.8	24.0	11.6	6.6	17.1	-25.4	-46.4	-2.5	-6.1	-23.2	14.0
	Summer	-0.2	-14.9	13.7	6.7	-4.8	18.8	58.2	36.5	122.2	3.7	-11.8	45.1	8.6	-1.3	22.6	-40.2	-70.7	4.6	-10.2	-36.0	5.2
	2075-2099																					
	Annual	3.1	-15.0	14.9	8.0	-12.3	25.8	39.2	-0.1	130.4	-20.5	-38.8	1.5	14.1	-6.8	39.6	-30.4	-48.6	-5.7	-7.5	-23.4	2.6
	Winter	6.1	-17.4	20.6	8.3	-16.9	32.4	31.3	-13.9	132.8	-24.0	-45.1	-3.4	15.6	-10.1	52.5	-23.8	-49.2	4.2	-4.9	-28.5	8.6
Summer	-2.3	-17.4	30.3	7.5	-19.3	45.3	74.7	27.3	205.5	7.4	-9.0	35.0	10.2	-9.0	53.5	-45.8	-75.1	2.0	-11.8	-37.4	22.0	

Impact of Agricultural BMPs on Hydrology under Climate Change

Most BMPs have little to no effect on annual, and seasonal model mean watershed level discharge compared to the No Practice scenario during both scenario periods and across both RCPs (Figs. 4-2a and 4-3a). For RCP26 scenario data, tile drainage reduced annual model mean discharge by 1.1% and 5.1% for the mid and end-of-century periods respectively. RCP85 scenario data resulted tile drainage reduced annual model mean discharge by 2.3% and 2.4% for the mid and end-of-century periods respectively. These tile drainage effects are also reflected in the combined BMP scenario (Fig. 4-2a and 4-3a). Figure 4-2a and 4-3a show that while there is not any substantial change in flow for mid-century, there is a significant increase in flow for late century, and again, only tile drainage has any noticeable effect on discharge for both RCP scenarios. However, runoff generation in the watershed was affected by the BMPs (Fig. 4-2a and 4-3b). Tile drainage reduced annual model mean runoff generation by 27.8% and 26.3% for the RCP26 scenario and 25.7% and 24.5% for the RCP85 scenario for the mid and end-of-century periods, respectively. Strip crop resulted in a reductions of 6.8% and 5.0% for the RCP26 scenario and 3.5% and 0.5% for the RCP85 scenario during 2041-2065 and 2075-2099 periods, respectively. The combined effect of all the BMPs resulted in an annual model mean runoff reduction of approximately 35.8% and 34.5% for the RCP26 scenario and 32.6% and 31.4% for the RCP85 scenario during mid and end-of-century periods. The no-till and buffer strip BMPs had no appreciable impact on annual or seasonal model mean runoff generation for both RCPs and scenario periods (Fig. 4-3b).

Impacts of Agricultural Conservation Practices on Water Quality under Climate Change

When agricultural BMPs are installed across all agricultural HRUs in the watershed, the sediment load was greatly reduced compared to the No Practice scenario for both RCPs. For the tile drainage and buffer strip BMPs the reduction in sediment export approached or, in some cases lower than the historical export, particularly during the winter/spring seasons (Fig. 4-2c and 4-3c). For the RCP26 scenario, annual model-mean sediment reductions (compared to the No Practice scenario) range from 2041-2065) to 8.1% (2075-2099) for the strip crops (Fig. 4-2c). For the RCP85, scenario annual mean sediment reductions (compared to the No Practice scenario) resulted in 18.4% (2041-2065) and 18.1% (2075-2099) for tile drainage, 18.3% (2041-

2065) and 18.6% (2075-2099) for buffer strips, 8.7% (2041-2065) and 7.7% (2075-2099) for strip crops, and 19.2% (2041-2065) and 18.5% (2075-2099) for combined BMPs (Fig. 4-3c).

Most BMPs resulted in 18.3% (2041-2065) to 18.7% (2075-2099) for tile drainage, 18.4% (2041-2065) to 16.1% (2075-2099) for buffer strip, and 8.2 % (a decrease in annual and seasonal model mean NO₃⁻ export compared to the No Practice and the historical model (Fig. 4-2d and 4-3d). For the RCP26 scenario, buffer strips reduced NO₃⁻ export by 7.4% for the 2041-2065 period, and 16.9% for the 2075-2099 period. For the RCP85 scenario buffers strips reduced NO₃⁻ export by 7.9% and 7.5% during the mid and end-of century periods, respectively. Tile drainage substantially increased annual and seasonal NO₃⁻ export particularly annual export by 22.3% for the 2041-2065 period and 22.4% for the 2075-2099 periods for RCP26, while for the RCP85 scenario the increases were 23.0% for 2045-2065 period and 25.7% for 2075-2099 period, compared to the No Practice scenario (Fig. 4-2d and 4-3d). This increase is primarily due to increased nitrification occurring after tile drainage is installed; tile drainage increases root zone aeration, increasing the conversion of ammonium to NO₃⁻, which is considerably more mobile in the soil. Tile drainage also removes excess soil moisture, which, when coupled with higher soil NO₃⁻ levels, dramatically increases N export. For the RCP26 scenario and compared to the historical export buffer strips decrease annual NO₃⁻ by 20.2% for the 2041-2065 and 20.9% for the 2075-2099. Strip crops result in decreases of 13.7% for the 2041-2065 period and 14.5% for 2075-2088 period. No-till results in decreases of 13.7% for the 2041-2065 period and 14.5% for the 2075-2099 period. For the RCP85 scenario, buffer strips reduced NO₃⁻ export by 15.9% for the 2041-2065 period and 26.5% for the 2075-2099 period. Strip crops reduced NO₃⁻ export by 9.2% for the 2041-2065 period and % for the 2075-2099 period No-till resulted in a decrease of 9.2% for the 2041-2065 period and 20.4% in 2075-2099 period (Fig. 4-3d).

For TN, BMPs result in a slightly different response in annual and seasonal TN export compared to the more mobile NO₃⁻ (Figs. 4-2e and 4-3e), with all BMPs, including tile drainage, reducing TN export compared to the No Practice scenario. This was consistent for both RCP scenarios. The buffer strip BMP was most effective in reducing TN export, resulting in decreases of 12.6% and 12.2% for the 2041-2065 and 2075-2099 periods, respectively for RCP26. For RCP85 the buffer strip reduced TN export by 13 for the 2041-2065 and 12.8% 2075-2099 periods, respectively. Tile drainage reduced TN export by 5.8% and 5.7% during the 2041-2065 and

2075-2099 periods, respectively for RCP26 and 6.1% and 6.0% during the 2041-2065 and 2075-2099 periods, respectively for RCP85. No-till and strip crops produced lower reductions, ranging from 0.1 to -0.5% for no-till and 2.3- to 2.6% for strip crops. The BMPs also lowered the seasonal variability in TN export (Figs. 4-2e and 4-3e).

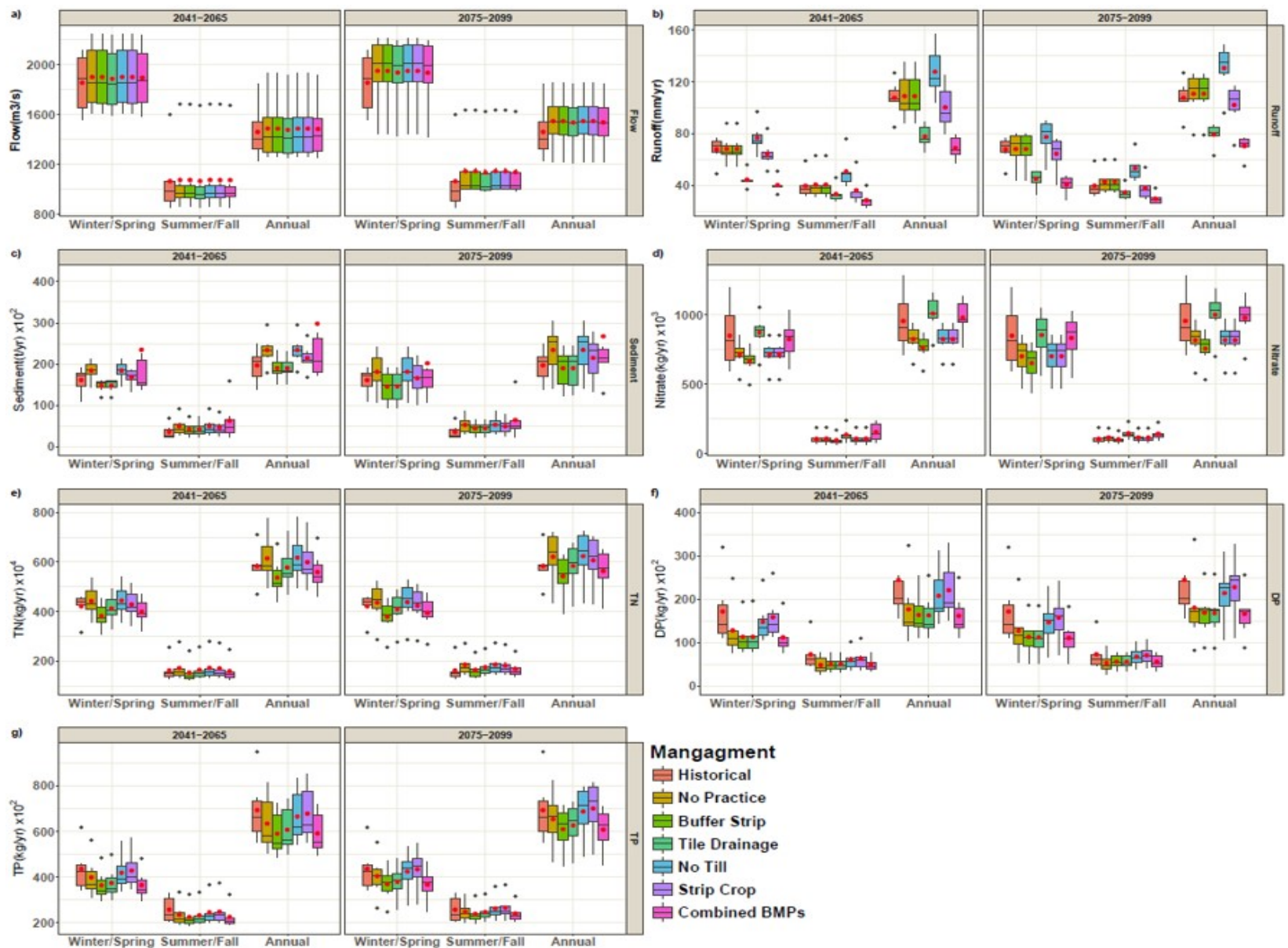


Figure 4-2: Box plot (1st, median, mean (red dot) and 3rd quartiles) for the RCP26 scenario climate models average-by-year streamflow (a), runoff (b), sediment (c), nitrate (d), total nitrate(e), dissolved phosphorus (f), and, total phosphorus (g) for five agricultural management practices under the six climate models, at the watershed outlet

All BMPs were effective in reducing both annual and seasonal DP and TP export compared to both the historical and future No Practice scenario and for both RCPs. Tile drainage and buffer strips tended to be the most effective at reducing annual and seasonal P export, with buffer strips slightly more effective at reducing TP and tile drainage slight more effective at reducing DP (Figs.4-2f, 4-2g and 4-3f, 4-3g). When tile drainage was implemented, annual DP export decreased by 4.5% and 3.0% for RCP26 for the 2041-2065 and 2075-2099 periods, respectively and 4.7% and 1.1% for RCP85 for the 2041-2065 and 2075-2099 periods, respectively/ For TP tile drainage resulted in a decrease of 3.8% and 3.7% for RCP26 for the 2041-2065 and 2075-2099 periods, respectively and 3.8% and 2.4% for RCP85 for the 2041-2065 and 2075-2099 periods, respectively (Figs. 4-2f, 2g and 4-3f, 3g). This is due to capability of tile drains to reduce surface erosion and surface runoff (Figs. 4-2b, 2c and 4-3b, 3c), which are the main drivers for sediment-associated TP export.

