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Integrating Multi-Media Models to Assess Nitrogen Losses from the Mississippi River Basin to the Gulf of Mexico

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Abstract

This study describes and implements an integrated, multimedia, process-based system-level approach to estimating nitrogen (N) fate and transport in large river basins. The modeling system includes the following components: 1) Community Multi-Scale Air Quality (CMAQ); 2) Water Research and Forecasting (WRF); 3) Environmental Policy Integrated Climate (EPIC); and 4) Soil and Water Assessment Tool (SWAT). The previously developed Fertilizer Emission Scenario Tool for the Community Multiscale Air Quality (FEST-C) system integrated EPIC with the WRF model and CMAQ. FEST-C, driven by process-based WRF weather simulations, includes atmospheric N additions to agricultural cropland, and agricultural cropland contributions to ammonia emissions. Watershed hydrology and water quality models need to be integrated with the system (FEST-C),

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however, so it can be used in large river basins to address impacts of fertilization, meteorology, and atmospheric N deposition on water quality. Objectives of this paper are to describe how to expand the previous effort by integrating a watershed model with the FEST-C (CMAQ/WRF/EPIC) modeling system, as well as demonstrate application of the Integrated Modeling System (IMS) to the Mississippi River Basin (MRB) to simulate streamflow and dissolved N loadings to the Gulf of Mexico (GOM). IMS simulation results generally agree with USGS observations/estimations; the annual simulated streamflow is 218.9 mm and USGS observation is 211.1 mm and the annual simulated dissolved N is 2.1 kg/ha. and the USGS estimation is 2.8 kg/ha. Integrating SWAT with the CMAQ/WRF/EPIC modeling system allows for its use within large river basins without losing EPIC's more detailed biogeochemistry processes, which will strengthen assessment of impacts of future climate scenarios, regulatory and voluntary programs for nitrogen oxide air emissions, and land use and land management on N transport and transformation in large river basins.

Key Words: Multi-Media Models, IMS-Integrated Modeling System, MRB-Mississippi River Basin, and nitrogen loading.

1 Introduction

Increased nitrogen (N) fluxes from the Mississippi River Basin (MRB) have been linked to increased occurrences of seasonal hypoxia in the northern Gulf of Mexico (GOM) (NSTC, 2000; USEPA, 2014; Alexander et al., 2008; Rabalais et al., 2001). Hypoxia is an environmental phenomenon in which concentration of dissolved oxygen in the water column decreases to a level that can no longer support living aquatic organisms which, in turn, depletes valuable fisheries and disrupts ecosystems. Modeling studies have been conducted to improve understanding of factors and

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sources contributing to increased N export from the MRB (Alexander et al., 2008; David et al., 2010; Donner and Kucharik, 2008; Donner and Scavia, 2007; Mayorga et al., 2010; McCrackin, et al., 2014; NSTC, 2000; Santhi et al., 2014). Those focused on interactions of land and water; and the NSTC (2000) concluded that N loading to the GOM is related to runoff, agricultural activity and human population densities. The current strategy of the Hypoxia Task Force (HTF), a collaborative effort of federal and state agencies, and tribes, is to reduce both N and phosphorous (P) losses through state-level nutrient reduction strategies and by targeting actions within watersheds where they will be most effective. There is an interim target of reducing N and P loading by 20% (relative to the 1980-1996 baseline period) by 2025, and a goal of reducing the summer hypoxic zone to less than 5,000 km^2 by 2035 (USEPA, 2014).

However, it is not clear how atmospheric N deposition contributes to the total N load and its impact on rivers, lakes and estuaries in the MRB, particularly impacts of Clean Air Act (CAA) regulations on abatement. Furthermore, climate is changing: temperatures are rising, snow and rainfall patterns are shifting, and more extreme climate events such as heavy rainstorms and record high temperatures are happening (USEPA, 2016). Considering the expected changes in climate during N assessment is also critical for the MRB (Donner and Scavia, 2007), because future climate scenarios may impact streamflow generation, and thus, N loads from the watershed. Finally, due to the complex N cycle and its dynamics from the atmosphere to the biosphere, through dry deposition of gaseous N species and wet deposition of dissolved N species in precipitation, the USEPA Science Advisory Board (USEPA, 2011) and the European Nitrogen Assessment (Sutton et al., 2011) emphasized the need for integrated, multimedia and transdisciplinary approaches to evaluate N fate and transport comprehensively. Therefore, an Integrated Modeling System (IMS) linking air, land surface, and stream processes is needed to fill the research gap for integrated, multi-media modeling for N studies in large river basins.

The USEPA developed the Fertilizer Emission Scenario Tool for the Community Multiscale Air Quality (FEST-C) system (Cooter et al., 2012; Ran et al., 2011); it simulates daily fertilizer application to agricultural lands for bi-directional ammonia (NH_3) modeling (Bash et al., 2013; Pleim et al., 2013) in the Community Multiscale Air Quality (CMAQ) model (Byun and Schere, 2006; Appel et al., 2016). FEST-C integrates the Environmental Policy Integrated Climate (EPIC) model (Williams, 1995; Williams, 1990; Williams and Arnold, 1996), a field-scale agricultural biogeochemical model, with the Weather Research and Forecast (WRF) model (Skamarock et al., 2008) and CMAQ; WRF/CMAQ simulates mesoscale meteorology and air quality (Fig. 1). The FEST-C system (EPIC/WRF/CMAQ) is useful for assessing impacts of agricultural fertilization and management practices not only on air quality (NH_3) (Fu et al., 2015) and climate (nitrous oxide (N_2O)) (Cooter et al., 2010), but also on crop yield, soil erosion, and hydro-ecosystems. The FEST-C system consist of field-scale models, however. To address impacts of fertilization, meteorology, and N deposition from the FEST-C modeling system on water quality, watershed hydrology and water quality models must be integrated. The next step toward a full multimedia assessment is integration of these atmospheric interactions with watershed processes and/or watershed hydrology and water quality models. We fill this gap by proposing to integrate the Soil and Water Assessment Tool (SWAT) with the FEST-C system.