Buffer strips reduced TP export by 6.5% and 10.0% for RCP26 for the 2041-2065 and 2075-2099 periods, respectively and 6.5% and 5.2% for RCP85 for the 2041-2065 and 2075-2099 periods, respectively (Fig. 4-2g and 4-3g). Dissolved P export decreased for the buffer strip by 33.2% and 33.1% for RCP26 for the 2041-2065 and 2075-2099 periods, respectively and by 33% and 31.3% for RCP85 for the 2041-2065 and 2075-2099 periods, respectively. No-till decreased export by 15.1% and 12.5% for RCP26 for the 2041-2065 and 2075-2099 periods, respectively, and 14.3% and 11.7% for RCP85 for the 2041-2065 and 2075-2099 periods, respectively. Strip crops resulted in a decrease of 9.7% and 6.9% for RCP26 for the 2041-2065 and 2075-2099 periods, respectively and 8.7% and 5.5% for RCP85 for the 2041-2065 and 2075-2099 periods, respectively (Fig. 4-2f and 4-3f).

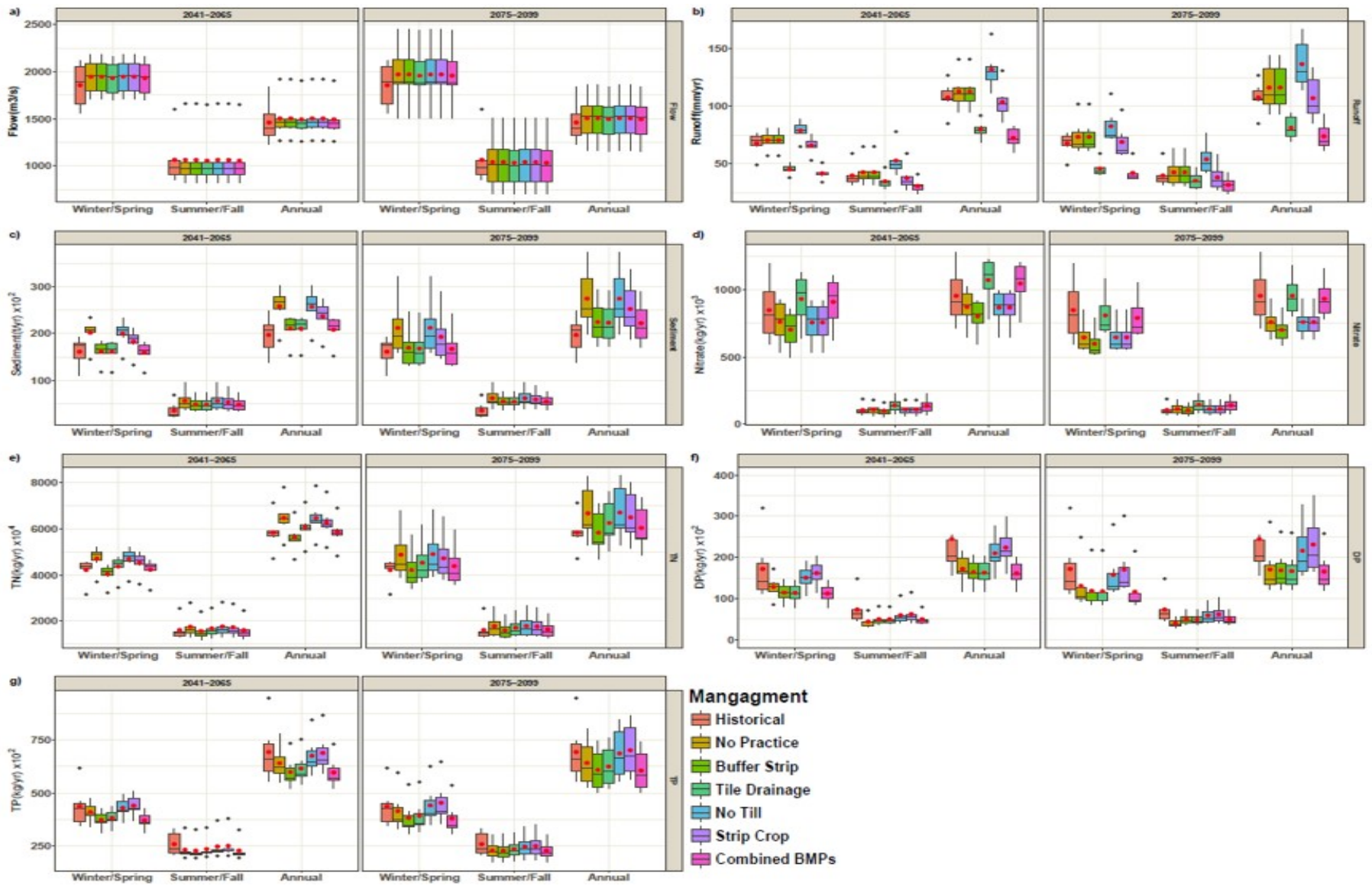


Figure 4-3: Box plot (1st, median, mean (red dot) and 3rd quartiles) of RCP85 scenario climate models average-by-year streamflow (a), runoff (b), sediment (c), nitrate (d), total nitrate(e), dissolved phosphorus (f), and, total phosphorus (g) for five agricultural management practices under the six climate models, at the watershed outlet.

Figure 4-4 and 4-5 compares the relative reductions achieved by widespread BMP implementation (BMPs installed across all agricultural land equally) and CSA targeting (BMPs applied to the 30% of the agricultural land that generates the most runoff). Across almost all BMPs there was very little difference between the widespread implementation and CSA targeting for both scenarios. For total watershed flow for both scenarios, widespread implementation of BMPs slightly reduces flow during both scenario periods (Figs. 4-4a and 4-5a). For runoff for both scenarios, widespread implementation of tile drainage and no till reduced runoff during both scenario periods (Figs. 4-4b and 4-5b). For sediment, widespread BMP implementation reduced sediment export more than for CSA targeting, particularly for the buffer strip, tile drainage, and strip crop BMPs (Fig. 4-4c and 4-5 c) for both scenarios and during both scenario periods. No-till did not result in appreciable differences between widespread implementation and CSA targeting in both RCP scenario. For NO₃⁻, only the buffer strip BMP and tile drainage provided greater relative reductions for widespread implementation while the other BMPs reduced NO₃⁻ export similarly across CSAs and widespread implementation (Fig. 4-4d and 4-5 d). Similar results occur for TN; widespread implementation of buffer strips reduced TN loss substantially more than CSA targeting for both RCP scenarios and both periods Fig. 4-4e and 4-5e). Tile drainage resulted in greater TN loss when implemented widely during both periods (Fig. 4-4e and 4-5e), however the export was still less than the No Practice scenario. Results of CSA targeting for both DP and TP show that buffer strip and tile drainage reduced losses slightly more when implemented widely than for CSA targeting for both RCP scenarios, with additional reductions of approximately 1-5% depending on practice, time periods, and RCPs (Figs. 4-4f and g and 4-5f and g).

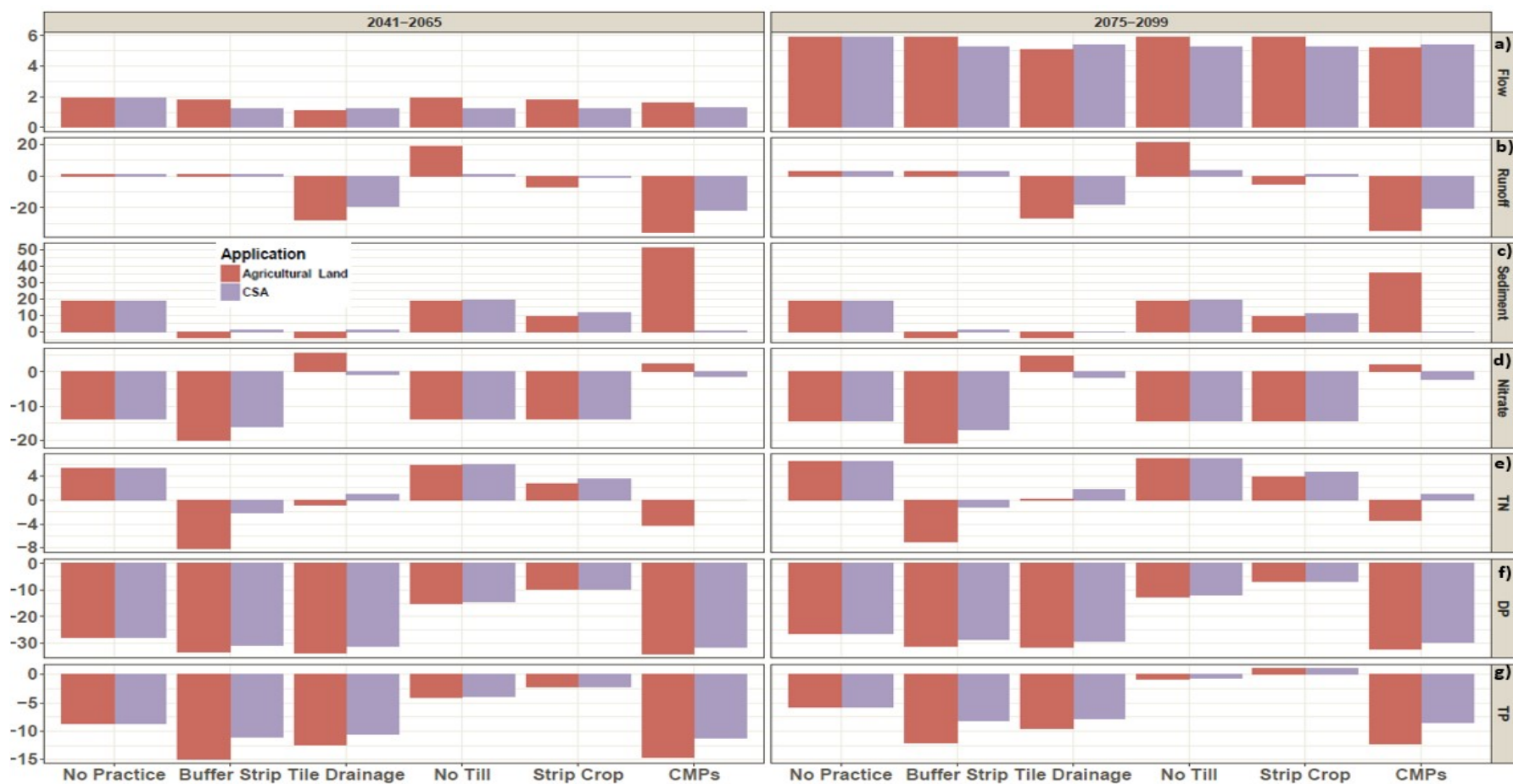


Figure 4-4: Comparison of annual changes (%) of RCP26 scenario for two future (2041-2065 and 2075-2099) time periods for flow (a), runoff (b), sediment (c), nitrate (d), total nitrogen (e), dissolved phosphorus (f), and total phosphorus (g) for four agricultural practices (note: CMPs in the figure stands for combination of all management practices) and no the BMP scenario, implemented on all agricultural landuses and only on critical source areas (CSA) relative to the historical scenario (1990 -2014) for the watershed outlet

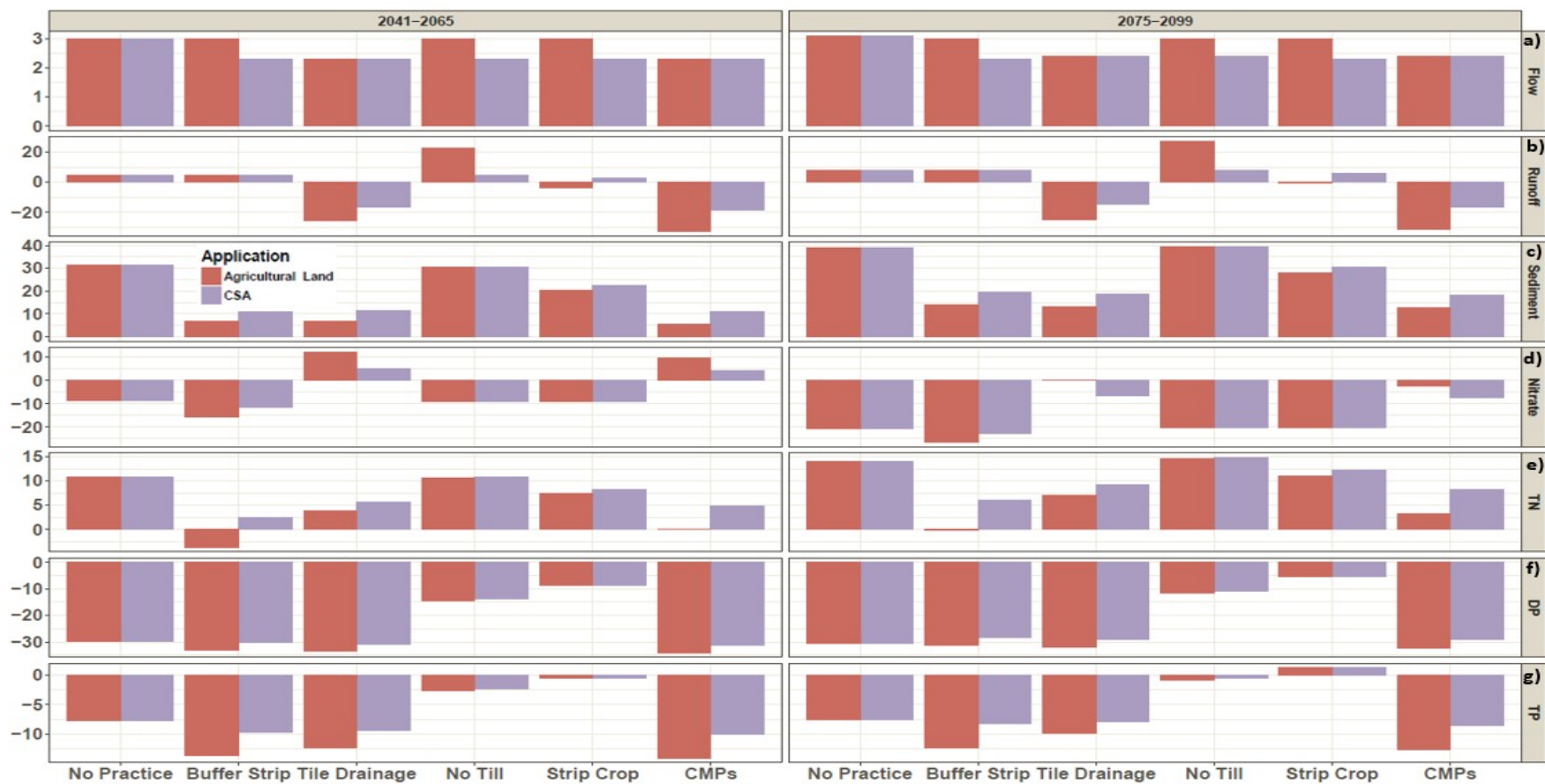


Figure 4-5: Comparison of annual changes (%) for RCP85 scenario for two future (2041-2065 and 2075-2099) time periods for flow (a), runoff (b), sediment (c), nitrate (d), total nitrogen (e), dissolved phosphorus (f), and total phosphorus (g) for four agricultural practices (note: CMPs in the figure stands for combination of all management practices) and no the BMP scenario, implemented on all agricultural landuses and only on critical source areas (CSA) relative to the historical scenario (1990 -2014) for the watershed outlet.

Discussion

Climate change is likely to affect the water quality of the Susquehanna River Basin. However, implementing BMPs on agricultural lands can offset much of the impact. The river basin is predicted to receive more annual precipitation by the mid and end-of-century periods (Table 4-2) with a concomitant increase in temperature (Table 4-3). The predicted increase in mean annual precipitation (3.8%) by the mid-century and (6.5%) the end-of-century are consistent with work of Najjar *et al.* (2009b), who predicted increases in precipitation over the Chesapeake Bay watershed of 3% to 12% using the CMIP3 A2 (medium high emission scenario) dataset and Howarth *et al.* (2006) who predicted an increase in precipitation of 4% and 15% during the 2030 and 2095 periods, respectively. These increases in precipitation and temperature affect processes such as nitrogen cycling, snowfall, and soil moisture, which translate into altered water quality, and affect BMP performance (Bosch *et al.*, 2014).

Increases in flow and surface runoff relative to the historic period result in substantial increases in sediment export, although the magnitude of the change differs among the climate models. Hayhoe *et al.* (2007) predicted similar increases in flow during spring driven by greater precipitation and decreases in summer driven by increased evapotranspiration. The predicted increase in flow will force existing BMPs to deal with more runoff and can impact their effectiveness and/or force water managers to design new practices to accommodate increased runoff. Because of these predicted increases in runoff and sediment export, BMPs become that much more important to achieve current water quality goals in the Chesapeake Bay, and to maintain the current export into the future.

Most BMPs had no effect on surface runoff, implemented either widely or targeted to CSAs except, perhaps for tile drainage (Figs. 4-2a, 4-3a). When tile drainage is installed on agricultural lands, there is a decrease in flow compared to corresponding periods without tile drainage (Figs. 4-2a, and 4-3a). Tile drainage removes free soil water, increasing the soil moisture storage capacity and infiltration (Madramootoo *et al.*, 2007), consequently reducing runoff and the associated soil erosion and TP loss (King *et al.*, 2014), but increases NO₃⁻ loss (Figs. 4-2d and 4-3d). The substantial increase in NO₃⁻ loss associated with tile drainage has been well documented (Randall & Goss, 2008), and occurs due to several factors. Tile drainage, by way of

increased soil aeration, increases nitrification (Stark & Firestone, 1995), making more NO_3^- available (Dinnes *et al.*, 2002), and since NO_3^- is soluble, it is easily exported from tile-drained fields. The strip crop and buffer strip BMPs did not affect surface runoff, but were effective in reducing NO_3^- export, even below the historic value (Figs. 4-2a and 4-3a), due primarily to increased nutrient uptake in plant biomass and their ability to reduce surface runoff generation. Although most model scenarios predicted a decrease in NO_3^- , all climate scenarios predicted an increase in TN (Table 4-4). This decrease in NO_3^- is due to increased denitrification from higher temperatures and higher soil moisture, while the increase in TN is driven primarily by decrease in both mineralization and nitrification, particularly during the drier summer periods (Groffman, Hardy, *et al.*, 2009; Schaefer & Alber, 2007) allowing more soil TN build up. Most BMPs were able to reduce TN export, and buffer strips were able to reduce export below the historic value (Figs. 4-2e and 4-3e). Tile drainage was more effective at reducing TN loss than NO_3^- loss because TN is not as mobile in the soil.

The increase in sediment export is mainly driven by increases in runoff (Fig. 4-2b, and 3b) and precipitation intensity causing erosion from upland areas (Langland & Cronin, 2003). The predicted increase in sediment export would have major impacts on Chesapeake Bay function, reducing clarity, and burying aquatic vegetation (Zhang *et al.*, 2013), and on watershed infrastructure. Indeed, Cerco (2016) found that the Conowingo reservoir on the lower Susquehanna (the largest reservoir in the basin) is currently in a state of dynamic equilibrium in which the sediment inflow and outflow are balanced; thus, the projected increases in sediment are unlikely to be stored in the watershed, but rather will be exported to the Bay. Our results show implementing BMPs reduces the effect of climate change on sediment export by 1.3% to 20.8%, particularly tile drainage and buffer strips (Fig. 4-2c and Fig. 4-3c). The effect of tile drainage is entirely realized through reductions in surface runoff, while the buffer strip effect is a result of sediment trapping by the buffer vegetation. Others have also shown buffer strips to be effective at controlling sediment export from agricultural fields (Arabi *et al.*, 2008; Blanco-Canqui *et al.*, 2004; White & Arnold, 2009). Surprisingly, no-till had a relatively small effect on sediment export, reducing it by only 1.3%. However, that these BMPs are applied only to agricultural HRUs in the watershed, and no-till is only applied to row crop HRUs, and even smaller fraction of HRUs, thus presenting the results at the watershed outlet dampens the effect. Across all agricultural HRUs, no-till reduced sediment export by 5.1 and 5.7% during the mid

and end-of century, respectively, and by 2.8 and 4.8% during the mid and end-of century, respectively, when implemented on CSAs. Bosch *et al.* (2014) and Woznicki and Nejadhashemi (2012) report similar results; averaging over the entire watershed tends to underestimate BMP effectiveness implemented at the field scale.

Both DP and TP export decrease in the basin under climate change; for DP the reductions range from 27.8% to 26.3% for RCP26 and 29.8% and 30.4% for RCP85, respectively for the 2041-2065 and 2075-2099 periods, respectively, while for TP the reductions range from 8.6% to 5.8% for RCP26 and 7.7% and 7.5% for RCP85 for the 2041-2065 and 2075-2099 periods, respectively (Table 4-4), which was consistent with Roberts *et al.* (2009) for the Chesapeake Bay, who predicted a 19% reduction in P. It is somewhat surprising that both DP and TP decreased in the future, although the TP decrease was relatively small, and there was considerable variability among models (Table 4-4), given the large increases in runoff and sediment export. However, more P was taken up in plant and microbial biomass associated with climate change, which would utilize DP rather rapidly if it was not buffered by desorption and dissolution reactions (Fitter & Hay, 2012), and increasing soil TN may stimulate plant growth resulting in increased P uptake by plant, this may also partially explain the decline in NO₃-. When BMPs are installed, P export decreases compared to future periods with no BMPs, although there is variability in magnitude of the changes among practices (Fig. 4-2f and 4-3f). Tile drainage and buffer strips resulted in the greatest reduction in both DP and TP export compared across all time periods and climate scenarios, substantially below the historic P export. The no till and strip crop BMPs resulted in smaller P reductions than the tile drainage and buffer strips, but were still able to offset the impact of climate change during both future periods (Figs. 4-2e and 4-3e). Reductions achieved by installing BMPs on CSAs were only slightly lower than widespread BMP installation.

These results indicate that for sediment and TN, maintaining current BMP extent will not be sufficient to meet water quality goals in the region under a changing climate. For pollutants such as sediment and TN, significant remediation effort will be required to offset or at least reduce the impact of changing climate on water quality in the basin. However, the effectiveness of BMP implementation depends on the types of practices used and the pollutant of concern. For instance, implementing tile drainage over buffer strips or strip crops might result in pollution swapping

(e.g., increased NO₃⁻ loss, but decreased sediment and P loss). Thus, managers tasked with improving water quality will need to weight, the relative performance of BMPs for specific pollutants before deciding which to install. Furthermore, it should be noted that maintaining current levels of nutrient and sediment export is not sufficient to meet the TMDL currently in place, which calls for reductions of 25%, 24%, and 20% for nitrogen, phosphorus, and sediment by 2025.

Conclusions

Climate change is likely to impact water quality in the Chesapeake Bay watershed; however, implementing BMPs can reduce this impact. Our results suggest that climate change will result in an increase in flow, surface runoff, sediment, and TN. However, installing BMPs on agricultural land can sustainably reduce these losses. Irrespective of BMP installation, increased crop growth and altered biogeochemical processes associated with a changing climate can also reduce losses, particularly for soluble nutrients such as DP and NO₃⁻, and BMPs can further reduce these losses. Maintaining current conditions will not be sufficient to meet water quality goals of the Susquehanna River and Chesapeake Bay under changing climate. Thus, managers need to focus on developing new agricultural conservation practices and/or use a combination of agricultural conservation practices to fully offset the effect of changing climate on water quality.

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CHAPTER 5

QUANTIFYING STRUCTURAL MODEL UNCERTAINTY USING A MULTI-MODEL ENSEMBLE

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Abstract

Watershed models are essential tools to understand, quantify, and predict hydrologic processes and nutrient export. However, the reliability of watershed models in a management context depends largely on associated uncertainties. The objective of this study is to quantify structural uncertainty of flow, sediment, total nitrogen (TN), and total phosphorus (TP) predictions using three models: the Soil and Water Assessment Tool-Variable Source Area model (SWAT-VSA), the standard Soil and Water Assessment Tool (SWAT-ST), and the Chesapeake Bay watershed model (CBP-model). We initialize each of the models using weather, soil, and land use data, and analyze outputs of flow, sediment, TN, and TP fluxes for the Susquehanna River basin at the Conowingo Dam in Conowingo, Maryland. Using these three models we fit Bayesian Generalized Non- or Linear Multilevel Models (BGMM) for flow, sediment, TN, and TP fluxes and obtain estimated outputs with 95% confidence intervals. We compare the BGMM results against the individual model results and straight model averaging (SMA) results using a split time period analysis (training and testing periods) to assess the BGMM in a predictive fashion. The BGMM provided better predictions of flow, sediment, TN, and, TP compared to individual models and the SMA during the training period. However, during the testing period the BGMM was not always the best predictor, in fact, there was no clear best model during the testing period. Importantly, the BGMM provides estimates of prediction uncertainty, which can enhance decision making and improve watershed management by providing a risk-based assessment of outcomes.