SWAT (Arnold et al., 2012; Gassman et al., 2007; Neitsch et al., 2011) has been widely applied to evaluate best management practices, alternative land use/land management, and climate change on pollutant losses to streams within a watershed (Chaplot et al., 2004; Gassman et al., 2007; Johnson

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et al., T., 2015; Santhi et al., 2006; Vaché et al., 2002). In the past, SWAT applications focused on evaluating land use/land management and/or climate change on water quality, but none focused on an integrated modeling approach that accounted for air deposition as well as its interaction with climate and agricultural activities. SWAT can consume user-defined atmospheric deposition and wet deposition data from the National Atmospheric Deposition Program (http://nadp.sws.uiuc.edu/) from 1980 to 2010, which are precipitation-weighted means (mg/L) at a monthly time step (Neitsch et al., 2011; Yen et al., 2016). Neither climate nor agricultural activities interact with atmospheric deposition during a SWAT simulation. Integrating SWAT with FEST-C systems not only allows the FEST-C systems to work at large watershed scales, but also allows SWAT to take in dynamic atmospheric N deposition (bi-directional CMAQ) data so it can account for interaction of air, climate and agricultural activities. Furthermore, EPIC can provide more detailed field-level biogeochemical processes simulation than SWAT. This integrated modeling system allows us to look at all potential sources of N from a watershed in a dynamic way and assess the impact of CAA amendment regulations, climate change, and land use/land management changes on N loadings in large river basins such as the MRB. This effort marks a significant step forward in a more complete systems-level framework for N assessment.

Due to the complexity of the modeling system and the scale of targeted application, our study focuses on model integration and proof of concept. The objectives were to 1) describe integration of SWAT with FEST-C (EPIC/WRF/CMAQ) and 2) demonstrate application of the integrated multi-media modeling system to the MRB to assess N loading.

2 Methodology

2.1. Overview of N Transformation and Transport

Nitrogen has the most complex nutrient cycle of all the mineral nutrients because it can exist in both dissolved forms and as gaseous NH_3 or N_2 (Burt et al., 1993). The nitrogen cycle and its dynamics in agricultural soils are complicated biological and chemical processes. Generally, major forms of N in soils are organic N associated with humus (active and stable in organic pool) and soluble forms of mineral N (mainly nitrate (NO_3^-) and ammonium (NH_4^+), with low concentration of nitrite (NO_2^-)). Nitrogen cycling and losses consist of the following processes: atmospheric N deposition; mineralization; immobilization; nitrification; denitrification; volatilization; biological N fixation from the atmosphere; decomposition of fresh residue; plant uptake; organic N transport in sediment; and nitrate and nitrite N losses in leaching, surface runoff and lateral subsurface flow (Yuan et al., 2017). To simulate N transformation and transport, N mass balances summarizing N gains (mineralization, fixation, and fertilizer application) and losses (plant uptake, denitrification, volatilization, and immobilization) are established in simulation models. Usually, N mass balance is maintained for both the organic and inorganic pools. Potential N losses from agricultural soils may occur through nitrate and nitrite leaching to the subsurface or through surface runoff and organic N transport in sediment.

2.2. FEST-C System

EPIC is a semi-empirical biogeochemical process model that assesses the effect of wind and water erosion on crop productivity and evaluates management solutions that maximize crop production while reducing soil and nutrient losses (Williams et al. 1984, 2008). It is a daily time-step, field-scale model, and the computational "fields" can extend up to 100 ha in area. EPIC has

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been modified to provide a full biogeochemical characterization of agricultural systems since its original development.

EPIC simulates the complete N cycle: atmospheric N inputs; fertilizer/manure N applications; crop N uptake; nitrification (transformation of the NH_4^+ pool to NO_3^-); denitrification (conversion of NO_3^- to produce N_2 and N_2O); ammonia volatilization (gaseous loss of NH_3 that occurs when NH_4^+ is surface applied); decomposition; mineralization and immobilization; organic N transport on sediment; and nitrate-N losses in leaching, surface runoff, lateral subsurface flow and tile flow. Mineralization is the process that breaks down organic N compounds in the soil to release NH_4^+, with concurrent release of carbon as CO_2 in most cases (Vinten and Smith, 1993); the reverse process is immobilization by which NH_4^+ pool to NO_3^- are microbially transformed into organic forms. Decomposition and mineralization of fresh organic N are controlled by a decay rate constant. Denitrification occurs only when soil moisture content is above field capacity. The fertilizer N is considered to dissolve immediately and contribute to the mineral N pool. Plant uptake of N is controlled by plant demand, but limited by soil supply of the N. Organic N in each soil layer is partitioned into fresh and stable pools. The organic N loss is estimated using sediment yield, organic N on the soil surface layer, and an enrichment ratio; the soluble N loss is estimated by considering soluble N concentration changes in soil layers (Wang et al., 2012). EPIC was modified to accept time series of wet and dry atmospheric deposition of oxidized and reduced N from WRF/CMAQ through the FEST-C system (Cooter et al., 2012; Ran et al., 2011).

EPIC options include characterization of various tillage practices (e.g., conventional, reduced-till, no-till, and contour plowing) and engineering changes (e.g., construction of terraces and installation of tile drainage). It also includes a heat unit-driven, above- and below-ground plant

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growth model, soil hydrology and soil heat budgets for multiple soil layers of variable thickness. Simulation output frequency is user-specified, ranging from daily to annual summaries of biogeochemical process rates, nutrient pools and management activity, as well as edge-of-field runoff, sediment, and nutrients.

The WRF model developed at the National Center for Atmospheric Research is a numerical weather prediction and atmospheric simulation system (Skamarock et al., 2008). It considers atmospheric thermodynamic properties and is applicable to horizontal spatial scales ranging from meters to thousands of kilometres. It has been used extensively for research and real-time forecasting throughout the world (http://www.wrf-model.org/index.php). WRF was used to generate EPIC weather inputs including daily maximum and minimum temperature, precipitation, solar radiation, relative humidity and wind speed.

The CMAQ model is a community-based atmospheric chemistry and transport model designed to simulate photochemical (e.g., ozone), aerosol (e.g., PM2.5), and toxic (e.g., benzene) air pollutants (Byun and Schere, 2006; Appel et al., 2016). It simultaneously models multiple air pollutants including ozone, particulate matter and a variety of gaseous elements (including N) to help air quality managers determine the best management scenarios for their communities, regions and states. The tool can provide detailed information about air pollutant concentrations in a given area for any specified emission or climate scenario (http://www.epa.gov/air-research/community-multi-scale-air-quality-cmaq-modeling-system-air-quality-management). Integrating CMAQ with EPIC through the FEST-C system provides a more dynamic, flexible, and spatially- and temporally-resolved estimate of NH_3 emissions from application of N fertilizers to agricultural soils than previous factor-based NH_3 inventories. Application of this integrated system produced a modified geospatial pattern of seasonal NH_3 emissions that improved simulations of observed atmospheric particle nitrate concentrations which, in turn, provided EPIC with better atmospheric N inputs than inventories (Cooter et al., 2012).