Introduction

Ecosystems operate under dynamic and complex physical, chemical, and biological interactions. The complexity of the interactions leads to difficulties in conceptualizing the processes mathematically, which in turn makes accurately modeling systems challenging. Uncertainty can be classified from two primary sources: epistemic and aleatory uncertainty. Epistemic uncertainty arises from a lack of knowledge or data necessary to estimate probabilities. Aleatory uncertainty, in contrast, derives from the inherent randomness in the system (e.g., weather-related variation).

Although complex and sophisticated physical models have been built to approximate real-world processes and to assist in effective decision-making, quantifying structural uncertainties (uncertainty related to the configuration of a system) of watershed models in model process conceptualization, initial conditions, and input data remains a challenge. Most previous research into model uncertainty has focused on model parameter or input data uncertainty (Renard *et al.*, 2010), and less on structural model uncertainty (e.g., the mathematical form or expression of the model processes). Thus, structural model uncertainty of watershed models can occur even if the true input values for all model parameters are known. Sources of structural model uncertainty include exclusion of important controlling variables, processes either missing or incorrectly represented, and misaligned boundary conditions (Ascough *et al.*, 2008). All these uncertainties propagate to total model prediction uncertainty (Shen *et al.*, 2015; Vrugt *et al.*, 2005). Thus, quantifying uncertainties associated with the watershed models cannot be neglected and should be explicitly considered to obtain credible model outputs with associated prediction uncertainty bounds to make effective management decisions.

Numerous approaches have been proposed to quantify uncertainties in watershed models, including Bayesian Model Averaging (Raftery *et al.*, 1997; Vrugt *et al.*, 2008), Generalized Likelihood Uncertainty Estimation (GLUE) (Blasone *et al.*, 2008; Vrugt *et al.*, 2005), multiple objective function criteria (Blasone *et al.*, 2008), sequential data assimilation (Moradkhani *et al.*, 2005), Bayesian Recursive Estimation (Thiemann *et al.*, 2001), and the Ensemble Kalman Filter (Abaza *et al.*, 2014). However, only a few methods, such as multi-model ensembles (MME) (Duan *et al.*, 2007; Stoica *et al.*, 2004), have been proposed for quantifying structural model

uncertainties. This is due to the complexity and difficulty of separating structural uncertainties from model parameter or input data uncertainty (Zhang *et al.*, 2011). Sharifi *et al.* (2017) evaluated the performance of different watershed models to assess water quality impacts on Queenstown drainage, Stow *et al.* (2009) demonstrated improved performance in estimating hypoxia in the Chesapeake Bay using a hierarchical Bayesian ensemble approach, but the study is limited to processes within the Bay and does not describe upland watershed processes. Boomer *et al.* (2013) and Exbrayat *et al.* (2010) also suggested use of multi model ensemble. However, research describing ensembles used to quantify structural uncertainty in watershed models is lacking, and no consensus on application of methods or evaluation guidelines has been reached.

Multi-model ensembles (MMEs) combine two or more models in an effort to improve model prediction and objectively evaluate model uncertainty (Boomer *et al.*, 2013). MMEs utilize the diversity of skillful predictions from different models and improve the estimation of structural uncertainties associated with model outputs (Duan *et al.*, 2007). MMEs are commonly used in weather forecasting (Krishnamurti *et al.*, 2000) and climate change analysis (Christensen *et al.*, 2006). For instance, climate forecasters used an MME approach to include the weaknesses and strengths of each model in the forecast (Wiley *et al.*, 2010), river flood forecasters also developed and used multi-model approach to exploit diversity of skillful predictions from different models (Cloke *et al.*, 2009; Duan *et al.*, 2007). There are different ways to implement MME approaches. Ensembles can be used to sample uncertainty in forcing assumptions, initial conditions, process conceptualization, input data, and training/calibration data. Generally, MMEs use multiple models to simulate responses to identical driving forces (e.g., climate inputs). Model projections are aggregated and compared to estimate uncertainty in system responses. For example, an MME could be used to evaluate management practices needed to achieve a water quality standard. Multiple solutions would be obtained from several models, and then be aggregated to obtain an estimated mean nutrient reduction achieved and the probability that the target will achieve the desired water quality improvements. Average model projections have been found to reproduce historical observations more accurately than individual models in a number of fields (Najafi *et al.*, 2011; Reichler *et al.*, 2008), and historically the variability in model projections has been used as a measure of uncertainty. Under these assumptions, solutions that generate smaller uncertainty ranges theoretically represent more conservative management approaches.

Little research has been carried out to quantify structural uncertainties of watershed models using MME (Duan *et al.*, 2007), and the application and analysis of ensemble methods remains a challenge in this field. Raftery *et al.* (2005) proposed Bayesian model averaging (BMA) post-processing methods to ensemble weather prediction models, however, the method requires accurate estimates of the weights and variances of the individual competing models in the ensemble (Vrugt *et al.*, 2008), additionally, the proposed algorithm cannot be guaranteed for global convergence (Vrugt *et al.*, 2006).

The BMA approach requires accurate estimation of weights and variances of each model and then averages over all possible models (Vrugt *et al.*, 2008). For instance, in the BMA approach, model averaging refers to estimating some quantity from each model and then averaging the estimates based on how likely each model predicts the data by assigning weights for each model (Wasserman, 2000). The BMA approach sometimes underperformed compared to simple unweighted averages because the process does not consider two equally performing models with the same weights. For instance, if two models perform equally well (i.e., have the same weights) BMA selects only one model (Graefe *et al.*, 2015). The Ensemble Kalman Filter approach assumes all probability distributions are Gaussian in shape, which is suitable for large state variables, but problematic for constituents that exhibit Non-Gaussian behavior (Evensen, 2003; Mandel, 2009). Thus, for this research we use new approach, namely Bayesian Generalized (Non-) Linear Multilevel Models (BGMM) (Bürkner, 2017), which integrates different probability distributions, explicitly incorporates prior knowledge about parameter distributions, allows predictor variables to be linear or nonlinear, and incorporates information from all predictors. This method offers a more complete quantification of uncertainty rather than primarily attempting to improve prediction skill.

In this study, we develop a BGMM as an ensemble capable of quantifying structural uncertainty of multiple models used to predict watershed response based on different forcing data. We employ the Hamiltonian Monte Carlo method using the No-U-Turn Sampler (NUTS) extension, which has been shown to converge to optimal Bayesian coefficients faster and more reliably than other Markov-Chain Monte-Carlo (MCMC) algorithms (Betancourt *et al.*, 2017; Bürkner, 2017). Structural uncertainties and credible intervals of model predictions for flow, sediment, total nitrogen (TN), and total phosphorus (TP) fluxes for the Susquehanna River basin at the

Conowingo dam in Conowingo, Maryland, were developed using the BGMM method. Specifically we: 1) developed and evaluated two watershed models, the Soil and Water Assessment Tool-Variable Source Area (SWAT-VSA) model (Easton *et al.*, 2008), the SWAT-standard (SWAT-ST) model (Arnold *et al.*, 2012), and obtained outputs from the Chesapeake Bay Phase 6 Watershed Model; 2) developed a BGMM using outputs from the three models as predictors and observed data as the response variable; and 3) developed regression coefficients obtained using the Hamiltonian Monte Carlo-NUTS algorithm. We analyzed the ensemble model performance based on two statistical metrics: percent bias (PBias), and root mean square error (RMSE), evaluated the weights of each model derived from the regression, and compared the BGMM model result with simple average of the three models.

Materials and Methods

Study Area Description

The Susquehanna River, the largest contributor of fresh water to the Chesapeake Bay, drains approximately 42% of the Bay watershed and contributes more than 50% of the fresh water flows to the Bay (Ko *et al.*, 2004) and largely controls salinity in the Bay (Gibson *et al.*, 2000). The basin is approximately 71,000 km², with elevation ranging from -10 to 960 m, and covers parts of the states of New York, Pennsylvania, and Maryland (Fig. 5-1). The Susquehanna River Basin has six major subbasins: Upper, Chemung, Middle, West Branch, Juniata, and Lower subbasins (Fig. 5-1). The climate varies along a north-south gradient, with the northern portion receiving more precipitation (1245mm) than the lower basin (838 mm), which experiences hotter and longer summers (DePhilip *et al.*, 2010). The land use of the basin is primarily forest (70%), agriculture (22%), and developed (7%). The major soil type is silt loam (70%), and the soil depth in most parts of the basin ranges from 0.5 to 2 m (Ray *et al.*, 2016).

Watershed Models

SWAT and SWAT-VSA Models Description

The Soil and Water Assessment Tool (SWAT) model is a process based, semi-distributed watershed model developed to simulate landscape processes and predict the impact of land management practices on water availability and water quality (Arnold *et al.*, 1998). SWAT

requires weather, soil, land cover, and land management data to simulate surface and subsurface hydrology and various chemical, nutrient, and sediment fluxes. In SWAT, the watershed is divided into sub watersheds and then further in to hydrologic response units (HRUs), which are unique combinations of soil type and land use. SWAT-VSA re-conceptualizes the standard SWAT to account for areas of the landscape subject to variable saturation dynamics (Easton *et al.*, 2008). In SWTA-VSA the area of each HRU is defined by the coincidence of land use and wetness index class determined from a Topographic Index (TI) to differentiate areas of the landscape with respect to their moisture storage and saturation index (Easton *et al.*, 2008). SWAT-VSA has been shown to provide better predictions of soil moisture and runoff generation than the standard SWAT model in watersheds with similar physical characteristics and climate to the study watershed (Easton *et al.*, 2008).

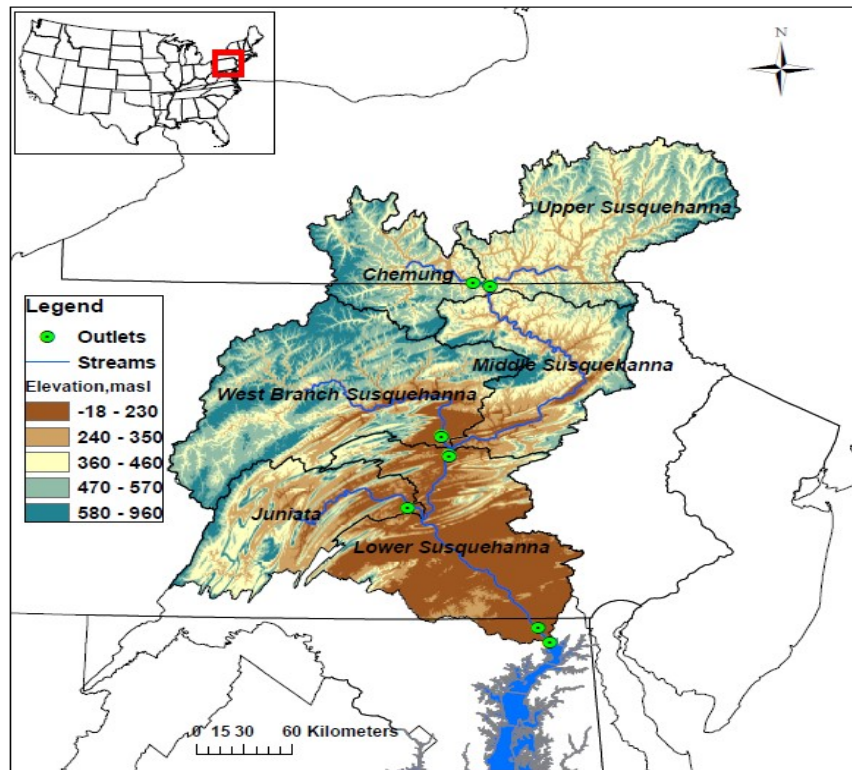


Figure 5-1: Location of Susquehanna River basin, major subbasins, and elevation features.

SWAT Model Inputs

The Susquehanna River SWAT-ST and SWAT-VSA models were initialized with 10 m digital elevation models (DEM) obtained from the United States Geologic Survey (USGS) National Elevation Dataset (NED) (Guenther *et al.*, 2007) using ArcSWAT 2012 and TopoSWAT (Fuka & Easton, 2016). TopoSWAT automates the SWAT-VSA initialization process by assimilating soil data, creating the TI map, overlaying the soil and TI maps, and developing the required database for model initialization. Soils data included in TopoSWAT are based on the Food and Agriculture Organization (FAO) soils database (FAO, 2007). The land use of the watershed was obtained from the National Land Cover Database 2011, the most recent national land cover product created by the Multi-Resolution Land Characteristics (MRLC) Consortium (Homer *et al.*, 2015). The model was forced with daily weather data from the Climate Forecast System Reanalysis (CFSR), including precipitation, temperature (min and max), relative humidity, wind speed and solar radiation (1990 to 2014) at the centroids of the six major sub basins. The dataset consists of hourly weather forecasts generated by the National Weather Service's NCEP Global Forecast System and has been successfully used for watershed modeling in different hydrologic settings (Fuka *et al.*, 2014).

SWAT model calibration and evaluation

Both SWAT-VSA and SWAT-ST calibration followed a cascading procedure, first calibrating all headwater basins (Upper Susquehanna, Chemung, West Branch, and Juanita sub basins) to observed data. Next, the second-order basin (Middle Susquehanna) was calibrated, leaving all parameters values for the headwater basins unchanged. Finally, the Lower Susquehanna basin outlet was calibrated, leaving all parameter values for the headwater and second-order basins unchanged. The model was calibrated and evaluated using the SWAT Calibration and Uncertainty Procedure, SWAT-CUP (Arnold *et al.*, 2012) and the SUFI2 (Sequential Uncertainty Fitting) optimization algorithm with the objective function set to percent bias (PBIAS) method. The model was calibrated for flow, sediment, TN, and, TP fluxes from 1985 to 1994 and evaluated from 2002 to 2011 at each of the six sub basins in the watershed.

Chesapeake Bay Watershed Model

The Chesapeake Bay Phase 6 Watershed Model (CBP) was developed to simulate hydrology, and fate of nutrients and sediment that contribute to Chesapeake Bay water quality degradation. The hydrological component of the Chesapeake Bay watershed model is based on the HSPF model (Hydrologic Simulation Program FORTRAN), which was derived from the Stanford Watershed Model (Boomer *et al.*, 2013). HSPF uses a mass-balance approach to solve a linked set of equations representing natural and anthropogenic mechanisms and lumped parameters, and uses hourly metrological data (Sharifi *et al.*, 2017). The CBP model consists of approximately 1,000 modeling segments/subbasins, with the average size approximately 64 square miles (Boomer *et al.*, 2013). The model input includes land use, weather, elevation features, fertilizer applications, wastewater plant discharges, septic systems, air deposition, farm animal populations, and other variables to estimate the amount of nutrients and sediment reaching the Chesapeake Bay (EPA, 2010). For the purpose of this research, monthly flow, sediment, TN, and TP fluxes data were obtained for Susquehanna River watershed at the Conowingo Dam from the outputs of Chesapeake Bay Phase 6 Watershed Model. The model was calibrated for flow, sediment, TN, and TP from 1985 to 2005 from 20 monitoring stations in the Chesapeake Bay watershed (Shenk *et al.*, 2012).

Observed Data

The daily observed flow in the six sub basins was obtained from the USGS waterdata website (<https://waterdata.usgs.gov/nwis/sw>). Monthly sediment, TN, and TP fluxes for the six subbasins were obtained from Hirsch *et al.* (2010) from (<https://cbrim.er.usgs.gov/methods.html>) using the Watershed Regression on Time Discharge Season (WRTDS) method. WRTDS was developed to understand and analyze water quality in Chesapeake Bay watershed.

Multi-Model Ensemble Approach

The BGMM procedure and a statistical post-processing method were fitted using the Stan package in R (Carpenter *et al.*, 2016) and developed based below equations (Buerkner, 2016).

$$y_i \sim D(f(\eta_i), \theta) \quad (1)$$

$$\boldsymbol{\eta} = \boldsymbol{\beta}\boldsymbol{X} + \boldsymbol{Z}\boldsymbol{u} \quad (2)$$

Where: \boldsymbol{y}_i is response \boldsymbol{y} through the linear combination of $\boldsymbol{\eta}$ of predictors transformed by inverse functions f assuming a certain distribution D , $\boldsymbol{\beta}$ and \boldsymbol{u} are the coefficients at the population level and group level, respectively, and \boldsymbol{X} and \boldsymbol{Z} are the corresponding design matrices. $\boldsymbol{\beta}$, \boldsymbol{u} , and $\boldsymbol{\theta}$ are the model parameters being estimated using the Hamiltonian Monte Carlo-NUTS algorithm (Buerkner, 2016).

Stan is a probabilistic programming language for full Bayesian Inference and Optimization (Carpenter *et al.*, 2016), incorporates the Hamiltonian Monte Carlo-NUTS algorithm (Bürkner, 2017), and provides flexibility for modeling and fitting different complex functions and distributions. Bürkner (2017) developed the brms R package using the Stan programming language by deploying the Hamiltonian Monte Carlo-NUTS algorithm for optimization of high-dimensional multi-level models. Stan is integrated with the R software environment through an interface called RStan. A wide range of distributions and linkage functions are supported in the package, allowing users to fit linear and nonlinear models, incorporate prior knowledge of all parameters in the response distribution, and also incorporate predictor variable distributions with different priors. Model fit can easily be evaluated and compared against observed data with a posterior predictive check and/or leave-one-out cross-validation (Bürkner, 2017).

We trained flow, sediment (log transformed), TN, and TP (log transformed) fluxes from 1985 to 1994 and then tested the model predictions from 2002 to 2011 using BGMM in Stan by defining family functions for response variables: for flow and TN using normal distributions while lognormal distributions were employed for sediment and TP. The trained and tested model ensemble performance was evaluated using two metrics, PBIAS and RMSE and also the data were split into two data sets to minimize model overfitting and under fitting (Kharin & Zwiers, 2002). The weights for each model for each constituent were obtained by summing up the absolute value of the fitted coefficient values and then dividing each coefficient by the sum of the absolute value of the coefficients obtained during training period. The results of the Bayesian model ensemble are compared against the performance of each individual model and the straight model averaging(SMA) during the training and testing period based on the above two statistical

metrics; additionally, the graphical time series of the BGMM with 95% credible interval was produced (structural uncertainty) from the three models.

$$Weights(i) = \frac{|(\beta_i)|}{\sum_{i=1}^n |(\beta_i)|} \quad (1)$$

Where the sum of all *Weights* across *i* is equal to one, and coefficient, β are fitted absolute coefficient values of each predictor.

Results

Individual Model Evaluation

Figure 5-2 shows a comparison of the three individual model predictions as well as the BGMM and SMA models for annual flow, sediment, TN, and TP with respect to observed data (WRTDS) during the training and testing periods. All models predicted flow reasonably well, with monthly PBIAS values ranging from -3.5% to 9.7% during both periods (Fig. 5-2a, Table 5-1). All models predicted slightly less inter-annual variability than the observed flow, although the BGMM captured the range most accurately (Fig. 5-2a). For sediment, the CBP-model under-predicted during the training period and over-predicted during the testing period, where it also predicted much greater variability than any of the other models or the observed data (Fig. 5-2b). The BGMM reproduced the observed response most accurately during the training period, but significantly over-predicted during the testing period. Both SWAT-VSA and SWAT-ST predicted the sediment load well in both periods, although both under-predicted (Fig. 5-2b, Table 5-1). All models tended to under-predict the TN load (Table 5-1) during the training period and over-predict (with the exception of SWAT-VSA and SMA) during the testing period (Fig. 5-2c). Total P was well characterized by all models with PBIAS ranging from 0.2% to 4.2% (Table 5-1), with the BGMM providing the most accurate predictions. Across all constituents, the BGMM reproduced the observed variability in the data most precisely (e.g., the BGMM had very similar ranges between the 1st and 3rd quartiles), although it did not always provide the most accurate absolute prediction, one example being the sediment predictions in the testing period (Fig. 5-2b).

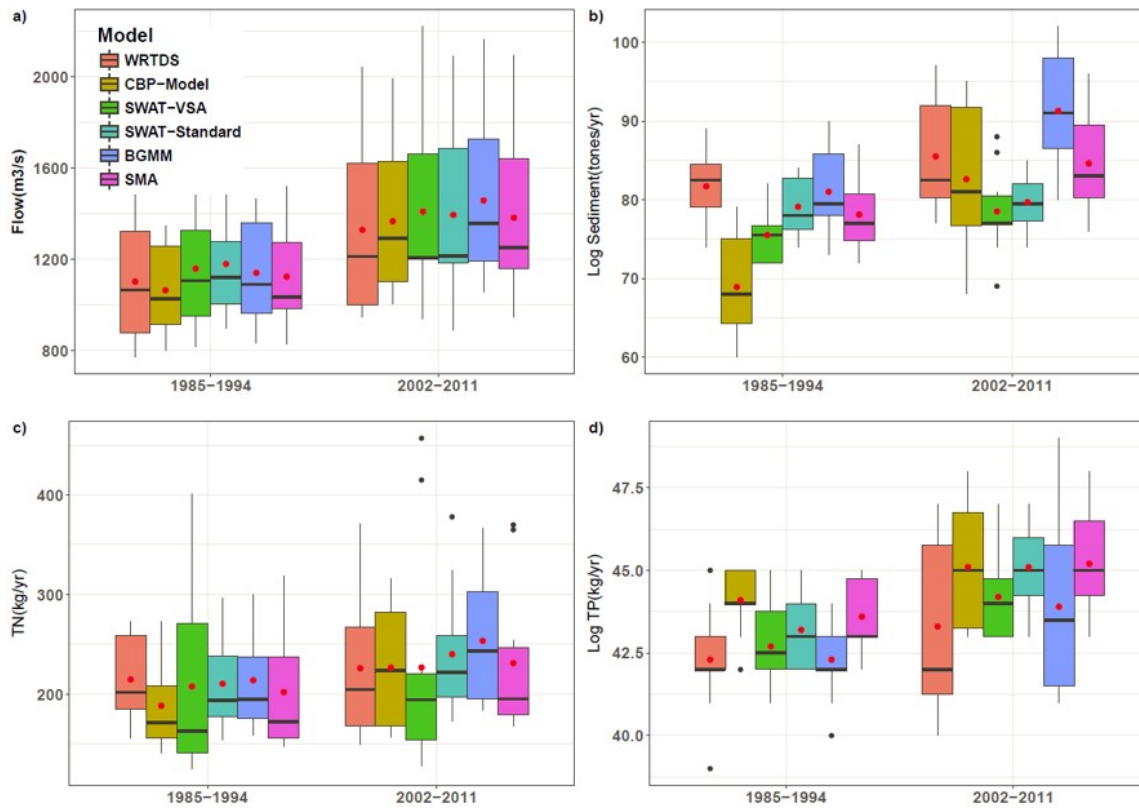


Figure 5-2: Box plot (1st quartile, median, mean (red dot) and 3rd quartile) of the three individual model predictions (CBP-model, SWAT-VSA, SWAT-ST), the BGMM, SMA, and annual observed data (WRTDS) for flow (a), sediment (b), total nitrogen (c), and total phosphorus (d) for the training (1985-1994) and testing (2002-2011) periods.

Ensemble Model Performance Evaluation

Table 5-1 shows the performance of each individual model, the SMA and the BGMM for monthly flow, sediment, TN, and TP fluxes during the training and testing period. Although the individual watershed models, the SMA, and the BGMM performed very well based on the PBIAS criterion recommended by Daniel *et al.* (2007; 2015), the models tended to predict the magnitude of constituents differently. For instance, during the training period flow was overestimated by SWAT-VSA and SWAT-ST but under predicted by the CBP-model. Differences in estimations drive the BGMM to weight the watershed models differently in the ensemble. The CBP-model was weighted higher compared to the other models (Table 5-2), likely due to the hourly calibration, which estimated flow at a higher resolution than the other models. During the testing period, flow was overpredicted by all watershed models compared to

observed data. The SMA outperformed the BGMM on flow predictions during both the training and testing periods. This is due to the BGMM underpredicting peak flows whereas the SMA captured the peak flows better (Figs. 5-3a, 5-3b). The SMA result follows Boomer *et al.* (2013), who found that straight model averaging outperformed individual model predictions of flow, sediment, TN, and TP fluxes in the Patuxent Estuary, USA, but also noted that there was no single best model for all constituents. These results are similar to ours, where no single model, or combination of models provided the best predictive power across all constituents (Table 5-1).

Table 5-1: Percent Bias (PBIAS) and Root Mean Square Error (RMSE) values for monthly model training and testing periods for Bayesian ensemble, straight averaging, Chesapeake Bay watershed model (CBP), SWAT-VSA, and SWAT-Standard (SWAT-ST).