This research builds on existing FEST-C system and uses the bidirectional flux version of CMAQ (bidi-CMAQ) which represents integration of EPIC and CMAQ models driven by WRF meteorology. The CMAQ version employs a compensation point approach to estimate the flux of NH_3 (emission or deposition) from underlying soil and vegetated surfaces to air (Bash et al., 2013; Cooter et al., 2012). EPIC was modified to take daily time series of Total Wet Oxidized N (g/ha); Total Wet Reduced N (g/ha); Total Dry Oxidized N (g/ha); Total Dry Reduced N (g/ha); and Total Wet Organic N (g/ha) from WRF/CMAQ (Cooter et al., 2012).

The FEST-C system guides users through generating land use and crop data needed for EPIC (BLED4 in Fig. 1), creating daily weather and N deposition input from WRF/CMAQ, preparing EPIC site, soil, and management inputs (Spatial Allocator Tools in Fig. 1) for EPIC simulations, and extracting EPIC output for quality assurance. In addition, it also extracts initial soil and pH conditions and daily N information required by CMAQ bi-directional NH_3 modeling. The Spatial Allocator Tools connect EPIC with WRF/CMAQ (Fig. 1). Our effort in this study further enhanced the FEST-C system to generate SWAT-needed inputs from EPIC/WRF/CMAQ.

The target EPIC simulation resolution for integration with a gridded regional air quality model is 144 km^2 (i.e.,12 km by 12 km rectangular grid-cells); land use at the start of the simulation period (2002) is used throughout. The 2002 County-level Census of Agriculture (fractional distribution of crops within the county with the total agricultural land use) was constrained by NLCD 2001 (Cooter et al., 2012). The area of each crop land on a given 12 km by 12 km grid cell is known,

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but the exact location is not. EPIC produces edge of field outputs including runoff, sediment, and nutrients on a daily basis for each crop within a grid cell; outputs are unit loadings (kg/ha).

2.3. Soil and Water Assessment Tool and Hydrologic and Water Quality System

SWAT simulates long-term impacts of land use and management changes on water, sediment and agricultural chemical yields, at various temporal and spatial scales, in a watershed (Arnold and Fohrer, 2005; Arnold et al., 1998; Gassman et al., 2007; Neitsch et al., 2011). It models the N cycle in the soil environment (in-field) and in stream water (in-stream). SWAT's in-field N treatment is similar to that in EPIC's, but it is less complex and does not have EPIC's new additions (Cooter et al., 2012; Yuan et al., 2017). SWAT models in-stream nutrient processes using kinetic routines from QUAL2E, an in-stream water quality model (Brown and Barnwell, 1987). In-stream transformation of different N species is governed by growth and decay of algae, water temperature, biological oxidation rates for conversion of different N species, and settling of organic N with sediment. The amount of organic N in the stream may be increased by conversion of N in algae biomass to organic N, and decreased by conversion of organic N to NH_4^+ and settling with sediment. The amount of ammonium may be increased by mineralization of organic N and diffusion of benthic ammonium N as a source, and decreased by conversion of NH_4^+ to NO_2^- or uptake of NH_4^+ by algae. Conversion of NO_2^- to NO_3^- is faster than conversion of NH_4^+ to NO_2^-; the amount of nitrite is therefore usually very small in streams. The amount of nitrate in streams can be increased by conversion of NO_2^- to NO_3^- and decreased by algae uptake. SWAT considers water runoff and loadings of sediment and other constituents, including point sources (e.g., sewage treatment plants), from land areas to and along the channel network, and can be summarized on a daily, monthly, yearly, or avarage annual basis (Neitsch et al., 2011).

The Hydrologic and Water Quality System (HAWQS 1.0) (https://epahawqs.tamu.edu/) was recently developed by the USEPA Office of Water to enhance usability of SWAT in simulating effects of land management practices based on an extensive array of crops, soils, natural vegetation types, land uses, and climate change scenarios on hydrology and water quality. HAWQS is a web-based, interactive water quantity and quality modeling system that employs SWAT as its core engine (Yen et al., 2016). It provides interactive web interfaces, maps, and pre-loaded input data including NHD Plus; land use/land cover (NLCD 2006 combined with CDL 2010 and 2011 crop data layer from USDA National Agricultural Statistics Survey (NASS) to differentiate agricultural land use); soil; climate; atmospheric deposition of N; and USGS data of streamflow and pollutants. Daily weather data implemented in HAWQS is from the the National Oceanic and Atmospheric Administration - National Centers for Environmental Information (NOAA-NCEI); the atmospheric deposition implemented in HAWQS is from the National Atmospheric Deposition Program which monitors precipitation chemistry (http://nadp.sws.uiuc.edu/NADP/). In addition, SWAT default parameters used by HAWQS have been preliminarily calibrated. HAWQS serves three different spatial resolutions (8-digit, 10-digit, and 12-digit HUCs) and varying temporal scales (time steps in daily/monthly/annual) (Yen et al., 2016).

2.4 Integrated Modeling System

2.4.1. Integration of SWAT and EPIC for the Integrated Modeling System

EPIC was used to simulate agricultural land because of its complexity in simulating agricultural production and related pollutant loadings, as well as its interaction and compatibility with CMAQ and WRF. EPIC is a field-scale model, however, and can only simulate edge of field loadings from agricultural land; landscape processes from fields to reaches, channel routing and in-stream water quality processes are not considered. Furthermore, EPIC does not simulate non-agricultural land. Therefore, SWAT was used to simulate non-agricultural land and stream processes for the Integrated Modeling System (IMS). SWAT divides a watershed into subwatersheds or sub-basins, which are further partitioned into a series of hydrological response units (HRUs), by setting a threshold percentage of dominant land use, soil type, and slope group. An HRU is assumed to be homogeneous in hydrologic response and consists of homogeneous land use and land management, soil, and slope (Gassman et al., 2007; Williams et al., 2008); Neitsch et al., 2011; Yen et al., 2016). Hydrological components, soil erosion and sediment yield, and nutrient cycles are simulated for each HRU, and yields from HRUs are aggregated for the subwatersheds. To integrate EPIC with SWAT in the IMS, loadings for all crops (agricultural land) from EPIC grids within each subwatershed or subbasin are aggregated into one value and expressed as mass (Table 1); the aggregated value is treated as a point source and directly introduced into the outlet of each subwatershed where it combines with loadings from non-agricultural land, as shown in Fig. 1. Together, loadings of runoff, sediment, and chemicals are routed from each subwatershed through a channel network to the outlet of the watershed.