Models	Constituents	PBIAS ^a		RMSE	
		Train	Test	Train	Test
BGMM	Flow(m ³ /s)	3.5	9.7	257.5	287.6
	Sediment(Log)(t/yr)	-0.7	6.8	0.7	1
	Total Nitrogen(kg/yr)	-0.4	12.3	42485.6	54250.1
	Total Phosphorus(Log)(kg/yr)	0.2	0.6	0.5	0.5
Straight Average	Flow(m ³ /s)	2.0	4.0	369	299.3
	Sediment(Log)(t/yr)	-4.3	-1.1	0.5	0.4
	Total Nitrogen(kg/yr)	-5.9	2.3	108538.8	114684.6
	Total Phosphorus(Log)(kg/yr)	3.1	4.2	0.3	0.3
CBP-Model	Flow(m ³ /s)	-3.5	2.9	362	301
	Sediment(Log)(t/yr)	-15.5	-3.3	1.3	1.1

	Total Nitrogen(kg/yr)	-12.3	0.3	64935.9	47743.6
	Total Phosphorus(Log)(kg/yr)	4.2	4.2	0.6	0.7
SWAT- VSA	Flow(m3/s)	5.5	6.1	582.7	506.7
	Sediment(Log)(t/yr)	-7.6	-8.3	1.4	1.5
	Total Nitrogen(kg/yr)	-3.3	0.3	255839.5	261368.1
	Total Phosphorus(Log)(kg/yr)	1.1	2.1	0.7	0.7
SWAT- ST	Flow(m3/s)	4.0	3.0	568.8	522.5
	Sediment(Log)(t/yr)	-3.0	-6.8	1.3	1.5
	Total Nitrogen(kg/yr)	-2.1	6.3	109842.3	126366.9
	Total Phosphorus(Log)(kg/yr)	2.0	4.1	0.7	0.8

^a +PBIAS indicates an over prediction, and -PBIAS indicates an under prediction

The BGMM predicted sediment (log), TN, and TP (log) fluxes very well compared to the individual watershed models and the SMA (Table 5-1) during the training period but performed less well during testing period. The poor performance of the BGMM during testing period might be due to the long, 10-yr prediction period and that the testing period occurred 9 yrs after the training period, an effect of the individual model verification periods. The aggregated effect of errors from the individual model predictions may also be contributing. The BGMM slightly under predicted sediment and TN during the training period, and over predicted TP during the training period and sediment and TN during the testing period. Table 5-2 shows the weights of each model during training and testing. The CBP-model performed very well compared to the other individual watershed models. The main reason for variability among model predictions and performance is the scale of model inputs and outputs. The CBP-model was developed at, fine temporal scale (hourly), but a coarse spatial scale (land-river segment), and was developed as a decision support/management model (e.g., to be used by decision makers in TMDL planning).

Both SWAT-VSA and SWAT-ST were developed at a coarser daily time step, but with finer spatial resolution (field scale), and were developed to address fine spatial scale watershed processes. Furthermore, SWAT-VSA has the most highly constrained calibration of the three models (Easton *et al.*, 2008; 2011). These differences are reflected in the BGMM model coefficients (Table 5-2), and are an example of structural uncertainty resulting from the different model initializations and formulations that are captured in the BGMM prediction.

Table 5-2: BGMM model coefficients from eq 2 for flow, sediment, total nitrogen, and total phosphorus

Constituent	CB-model	SWAT-VSA	SWAT-ST
Flow	0.62	0.24	0.14
Sediment	0.68	0.12	0.20
Total Nitrogen	0.74	0.01	0.25
Total Phosphorus	0.85	0.12	0.03

The monthly time series analysis for observed data, SMA, and BGMM with 95% credible intervals for flow, sediment (log), TN, and TP (log) fluxes are shown in Figure 5-3. The BGMM captured the low and high observed flow peaks very well compared to the SMA during the training period (Fig. 5-3a), with only 8% of observed flow falling outside the 95% credible interval (Table 5-3). During the testing period the PBIAS of the BGMM model increased from 3.5 to 9.7% (Table 5-1) but only 11% of the observed flow fell outside the 95% credible intervals (Table 5-3).

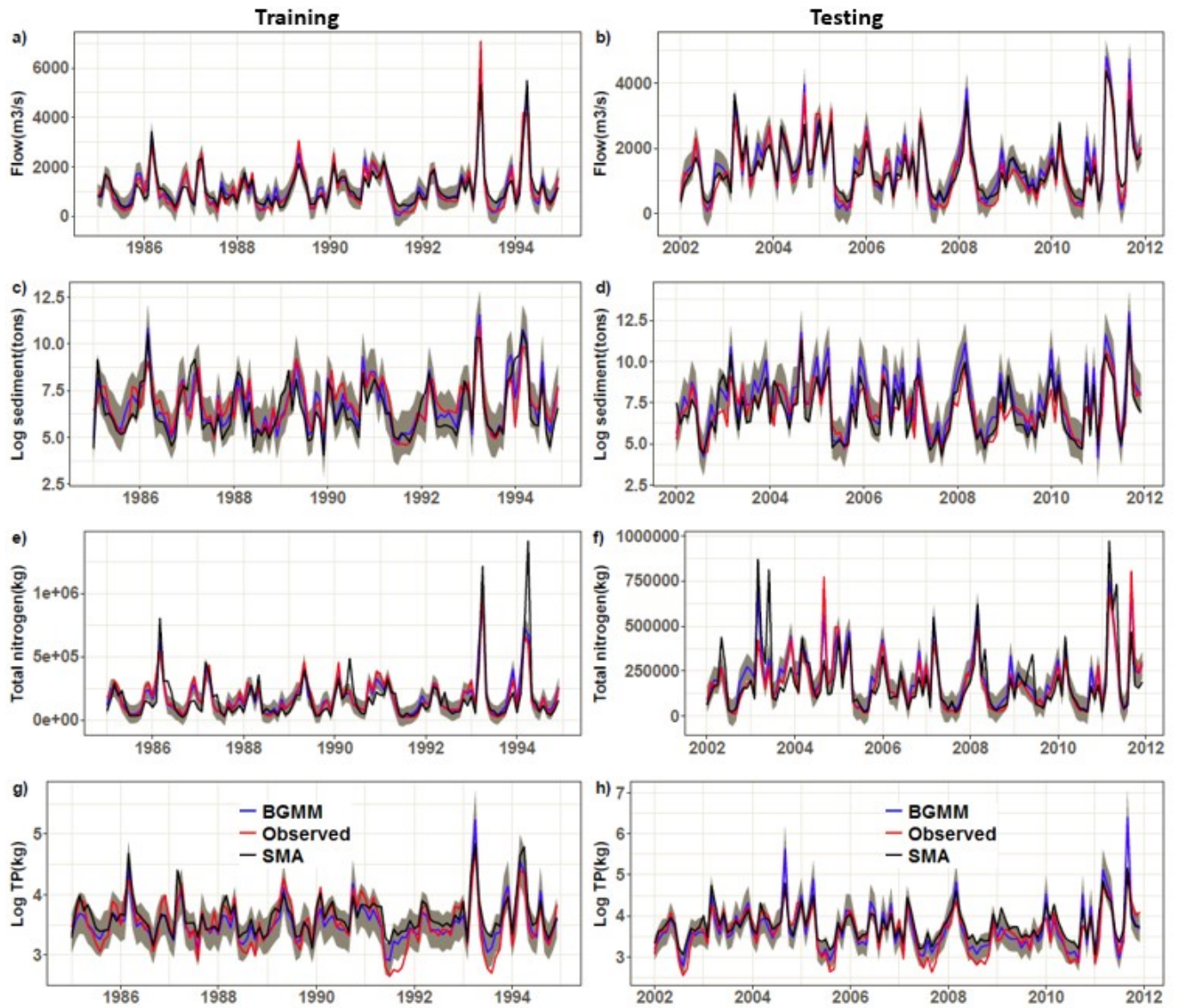


Figure 5-3: Model predictions for the SMA and BGMM ensembles and 95% credible interval for the BGMM (gray shading) for the training (1985 to 1994, left) and testing (2002 to 2011, right) periods for flow (a & b), log sediment (c & d), total nitrogen (e & f), and log total phosphorus (g & h).

Table 5-3: Percent of observed constituents falling outside of the 95% credible interval for the BGMM.

Constituent	Train	Test
Flow	8	11
Sediment	8	22
Total Nitrogen	8	13
Total Phosphorus	6	16

The BGMM captured the sediment (log) flux dynamics and peaks well during the training period with a low 8% of observed data falling outside of the 95% credible interval (Fig. 5-3c, Table 5-3). During the testing period the BGMM performed slightly worse, generally over predicting sediment export, with 22% of observed data falling outside of the 95% credible interval (Fig. 5-3d, Table 5-3), while the SMA tended to capture the peaks of sediment export more accurately (Table 5-1, Fig. 5-3d). For TN, the BGMM captured both the pattern and peaks of TN very well, with only 8% of observed data falling outside of the 95% credible interval (Fig. 5-3e, Table 5-3), and outperformed the SMA, which substantially over predicted the peaks. During the testing period the SMA outperformed the BGMM, which tended to miss peaks and have 13% of the observed data fall outside of the 95% credible interval (Fig. 5-3f, Table 5-3). Neither the BGMM or SMA were able to capture the low values of TP export, (Fig. 5-3g, h) but estimated the peaks and overall temporal dynamics well (Fig. 5-3g, h). Only 6% of observed TP data fell outside of the 95% credible interval during the training period, but this increased to 16% during the testing period (Table 5-3).

Figure 5-4 shows the marginal effects of each individual model on the different constituents. The marginal effect is the rate at which the dependent variable changes with respect to one predictor while holding other predictor variables constant (Leeper, 2017), or the change in the probability of the observed given a one-unit change in the model prediction. For flow the marginal effects of the CBP-model and SWAT-VSA were similar, as the observed flow increased the marginal

effect increased for each model and the 95% credible interval is relatively narrow and constant (Figs. 5-4a, b), which indicates that both models captured both low and high flow values fairly well, with low uncertainty. However, for both models high flows were associated with wider 95% credible intervals of the marginal effects relative to low flows, indicating greater model uncertainty. The SWAT-ST results (Fig. 5-4c) show that the marginal effect decreased as the observed values increased, and had a much wider 95% credible interval compared to other models, equating to greater uncertainty. Both SWAT-VSA and SWAT-ST also displayed smaller marginal effects than the CBP-model, marginal effect ranging from approximately 0.41 for SWAT-VSA to -0.27 from SWAT-ST, while the CBP-model remained nearly 1. For sediment (Figs. 5-4d, e, f), TN (Figs. 5-4g, h, i), and TP (Figs. 5-4j, k, l) the marginal effect for each model increased as respective predictors were changed while holding others constant. However, the marginal effect 95% credible interval was quite different for each of the three watershed models, narrower across the marginal effects for the CBP-model, and wider for both SWAT-VSA and SWAT-ST. Similar to flow, the marginal effects were smaller for SWAT-VSA and SWAT-ST, for TN in particular (Figs. 5-4g, h, i), less so for sediment (Figs. 5-4d, e, f) and TP (Figs. 5-4j, k, l). The 95% credible intervals for nutrients and sediments, being considerably wider than the 95% credible interval for flow, further indicate more uncertainty in these predictions, which is consistent with previous MME research (Boomer *et al.*, 2013).

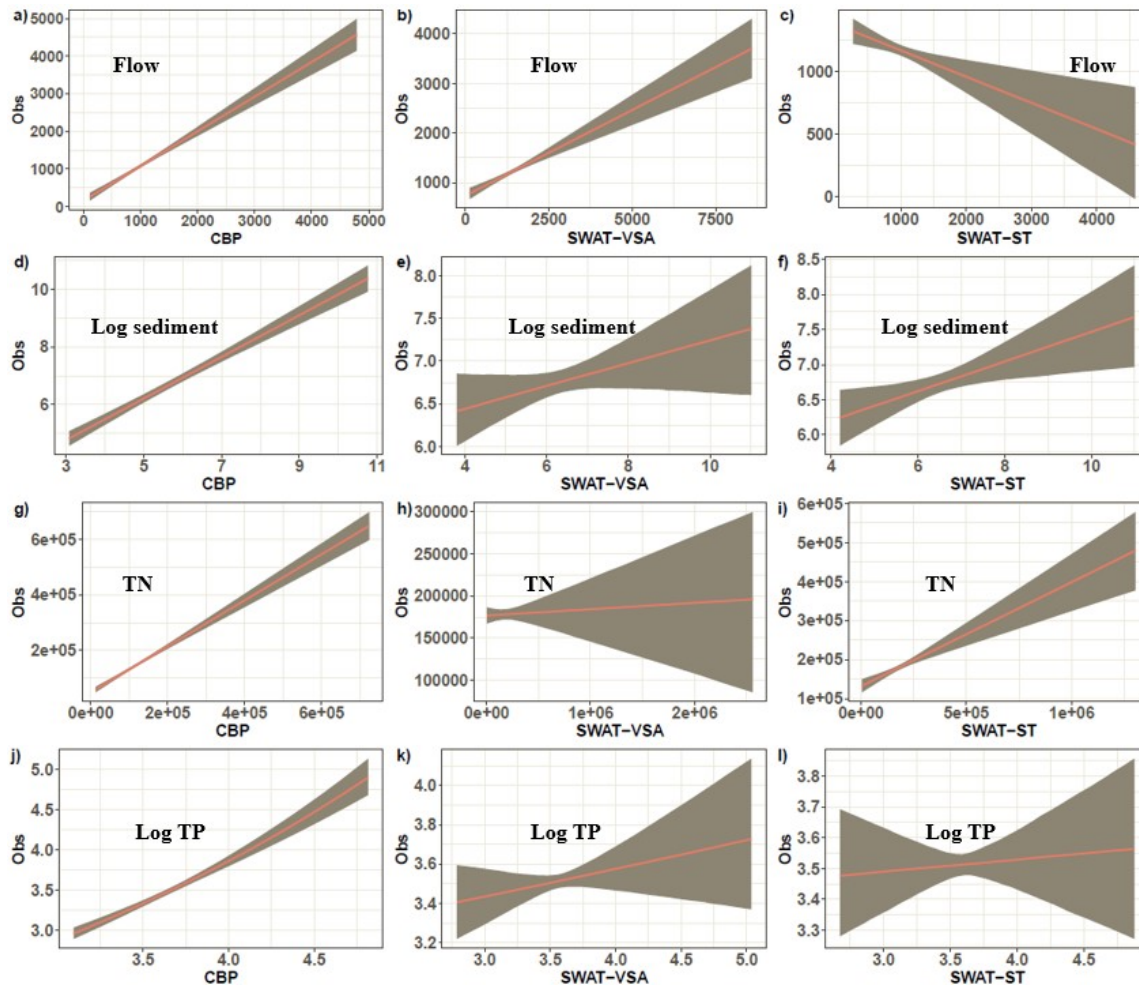


Figure 5-4: Plot of marginal effects (with 95% credible interval) of each model for flow (a, b, and c), log sediment (d, e, and f), TN (g, h, and i), log TP (j, k, and l) during the training period.

Discussion

The MME using the BGMM method presented here quantifies the structural uncertainty from three watershed models in the Susquehanna River watershed. Our results show that the BGMM provides better predictions of flow, sediment, TN, and TP compared to individual models and the SMA during the training period, although constituents were less well predicted during the testing period. The relatively poor performance during the testing period might be due to the aggregated effect of errors from the individual model predictions, or an indication that the stationarity of the constituents was violated (Ajami *et al.*, 2006). Indeed, the mean annual flow increased from $1140 \text{ m}^3 \text{ s}^{-1}$ during the training period to $1458 \text{ m}^3 \text{ s}^{-1}$ during the testing period, a good indication

that conditions in the basin were changing. These results are similar to other studies that concluded that MMEs outperformed single models and simple averaging methods in some, but not all cases (Ajami *et al.*, 2006; Stoica *et al.*, 2004; Weisheimer *et al.*, 2009). Indeed, the strength of the BGMM is not necessarily in the absolute predictions, but rather in the uncertainty associated with those predictions. For instance, the larger 95% credible intervals for sediment and nutrients suggest where more research is justified to provide better understanding of physical watershed processes (Boomer *et al.*, 2013) or where continued development of each of the individual models could improve the BGMM results.

The prediction variability among models is due to several factors including differences in model initialization, conceptualization of processes, and mathematical representation and expressions, which are also the sources of structural model uncertainty (Son & Sivapalan, 2007). Varying temporal resolution of model input data drive differences in model predictions as well. For instance, the CBP-model was initialized with hourly meteorological data and calibrated to hourly flow data, while both the SWAT-VSA and SWAT-ST models were initialized with daily meteorological data and calibrated with daily flow data.

The inherent structural uncertainty from three watershed models is well represented by BGMM with 95% credible intervals (Fig. 5-3). This uncertainty can be used in many fashions, but perhaps the most important in the water resources field is for decision-making and policy implementation. The BGMM uncertainty can help guide decision makers to identify and minimize the largest sources of uncertainty, an example of which might be the probability of meeting a water quality goal in the basin, such as a TMDL. Indeed, the BGMM method can provide quantitative estimates of the probability of meeting a TMDL by providing estimates of the risks associated with imperfect knowledge of watershed processes or the impact of landuse change (Breuer *et al.*, 2009) and climate change (Hashmi *et al.*, 2009) stressors. Others have explored risk, or uncertainty based decision making, for instance, Giorgi and Mearns (2003) used Reliability Ensemble Averaging (REA) to estimate the uncertainty range and reliability of regional climate change projections based on ensembles of climate models. Brekke *et al.* (2008) used ensembles of historical and future projections from the World Climate Research Programme's (WCRP's) Coupled Model Intercomparison Project phase 3 (CMIP3) multi-model dataset to determine how model credibility affects the apparent relative scenario likelihood in

regional risk assessments, one of the types of scenario likelihood associated with climate change (Brekke *et al.*, 2008).

The test of the marginal effects decomposes the BGMM into the individual models and provides some diagnostic measures to evaluate the performance of each model and the associated uncertainty bounds, which in turn is representative of structural uncertainty of each model (Fig. 5-4). Indeed, the marginal effect (Fig. 5-4) corroborates that the CBP-model, with finer temporal scale input and output data, predicted peak flows (and peak nutrient and sediment export) with greater accuracy, compared to the other watershed models, while SWAT-VSA and SWAT-ST tended to better capture base flows. These nuances are reflected in the BGMM coefficients (Table 5-2). However, the watershed model with the highest coefficients in BGMM or with more consistent marginal effect does not mean the individual model is a better predictor (Sheiner & Beal, 1981). For instance, the CBP-model individually had the worst prediction performance of TN, with a PBIAS of -12%, while both SWAT models had a PBIAS of approximately 3%, yet the CBP-model had a coefficient of 0.74 while SWAT-VSA and SWAT-ST had coefficients of 0.01 and 0.25, respectively. Yet the BGMM outperformed each of the individual models with a percent of -0.3. Clearly, being able to incorporate the best aspects of each model more than makes up for the deficiencies in each model (Doblas-Reyes *et al.*, 2005; Hagedorn *et al.*, 2005).

While the BGMM was not always the best performing model, particularly when tested outside of the range for which it was developed, the BGMM is the only one that can provide estimates of model uncertainty. The BGMM leverages the strengths of each individual watershed model. The use of multi-model ensembles has been proposed for use in watershed modeling (e.g., Boomer *et al.*, 2013; Exbrayat *et al.*, 2010) for predicting flow and nutrients, but much of the literature in watershed modeling describes the use of simple averaging techniques, or simply suggests using an ensemble model approach to improve upon current work and allow an assessment of model uncertainty. Thus, the BGMM approach developed here represents an incremental step towards realizing these goals. The BGMM method can be used to analyze the effects of different landuse and climate change scenarios on water resources and quality by obtaining the weights of models and the predictions with associated uncertainty bounds. Additionally, these bounds can help to enhance model prediction credibility and assist the decision-making process.

Conclusions

This study describes and evaluates a multi-model ensemble using the BGMM approach, which is capable of quantifying structural uncertainty and in some cases, improving predictions over individual models. Current research is lacking in this area and effective methods for quantifying structural uncertainty are paramount in a watershed management context. Three watershed models (CBP-model, SWAT-VSA, and SWAT-ST) tended to predict flow, sediment, and nutrients differently in the Susquehanna River basin. The CBP-Model model performed very well in predicting flow due to fine scale data input and hourly data calibration. Our results show the BGMM provided predictions of sediment, TN, and TP similar to the CBP-model, SMA, SWAT-VSA, and SWAT-ST in predicting flow. The BGMM method also provided 95% credible intervals capable of quantifying structural uncertainty associated with the watershed models, which can assist with the decision-making process in a management context.

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CHAPTER 6

CONCLUSIONS AND FUTURE WORK

Quantifying the impact of climate change on the hydrologic cycle and nutrient export in agroecosystems requires new tools and methods. Tools that link key biogeochemical processes and hydrologic processes are required to quantify N, P, sediment fluxes export, and GHG emissions from the landscape to surface waters under changing climate, and help to develop effective landscape management strategies to improve water quality. Challenges for researchers in building such tools that couple these processes are a lack of understanding of interaction of biogeochemical and hydrologic processes under a changing climate, and difficulty in refining the spatial and temporal representation of processes.

To address some of these problems, a new model (SWAT-GHG) that links environmental and soil factors was built to predict the impact of land management and climate change on water and air quality. The model predicted N₂O emissions with good spatial and temporal accuracy. While the model proved valuable in predicting GHG emissions (Chapter 2), further refinement could improve model utility. One area of further development would be inclusion of a dynamic soil pH routine, as currently pH is a user defined, static input. Including routines to model other GHGs, such as methane (CH₄), would further improve the model. The inclusion of CH₄ would provide a complete picture of GHG emissions from agricultural lands.

Chapter 3 details an application of SWAT-GHG to a small agricultural watershed with long-term, high-resolution water quality and land management data. This application highlighted the potential impact of climate change on nutrient cycling, including the effect on the nutrient export and GHG emissions, and on alterations to the hydrologic cycle. These types of model assessments highlighted the need for detailed crop rotation representation in the model, which is particularly important when evaluating the performance of best management practices (BMPs), as in Chapter 4.

Chapter 4 describes the potential for BMPs to reduce the impact of climate change on water quality. All of the BMPs evaluated, to varying extents, were capable of reducing the impact of climate change. The results also indicated that for NO₃-N and sediment more will need to be

done to ensure adequate water quality in a changing climate. One of the most important findings was that performance of BMPs is highly dependent on the land use classification and management practices employed, including detailed crop rotation data, which are often hard to obtain. Thus, future work in this area requires both better information to inform models, as well as better spatial representation of BMPs on the landscape. More could also be done by testing new BMPs or combinations of different BMPs or on methods to target critical source areas of the landscape.