This approach assumes no routing inside each subwatershed to the pour point (i.e., no field-to-field routing). A delivery ratio (DR) method is thus used to account for the stream processes inside each subwatershed (Santhi et al., 2011; Wang et al., 2011). DR refers to the fraction of total soil and nutrient loss from fields within the subwatershed that actually reaches the nearest stream.

2.4.2 Weather and Atmospheric N Deposition for the Integrated Modeling System

Both SWAT and EPIC require daily time series of radiation, maximum and minimum temperature, precipitation, relative humidity, and 10-m wind speed conditions. These data can come from historical observations, be simulated (e.g., data by WRF), or be a combination of both. Through the FEST-C system, EPIC receives WRF weather inputs for each 12 km by 12 km grid. WRF climate data of 12 km by 12 km grid were aggregated to an 8-digit HUC level to run a SWAT simulation on non-agricultural land, because SWAT requires one weather file for each subbasin. Again, through the FEST-C system, EPIC receives CMAQ atmospheric N deposition for each 12 km by 12 km grid (Table 2). Similarly, SWAT requires one deposition file for each 8-digit HUC; thus, the CMAQ deposition data for each 12 km by 12 km grid within each HUC8 were aggregated into one file and used for SWAT simulation on non-agricultural land (Table 2). The IMS simulation uses grid-based climate-forcing by WRF because it is fully integrated with the air-quality model CMAQ, which reflects N exchange between the land surface and atmosphere. Furthermore, the IMS simulation uses grid-based CMAQ atmospheric N deposition for agricultural land because it is fully integrated with air-quality model CMAQ. For non-agricultural land, both atmospheric wet deposition of ammonium (mg/l) and atmospheric wet deposition of nitrate (mg/l) for each subbasin were assumed to be zero. Daily total wet and dry oxidized N are summed to provide atmospheric deposition of nitrates; daily total wet and dry reduced N are summed to provide atmospheric deposition of ammonium (kg/ha/day), as shown in Table 2.

2.5. IMS Implementation on the MRB

The MRB including Missouri, Arkansas-Red-White, Ohio-Tennessee, and upper and lower MRBs (Fig. 2,) drains all or part of 31 US states (41% of the contiguous US). The river mainstem is 3700 km in length and runs from the southern Canadian border to the GOM. The watershed provides drinking water, food, industry, and recreation for millions of people. The largest hypoxic zone currently affecting the United States -- and the second largest hypoxic zone worldwide -- is the northern GOM, adjacent to the Mississippi River. SWAT was set up for the MRB through HAWQS at the 8-digit HUC level, where each 8-digit HUC is treated as a subbasin.

The HAWQS-SWAT simulation comprises 821 8-digit HUCs covering an area of 3173262.31 km^2 from northern Minnesota to Baton Rouge, LA, ending at the outlet of HUC08071000, on a daily timestep (black dot with white star in Fig. 2). Although the Mississippi River continues 100 more miles south to New Orleans where it meets GOM, the river bifurcates after Baton Rouge and not all basins contribute directly to the Mississippi River (Fig. 2). In addition, 8-digit HUCs in Canada, which also contribute to the Mississippi River, were not included, as HAWQS was developed only for the contiguous U.S. Finally, all of SWAT's necessary data (SWAT editor tables, input files and other associated data) were downloaded so they can be used by the SWAT editor program.

Each land use type within each 8-digit HUC was treated as one HRU: each cropland was treated as one HRU and urban land was treated as one HRU, etc., within a given 8-digit HUC. For IMS simulation, SWAT cropland output was muted by adjusting the cropland area fraction to zero (unit loading * area fraction = 0). EPIC loadings for all cropland (agricultural land) within each 8-digit HUC were aggregated into one value and introduced into the outlet of each 8-digit HUC. The IMS simulation for the MRB ends at the pour point of HUC 08070100. Since the time of travel is limited mostly to a single day within each 8-digit HUC, we assume that nutrient transformations en route to the stream are negligible. Furthermore, "Area" used in Table 1 (last column) refers to the agricultural land in HAWQS-SWAT; the ratio was applied to account for the agricultural land differences between EPIC and HAWQS-SWAT, if any.

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2.6. Model Simulations for the MRB

To evaluate the IMS, the following model simulations were performed:

1. HAWQS-SWAT: All SWAT inputs including climate (daily precipitation, maximum and minimum air temperature) were directly extracted from HAWQS system; the simulation was performed from 1999 to 2010 (weather in HAWQS 1.0 ends in 2010), with the first three years as a warm-up period. HAWQS-SWAT uses area-weighted NOAA-NCEI observations as climate input for each subbasin (8-digit HUC); these data are interpolated using the Theissian polygon method to create a pseudo station for each 8-digit HUC. Air deposition used in this simulation is from the National Atmospheric Deposition Program (http://nadp.sws.uiuc.edu/).
2. HAWQS-SWAT WRF: for this simulation, climate input (daily precipitation, maximum and minimum air temperature) were replaced with WRF-produced daily precipitation, maximum and minimum air temperature, solar radiation; the rest of the inputs remain the same as the above simulation (HAWQS-SWAT). This simulation was performed because the FEST-C system were driven by process-based WRF weather simulations.
3. IMS simulation: EPIC simulates agricultural land. SWAT takes in EPIC loadings, simulates non-agricultural land, and performs channel-routing processes. The IMS uses grid-based climate forcing by WRF because it is fully integrated with air-quality model CMAQ, which reflects N exchange between the land surface and atmosphere. The IMS simulation was performed for 2002 to 2010. CMAQ estimates of speciated wet and dry N deposition are used for non-agricultural land.

Results from the first and second simulation are the benchmark for the IMS evaluation. Comparing results from simulations 1 and 2 is helpful for understanding the effects WRF weather data have on a model's results. All simulations end in Baton Rouge, LA (pour point of the HUC08071000).