Finally, in Chapter 5 the inherent uncertainty associated with watershed/hydrologic modeling was assessed using a Bayesian Generalized Multi-Level Model (BGMM), and compared to individual ensemble model members and a Straight Model Averaging (SMA) method. While the BGMM was not always the best model for each constituent of interest, it was, on the whole the most consistent predictor. Furthermore, the BGMM provided quantitative estimates of prediction uncertainty, which none of the other models could provide. Future work should explore other multi model ensemble methods to better capture uncertainty associated with model structure, parameter input uncertainty, and calibration/numerical method representation in watershed models. Further investigation into calibration/numerical method representation of environmental models is critical to improving model utility, as the paradigm of “obtaining the right answer for the wrong reason” continues to plague environmental modelers, and with more and more powerful computational abilities threatens the validity of our models.


```

!! sol_wpmm(:,:) |mm H2O      |water content of soil at -1.5 MPa (wilting
!!                    |point)
!! sol_z(:,:) |mm          |depth to bottom of soil layer
!! n2o_nit(k,j) |Kg N/ha    |amount of nitrous oxide from nitrification
!!
!!
!! ~~~~~
!!
!! ~~~ OUTGOING VARIABLES ~~~
!! name      |units      |definition
!! ~~~~~
!! nitr_oxide |Kg N/ha    |Nitrous oxide in the soil profile
!! ~~~~~
!!
!! ~~~ LOCAL DEFINITIONS ~~~
!! name      |units      |definition
!! ~~~~~
!! j         |none       |number for HRU
!! k         |none       |counter
!! nly       |none       |number of layers
!! fd_co2(:,:) |g N/ha/day |the maximum total N gas flux for a given soil respiration or
!!                    |index function for carbon availability on total
!!                    |denitrification (N2O + N2) N gas flux
!! fd_ph(:,:) |none       |effect of PH on denitrification rate
!! fd_no3(:,:) |g N/ha/day |the maximum total N gas flux for a given soil No3 level
!! fd_tmp(:,:) |none       |effect of temperature on denitrification rate
!! fd_wfps(:,:)|%          |effect of wfps(water filled pore space on denitrification rate
!! fr_co2     |g N/ha/day |effect of soil respiration or carbon on ratio
!! fr_no3     |g N/ha/day |effect of soil nitrate on ratio
!! fr_wfps    |%          |effect of water filled pore space on ratio
!! sol_cmass  |kg c/ha    |amount of carbon stored in the soil layer

```

```

!!          |converted by using percent organic carbon
!!  sum_N20  |kg N/ha   |amount of N lost by denitrification in the soil profile
!!  wfps(:,) |%          |water filled pore space for each soil layer
!!  xx's     |none       |variables to hold value for denitrification
!!  xx_r's   |none       |Variables to hold for nitrous oxide calculation
!!  ~~~~~
!!
!!  ~~~ SUBROUTINES/FUNCTIONS CALLED ~~~
!!  Intrinsic: Exp, Max, Atan, Min
!!  SWAT:
!!
!!
!!  ~~~~~ END SPECIFICATIONS ~~~~~
!!
!!
    use parm
    integer :: j,k,nly,kk
    real :: sol_thick,xx,xx1,xx2,xx3,xx4,xx5,xx6
    real :: xx_r1,xx_r2,xx_r3,xx_r4,wc,sat
    real, parameter :: PI=3.141592653589793D0,convert= 0.001
    real ::fd_co2,fd_no3, fd_ph,fd_wfps
    real :: fr_co2, fr_no3, fr_ph,fr_wfps,nitr_N2_pro
    real :: ratio_N2_N2O,nitr_N2O_pro,nitr_N2O,sol_no3_load,nitr_N2
    real :: sol_mass,sol_cmass,fd_tmp,wfps,dent_flux,sol_tex
    real :: dent_flux_pro
!!  real :: fdr_no3_pro, fdr_co2_pro
!!
!! initialize local variables
!!
    k = 0
    j= 0

```

```
j = ihru
nly = sol_nly(j)
wc = 0.
sat = 0.
sum_N2O = 0.
sol_mass = 0.
sol_cmass = 0.
fd_co2 = 0.
fd_no3 = 0.
fd_ph = 0.
fd_wfps = 0.
fd_tmp = 0.
wfps = 0.
fr_co2 = 0.
fr_no3 = 0.
fr_ph = 0.
fr_wfps = 0.
sol_thick = 0.
xx = 0.;xx6=0.
xx1=0.;xx2 = 0.;xx3 =0.;xx4 =0.;xx5 = 0.
xx_r1=0.;xx_r2 =0.;xx_r3 = 0.;xx_r4 = 0.
ratio_N2_N2O = 0.
dent_flux =0.
sol_tex = 0.
nitr_N2O = 0.
    nitr_N2 = 0.
nitr_N2O_pro =0.
    nitr_N2_pro = 0.
nitr_oxide(j)=0.
    n2_den(j) = 0.
!den_tot =0.
```

```

sol_no3_load =0.
      dent_flux_pro =0.
!!   den_tot(j) = 0.
!!   nitr(j)  = 0.
!!   fdr_no3_pro =0.
!!   fdr_co2_pro =0.
!!
!!soil carbon mass from the soil and reduction function
!!calculation for each layer
!!
  !if (cden==1) then
  do k = 1,nly
    if (k == 1) then
      sol_thick = sol_z(k,j)
    else
      sol_thick = sol_z(k,j) - sol_z(k-1,j)
    end if
  !! kg/ha( 10,000 for ha, originally it was (kg/m2)
      sol_mass=(sol_thick/1000.)*10000.*sol_bd(k,j)
    &      * 1000.*(1- sol_rock(k,j)/100.)
  !! mass of carbon( kg/ha)
  !!
      sol_cmass=sol_mass *(sol_cbn(k,j)/100.)
      xx = 0.35*sol_cmass
      if (xx <= 35.) then
        xx = Exp(0.35*sol_cmass)
        xx = 200./xx
          xx= 1.+ xx
        fd_co2=(24000./xx)-100.
      else
        xx = Exp(35.)

```

```

xx = 200./xx
xx= 1.+ xx
fd_co2=(24000./xx)-100.
end if
!!
!!fd_co2 first in g N/ha and converted in to Kg N/ha
!!   fd_co2=fd_co2*convert
!!
!! soil_no3 level is in concentration (mg/kg ) not in Kg/ha;
!! so kg/ha is changed in to mg/kg
!! from .chm input file for each layer, fd_no3 in gN/ha
!!
xx6=sol_bd(k,j)*sol_thick*100.
sol_no3(k,j)=sol_no3(k,j)/xx6  !! sol_no3 is converted in to mg/kg
!if (sol_no3(k,j) > 0.) then
xx1=40000.*(Atan(PI*0.002*(sol_no3(k,j)-180.)))/PI
if (xx1 > -11000.) then
fd_no3=11000.+xx1
else
fd_no3 = 1.e-6
end if
!!   else if(sol_no3(k,j) <= 0.
!!           !fd_no3 = 0.
!!       !end if
!! fd_no3 in Kg N/ha
!!   fd_no3=fd_no3*convert
!!
!!calculates PH reduction factor for each soil layer based on
!!soil PH input provided in the .sol input file
!!
kk=k

```

```

if(k==1) kk=2
if (sol_tmp(kk,j) > 0. .and. sol_st(kk,j) > 0.) then
  !! microbial processes if temp > 0 C
  !! microbial processes if water > pwp
if (sol_ph(kk,j) <= 2.5) then
  fd_ph=1.e-6
else if( sol_ph(kk,j) > 2.5 .and. sol_ph(kk,j)< 6.5) then
  fd_ph=(sol_ph(kk,j) - 2.5)/4.
else
  fd_ph= 1.
end if
!! calculate the temperature reduction function based on
!! soil temperature of each layer
!!
  xx2=sol_tmp(kk,j)/(sol_tmp(kk,j)+
&   Exp( 9.93 + 0.312*sol_tmp(kk,j)))
  xx2= 0.9*xx2+0.1
  fd_tmp= Max(xx2,0.1)
!!
!! calculate wfps(water filled pore space) based on water content and
!! saturation level at each soil layer and determine the water content
!! effect on total denitrification based on the texture of soil in
!! each layer;three d/t equations depending on dominant soil texture
!! are used to determine the effect of water content
!! on denitrification rate as described in the
!! paper of Parton,Mosier et al. 1996
!!
  wc=sol_st(kk,j)+sol_wpmm(kk,j)
!!
!! wc units mm
  sat=sol_ul(kk,j)+sol_wpmm(kk,j)

```

```

!! sat units mm
    wfps=(wc/sat)
    sol_tex=MAX(sol_clay(k,j),sol_silt(k,j),
&        sol_sand(k,j))
    if (wfps >=0.30) then
        if(sol_tex == sol_clay(k,j)) then
            xx3=1.06*wfps
            xx3=18.**xx3
            xx3=22./xx3
            xx3=18.**xx3
            fd_wfps=60./xx3
        else if (sol_tex == sol_silt(k,j))then
            xx4=1.39*wfps
            xx4=14.**xx4
            xx4=16./xx4
            xx4=14.**xx4
            fd_wfps=4.82/xx4
        else
            xx5=2.01*wfps
            xx5=12.**xx5
            xx5=16./xx5
            xx5=12.**xx5
            fd_wfps=1.56/xx5
        end if
    else
        fd_wfps=0.
    end if
!!
!!Calculate the reduction functions / factors for ratio of N2:N2O
!!to determine GHG's particularly N2O for each layer based on
!!reduction function; first calculate the water filled pore space

```

```

!!for water content effect on ratio of N2: N2
!!
  if (wfps>=0.30) then
    xx_r1=2.2*wfps
    xx_r1=13.**xx_r1
    xx_r1=17./xx_r1
        xx_r1=13.**xx_r1
    fr_wfps=1.4/xx_r1
  else
    fr_wfps=0.
  end if
!!
!!Calculate PH reduction function/ factor effect on ratio of N2:N2O
!!
  xx_r2=Exp(-sol_ph(kk,j)*1.1)
  fr_ph=1./(1470.*xx_r2)
!!
!!calculate the effect of soil No3 on the ratio N2:N2O
!!
  xx7=sol_bd(k,j)*sol_thick*100.
  sol_no3(k,j)=sol_no3(k,j)/xx6
!!
  !if (sol_no3(k,j) > 0.) then
    xx_r3=1.*(Atan(PI*0.01*(sol_no3(k,j)-190.)))/PI
!!    if (xx_r3<-0.46) then
      xx_r3 = 0.5+xx_r3
      fr_no3=(1.- xx_r3)*25.
!!
!! Calculate the effect of the soil respiration on
!! the ratio N2:N20,in g N/ha
!!

```

```

        xx_r4=30.78*(Atan(PI*0.07*(sol_cmass - 13.)))/PI
!!     if (xx_r4 > -13.) then
        fr_co2=13.+xx_r4
!!     else
!!     fr_co2 = 1.e-6
!!     end if
!! in Kg N/ha
!!     fr_co2=fr_co2*convert
!!
!!
!! calculate the total denitrification flux(N2 + N2O) based on
!!the above reduction functions
!! Kg N/ha
        dent_flux=Min(fd_no3,fd_co2)*fd_tmp*fd_wfps*fd_ph
!!
!! calculate the ratio N2:N2O based on the above reduction functions
!! or factors and partition in to
!! Nitrous oxide(N2O) and di nitrogen(N2)
!!
        ratio_N2_N2O=Min(fr_no3,fr_co2)*fr_wfps*fr_ph
!!
!! amount of N lost as nitrous oxide for each layer
!!
        if(ratio_N2_N2O > 0.) then
            nitr_N2O = dent_flux/(1.+ratio_N2_N2O)
                nitr_N2 = dent_flux/ (1. + (1.0/ratio_N2_N2O))
        else
            nitr_N2O = 0.
            nitr_N2 = dent_flux
        end if
        if(sol_no3(k,j) > 0.001*dent_flux) then

```

```

        sol_no3(k,j) = sol_no3(k,j) - 0.001*dent_flux !! convert in to kg/ha
    else
        sol_no3(k,j) = 0.
    end if
    if(cden ==1) then
        wdnt1 = nitr_N2 + wdntl
    end if
!!         den_tot = den_tot + dent_flux

    end if
!!
!!for testing purpose only
!!
!! nitriuous oxide outputs for .hru file
!!
        nitr_oxide(j)=nitr_oxide(j)+nitr_N2O
        n2_den(j) = n2_den(j) + nitr_N2
!!     sol_no3(k,j) = sol_no3(k,j)- nitr_oxide(j)

!!     den_tot(j) = nitr_oxide(j) + nitr(j)
!!
!! amount of N lost as nitriuous oxide in the soil profile in Kg N/ha
!!     if(iyr == 2009) then
        write (1003,9000)iyр,i,k,j,sol_ph(k,j),sol_tmp(k,j),fd_ph,
&         sol_cmass,fd_co2,fd_no3,dent_flux,
&         ratio_N2_N2O,nitr_N2O,fd_tmp,sol_no3(k,j)
        write (1006,9002)iyр,i,k,j,wfps,fr_no3,fr_co2,fr_wfps,fr_ph,
&         fd_wfps,sol_cbn(k,j),sol_thick,sol_tex
!!     end if
!!
!!

```

```

!!   den_tot = den_tot + dent_flux
    dent_flux_pro=dent_flux_pro +dent_flux
    nitr_N2O_pro=nitr_N2O_pro+nitr_N2O
        nitr_N2_pro = nitr_N2_pro + nitr_N2
!!
    end do
    !end if
!!
!! writing daily output file
9000   format(i4,',',i4,',',i4,',',i4,11(',','f10.3))
9002   format(i4,',',i4,',',i4,',',i4,9(',','f10.3))
!!
        write (1002,3001)k,iyr,i,j,dent_flux_pro,nitr_N2O_pro,
&                nitr_oxide(j),nitr_N2_pro,n2_den(j)
3001   format(i4,1x,i4,1x,i3,1x,i4,1x,f10.3,1x, 2f10.3,1x,2f10.3)
    return
    end

```