2.7. Model Evaluation

Eighty-five U.S. Geological Survey (USGS) gauge stations across the country were used to calibrate HAWQS during its development; six were from Tennessee, eighteen from Ohio, and sixteen from the Upper MRB for a total of 40 in the MRB. Since default parameters used by HAWQS have been preliminarily calibrated as documented in the HAWQS Quality Assurance Project Plan (an unpublished EPA document), no further calibration was performed. And due to the complexities at this scale, calibration would be extremely difficult and require another standalone study. Our study focuses on model integration.

Although no calibration was performed, USGS gauge stations located at the main stem of the Mississippi River and close to the outlet of the MRB were identified to support model evaluation (Table 3). The location, size of the drainage area for each USGS gauge station, and time period for available flow, sediment and N data are listed in Table 3. Three USGS stations are identified (Fig. 2 and Table 3). The USGS 07373420 Mississippi River near St. Francisville, LA, with a drainage area of 2,914,515.747 km^2, is a long-term USGS National Water Quality Assessment monitoring station on the Mississippi River. Discrete water quality samples were collected, but continuous streamflow was not monitored at this station. Nutrient loads delivered to the GOM estimated by the USGS, are therefore a product of the concentrations of NO_3^- plus NO_2^- from USGS 07373420 at St. Francisville and streamflow from 07295100 at Mississippi River at Tarbert Landing, MS (also US Army Corps of Engineers site 01100). More information on how the load was estimated can be found in the USGS Open-File Report 2007-1080 (USGS Streamflow and Nutrient Delivery to the Gulf of Mexico, available at http://toxics.usgs.gov/hypoxia/mississippi/flux_ests/delivery/index.html). Nutrient loads estimated at this site were additionally evaluated for 2011 to 2013, using in-situ nitrate sensors and streamflow data collected at the USGS 07374000 station at Baton Rouge, LA, about 60 km from this station (Pellerin et al., 2015) (Fig. 2). Pellerin et al. (2015) concluded that the measured NO_3^- load with in-situ nitrate sensors underestimated the load at the St. Francisville station by only 3.5% for the entire study period. Much larger differences (5% to 20%) were observed at daily or monthly time steps, however. High frequency NO_3^- measurements captured the variation of the load at a daily or monthly time step and improved accuracy.

Results from all simulations were compared to available USGS data to evaluate the model's performance. Data from all three USGS stations were used (Fig. 2 and Table 3).

3 Results and discussion

3.1 Streamflow Evaluation

Comparisons of simulated and observed monthly streamflow (USGS stations 07295100 at Mississippi River at Tarbert Landing, MS and 07374000 at Baton Rouge, LA) for the simulation period 2002 to 2010 are shown in Fig. 3. Generally, the HAWQS-SWAT-simulated streamflow followed seasonal trends of the observed streamflow at 07295100, with an R^2 of 0.52; R^2 was not calculated for 07374000 due to the fact that 07374000 does not have complete data for the simulation period. Observations at 07374000 followed that of 07295100, with lower peaks (Fig. 3). The HAWQS-SWAT simulation over-estimated streamflow, however, particularly for high-flow months such as April in 2002, 2003, 2008 and May in 2009 (Fig. 3). It also under-estimated streamflow for the dry season such as December in 2009 and 2010 as well as January in 2006 and 2010. The average monthly flow observed at the USGS 07295100 was 17.6 mm and the simulated average monthly flow was 21.8 mm (Table. 4).

Since the IMS simulation uses WRF-generated weather data, a simulation with WRF-generated weather data was also performed using the same inputs of HAWQS-SWAT, called HAWQS-SWAT WRF. The HAWQS-SWAT WRF-simulated streamflow followed seasonal trends of the HAWQS-SWAT simulated streamflow well, with an R^2 of 0.83. The average monthly flow simulated by HAWQS-SWAT WRF is 18.0 mm, which is very close to observed mean monthly flow (Table 4). The IMS simulated streamflow is almost identical to the HAWQS-SWAT WRF-simulated flow, with an R^2 of 0.99. The average monthly flow simulated by IMS is 18.2 mm (Table 4).

The annual streamflow comparison of simulated and observed at the USGS station 07295100 at Mississippi River at Tarbert is shown in Fig. 4; observed streamflow from the USGS station 07374000 at Baton Rouge, LA was not shown because this station does not have all 9 years of data. Although the HAWQS-SWAT-simulated streamflow reflects annual variation of the observed streamflow well, with an R^2 of 0.90, it over-estimated streamflow for all years of the simulation period (Fig. 4 and Table 5).

Runoff was possibly overestimated because SWAT underestimated groundwater recharge. As flows approach the GOM, water levels rise, resulting in higher seepage and groundwater recharge, a condition not well-suited for SWAT modeling (Daggupati et al., 2016). Observations at 07374000 presented lower peaks (Fig. 3), which is consistent with this phenomenon. The lower groundwater recharge would result in lower baseflow which also explains the under-estimated monthly streamflow during dry season (Fig. 3). Another possible reason for over-estimation of the runoff is that water withdrawn for irrigation and other uses was not accounted for in the simulations.

In addition to the original calibration performed for 85 USGS stations where streamflow was available (HAWQS Quality Assurance Project Plan, an unpublished EPA document), further calibration is underway to expand on the initial calibration to improve HAWQS-SWAT's performance. Calibration at such a scale, however, may be extremely difficult, as is demonstrated in the HAWQS QAPP and other studies (Daggupati et al., 2016; Scherer et al., 2015), due to the level of variability and uncertainty in streamflow. Determining how to calibrate the model effectively at such a scale, and with such high levels of variability and uncertainty (even conflicting results), would require a standalone study in the future; this is supported by other studies (Daggupati et al., 2016; Scherer et al., 2015).

The HAWQS-SWAT WRF-simulated annual streamflow is lower than HAWQS-SWAT-simulated annual streamflow for all years but 2002. The average annual streamflow simulated by HAWQS-SWAT WRF is 211.7 mm, which matched the observed mean annual streamflow of 211.1 (Table 4). The HAWQS-SWAT-simulated annual streamflow is 261.1. The IMS-simulated annual streamflow is very close to the HAWQS-SWAT WRF simulated annual streamflow (Fig. 4). In the next section we will compare WRF precipitation and temperature to NOAA-NCEI to seek insights into WRF and explore reasons for lower streamflow from HAWQS-SWAT WRF and IMS.

3.2 Climate Forcing Comparison between NOAA-NCEI and WRF

Since the only difference between HAWQS-SWAT and HAWQS-SWAT WRF simulations is weather data, WRF-generated climate data were compared to HAWQS area-weighted NOAA-NCEI

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climate observations to understand how well the WRF model represents observed climate data in the study area. This is necessary because the FEST-C system were driven by process-based WRF weather simulations, thus the IMS uses grid-based climate forcing by WRF because it is fully integrated with air-quality model CMAQ. WRF climate data of 12 km by 12 km grid were aggregated to an 8-digit HUC level; this was also needed to run a HAWQS-SWAT WRF simulation, because HAWQS-SWAT requires one weather file for each subbasin. We compared spatial distribution of average annual precipitation and air temperature from 2002-2010 (Fig. 5). This helped to understand the difference of streamflow simulations between HAWQS-SWAT and HAWQS-SWAT WRF and provided insights into IMS simulation results.

The trends in spatial distribution of precipitation across the MRB is similar between WRF simulations and NOAA-NCEI observations (Fig. 5a vs. Fig. 5b); the southeast of MRB experienced higher annual precipitation than the northwest of the MRB. WRF systematically overestimated precipitation in western Missouri River Basin, however, and seemed to underestimate precipitation in the lower MRB (Fig. 5a vs. Fig. 5b). The trends in spatial distribution of temperature across the MRB is also similar between WRF simulations and NOAA-NCEI observations (Fig. 5c vs. Fig. 5d), but WRF seems to systematically overestimate temperature. Higher WRF precipitation would produce higher streamflow, but higher WRF temperature would result in higher evapotranspiration and, thus, lower streamflow. Overall, HAWQS-SWAT WRF simulated lower average monthly and annual streamflow than HAWQS-SWAT due to the combined effects of precipitation and temperature.

In addition to comparing the spatial distribution of average annual precipitation and temperature, we explored differences in daily precipitation patterns between NOAA-NCEI and WRF

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(Fig. 6). Daily precipitation accumulation curves from 2002 to 2010 at six randomly selected 8-digit HUCs (one from each 2-digit HUC) are presented in Fig. 6. The accumulative precipitation curve is similar between NOAA-NCEI observations and WRF simulations for all six 8-digit HUCs. WRF overestimated precipitation for the Ohio (Fig. 6a), Lower Mississippi (Fig. 6d) and Missouri River basins (Fig. 6e), and underestimated precipitation for the Upper Mississippi (Fig. 6c) and Arkansas Red White River basins (Fig. 6f). For the Tennessee river basin, WRF overestimated precipitation from 2003 to 2008, but was close to the observations at the end of the comparison period. Overestimation of rainfall in Missouri River basin is consistent with the spatial distribution presented in Fig. 6b. Since rainfall in the Ohio River basin is more than 10000 mm for 11-year accumulation, overestimation is small compared to total rainfall, and would not substantially affect streamflow. In contrast, rainfall overestimation in the Missouri River basin (Fig. 6e) could introduce greater bias in hydrological modeling, because precipitation is less than 4000 mm for 11 years of accumulation. Although more comparisons between NOAA-NCEI and WRF must be performed, the limited comparison shows that WRF can reproduce retrospective weather data.

3.3 Dissolved N Evaluation

Comparisons of simulated and observed monthly dissolved N (USGS stations 07373420 at the Mississippi River near St. Francisville, LA) from 2002 to 2010 are shown in Fig. 7. Generally, the HAWQS-SWAT simulated dissolved N followed seasonal trends of observed values, with an R^2 of 0.53. The HAWQS-SWAT simulation overestimated dissolved N, as it did for streamflow (Fig. 3), particularly for spring and early summer months such as May in 2002, 2003, 2009 and 2010, as well as June in 2008 (Fig. 7). Fertilizer timing impacts N simulation as demonstrated in Yuan and Chiang (2015); fertilizer timing in HAWQS may be based on actual fertilizer application data, but it is very challenging to accurately capture fertilizer timing and amounts at such a large scale. The average monthly dissolved N estimated at the USGS 07373420 is 0.23 kg/ha. and the simulated amount by HAWQS-SWAT is 0.35 kg/ha. (Table. 4).

The annual comparison between HAWQS-SWAT-simulated and observed dissolved N at the main outlet of the MRB (USGS 07373420) from 2002 to 2010 presents the same trends as the monthly results (Fig. 8). Model simulations of dissolved N correspond well to USGS estimations, with an R^2 of 0.81. HAWQS-SWAT overestimated the dissolved N for all years during the simulation period, however (Fig. 8).

Several potential factors could result in higher simulated dissolved N. First, higher runoff estimation could cause higher dissolved N results. In addition, fertilizer timing and amounts (as discussed above) could cause discrepancies. For the streamflow simulation, model calibration at such scale -- with so much variability and uncertainty -- would be a daunting task. Evaluation of model simulations on nutrients has not been offered by the HAWQS developers. Finally, other studies (Chu et al. 2004; Grunwald and Qi, 2006; Hu et al., 2007; Yuan and Chiang, 2015) have demonstrated the disadvantage of SWAT models in simulating dissolved N, particularly in representing the impact of in-field processes on dissolved N.

The HAWQS-SWAT WRF-simulated dissolved N followed seasonal trends of the HAWQS-SWAT-simulated dissolved N well, with an R^2 of 0.85, although it results in overestimations and underestimations of dissolved N over the simulation period (Fig. 7). The average monthly dissolved N simulated by HAWQS-SWAT WRF is lower than HAWQS-SWAT (0.29 kg/ha vs. 0.35 kg/ha) (Table 4). The lower simulated streamflow by HAWQS-SWAT WRF may result in lower simulated dissolved N. The IMS-simulated dissolved N is lower than the HAWQS-SWAT WRF-simulated

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dissolved N, but followed the seasonal trends of the HAWQS-SWAT WRF simulations, with an R^2 of 0.78. The IMS-simulated dissolved N compared well to USGS estimations (R^2 of 0.67), especially for the peaks, as shown in Fig. 7. The IMS, based on EPIC for agricultural land, simulates a wider variety of crop species and realistically represents crop growth and plant-nutrient relationships. Second, EPIC parameterizations have been selected to capture regional-scale crop production patterns, representative of a much finer scale of farm production practices. Finally, the IMS characterizes land-atmosphere N exchange in much greater detail. The IMS therefore demonstrated greater advantages in simulating N processes than any previous work.

In summary, the IMS model was able to reflect seasonal variation of streamflow and dissolved N at USGS gauges, regardless of the complexity of the model, and variability and uncertainty of the watershed at such a large scale. For this proof of concept demonstration, model calibration was not performed. Model calibration at a scale with such variability and uncertainty is extremely difficult and offers potential for a study in the future.

The IMS model integrated the previously developed FEST-C system with the SWAT model. The FEST-C system, driven by process-based WRF weather simulations, includes atmospheric N additions to agricultural cropland, and agricultural cropland contributions to ammonia emissions. The IMS can assess impacts from meteorology, atmospheric N deposition and agricultural management practices on water quality in large river basins.

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4 Conclusions and Future Work

The IMS is unique in its integration of climate, air deposition, landscape and watershed processes (WRF/CMAQ/EPIC/SWAT), as well as its inclusion of detailed field-scale biogeochemistry on regional to national-scale simulations. It is an improvement of the existing FEST-C (CMAQ/WRF/EPIC) modeling system because stream/channel processes can be simulated after integrating the most commonly used watershed model, SWAT. On the other hand, IMS also improved SWAT simulation results, because it incorporates more field-scale biogeochemical processes by using EPIC in the FEST-C system for agricultural land simulations. Preliminary application of the IMS on MRB showed that simulation results are comparable to USGS observations (streamflow) and estimations (dissolved N), particularly on dissolved N (annual simulated dissolved N of 2.1 kg/ha. vs USGS estimation of 2.8 kg/ha). Future work includes more evaluation of the model including baseflow, sediment and organic N, using it to investigate additional potential sources of N from the watershed in a dynamic way and assessing the impact of CAA amendment regulations and land use land management changes on N fate and transport in large river basins such as the MRB under alternative environmental scenarios. This marks a significant step forward toward a more complete systems-level framework for N assessment.

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Abbreviations

CAA - Clear Air Act

CMAQ - Community Multi-Scale Air Quality

EPIC - Environmental Policy Integrated Climate

FEST-C - Fertilizer Emission Scenario Tool for the Community Multiscale Air Quality

HAWQS - The Hydrologic and Water Quality System

MRB - Mississippi River Basin

NH_3 - ammonia

NH_4^+ - ammonium

NO_3^- - nitrate

NOAA - National Oceanic and Atmospheric Administration

NCEI - National Centers for Environmental Information

NSTC - National Science and Technology Council

SWAT - Soil and Water Assessment Tool

USEPA – US Environmental Protection Agency

WRF - Water Research and Forecasting

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Table 1. EPIC daily output variables converted to SWAT point source input

EPIC Output Variable Name	EPIC Variable Description	SWAT Point Source Variable Names	SWAT Point Source Variable Description	Conversion from EPIC to SWAT
Q/QDRN/SSF	Surface flow/Tile drainage/Subsurface flow (mm)	FLODAY	Contribution to stream flow for the day (m^3)	FLODAY= (Q+QDRN+SSF)*Area
MUSL	Sediment loss (kg/ha)	SEDDAY	Sediment loading to reach for the day (metric tons)	SEDDAY= (MUSL)*Area*Delivery Ratio
YON	N loss with sediment (kg/ha)	ORGNDAY	Organic N loading to reach for the day (kg N)	ORGNDAY= (YON)*Area *Delivery Ratio
YP	P loss with sediment (kg/ha)	ORGPDAY	Organic P loading to reach for the day (kg P)	ORGPDAY= (YP)*Area *Delivery Ratio
QNO3/DRNN /SSFN	N Loss in Surface Runoff/Tile drainage/Subsurface flow (kg/ha)	NO3DAY	NO_3 loading to reach for the day (kg N)	NO3DAY= (QNO3+DRNN+SSFN)*Area
QAP/SSFP	P loss in surface and subsurface flow (kg/ha)	MINPDAY	Mineral P loading to reach for the day (kg P)	MINPDAY= (QAP+SSFP)*Area

- Area refers to HAWQS-SWAT agricultural land

Table 2. N deposition variables used by SWAT and EPIC

SWAT		EPIC	
variable index	**variable name**	**variable index**	**variable name**
1	Atmospheric wet deposition of ammonium (mg/l) for entire watershed	1	Daily Total Wet Oxidized N (g/ha)
2	Atmospheric wet deposition of nitrate (mg/l) for entire watershed	2	Daily Total Wet Reduced N (g/ha)
3	Atmospheric dry deposition of ammonium (kg/ha/day) for entire watershed	3	Daily Total Dry Oxidized N (g/ha)
4	Atmospheric dry deposition of nitrate (kg/ha/day) for entire watershed	4	Daily Total Dry Reduced N (g/ha)
		5	Daily Total Wet Organic N (g/ha)
		6	Daily Total dry Organic N (g/ha)

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Table 3: USGS monitoring stations close to the outlet of the MRB; size of the drainage area; and the time period for available discharge, sediment and nitrogen data

<table>
<tr><th rowspan="2">USGS monitoring station number</th><th rowspan="2">USGS monitoring station location</th><th rowspan="2">Watershed drainage area (km²)</th><th colspan="2">Discharge</th><th colspan="2">Nitrogen (Nitrate plus nitrite)</th></tr>
<tr><th>Start</th><th>End</th><th>Start</th><th>End</th></tr>
<tr><td>07295100</td><td>Mississippi River at Tarbert Landing, MS</td><td>2913480</td><td>Jan-1930</td><td>Present</td><td colspan="2">N/A</td></tr>
<tr><td>07373420</td><td>Mississippi River near St. Francisville, LA</td><td>2914516</td><td colspan="2">No continuous flow monitoring</td><td>Oct-1943</td><td>Present</td></tr>
<tr><td rowspan="2">07374000</td><td rowspan="2">Mississippi River at Baton Rouge, LA</td><td rowspan="2">2915837</td><td>Apr-2004</td><td>Sep-2005</td><td rowspan="2">Dec-2011</td><td rowspan="2">Jan-2016</td></tr>
<tr><td>Oct-2006</td><td>Apr-2016</td></tr>
</table>

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Table 4. Model evaluation for monthly and annual streamflow (mm) and dissolved N (kg/ha.) for the simulation period 2002-2010

Constituents	Observation at USGS 7295100	Estimation at USGS 07373420	SWAT-HAWQS	SWAT-HAWQS WRF	IMS
Mean Monthly Streamflow (mm)	17.6		21.8	18.0	18.2
Mean Annual Streamflow (mm)	211.1		261.1	211.7	218.9
Mean Monthly Dissolved N (kg/ha.)		0.23	0.35	0.29	0.18
Mean Annual Dissolved N (kg/ha.)		2.8	4.2	3.5	2.1

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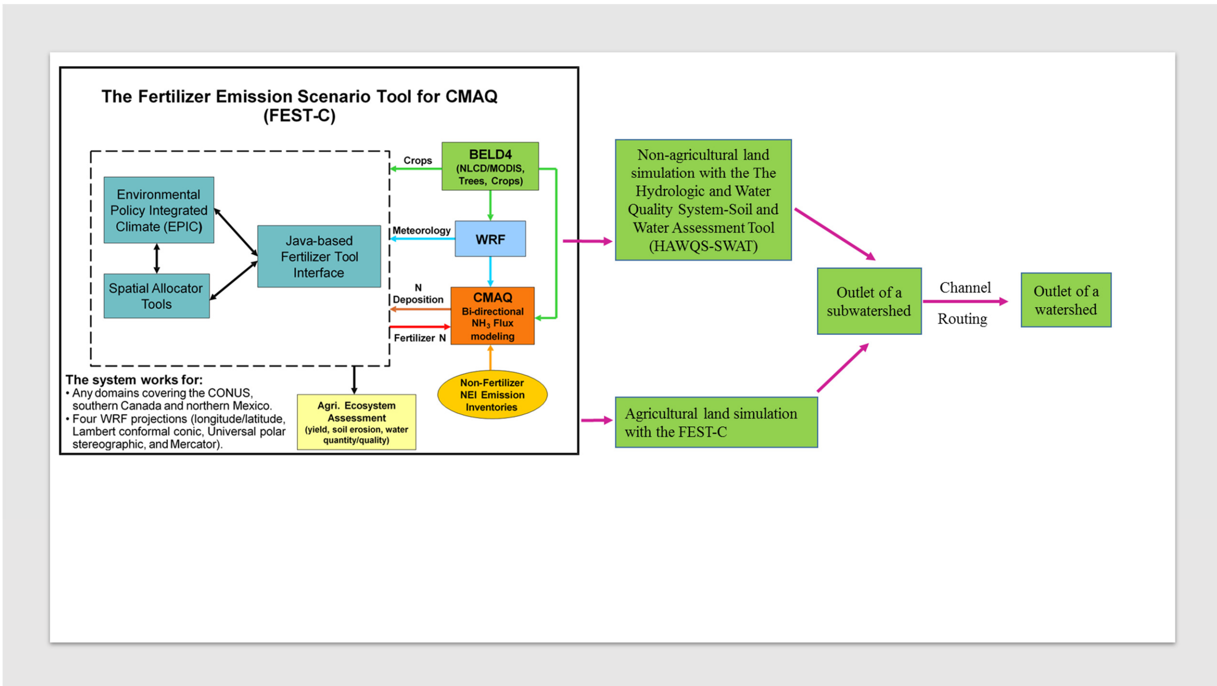

Fig. 1. Integration of FEST-C (EPIC/WRF/CMAQ) and SWAT: EPIC was used to simulate agricultural land because of its complexity in simulating agricultural production and related pollutant loadings, as well as its interaction with CMAQ and WRF. HAWQS-SWAT simulates non-agricultural land and takes in FEST-C output from agricultural land at an outlet of a subwatershed, then simulates stream/channel processes and routes combined loadings to the outlet.

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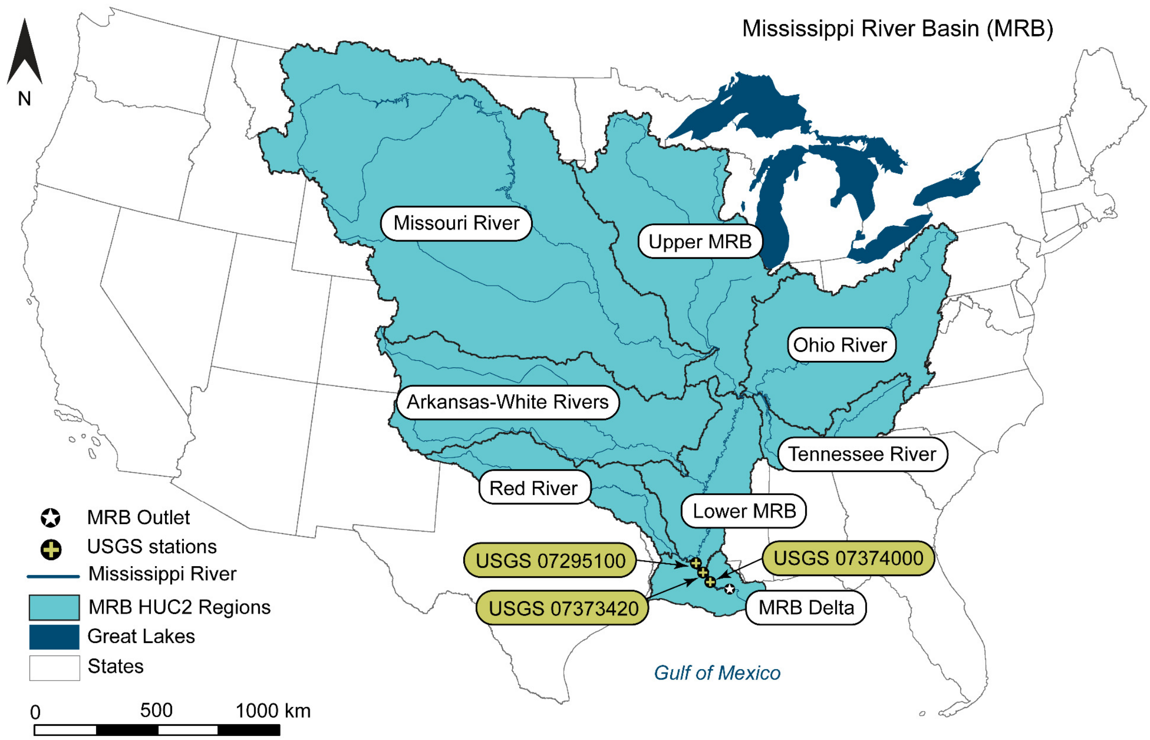

Fig. 2. Geographic location of Mississippi River Basin (MRB): black dots with a cross indicate the USGS stations, located close to the outlet of MRB and used to evaluate models' performance; the black dot with a star indicates the outlet of the MRB.

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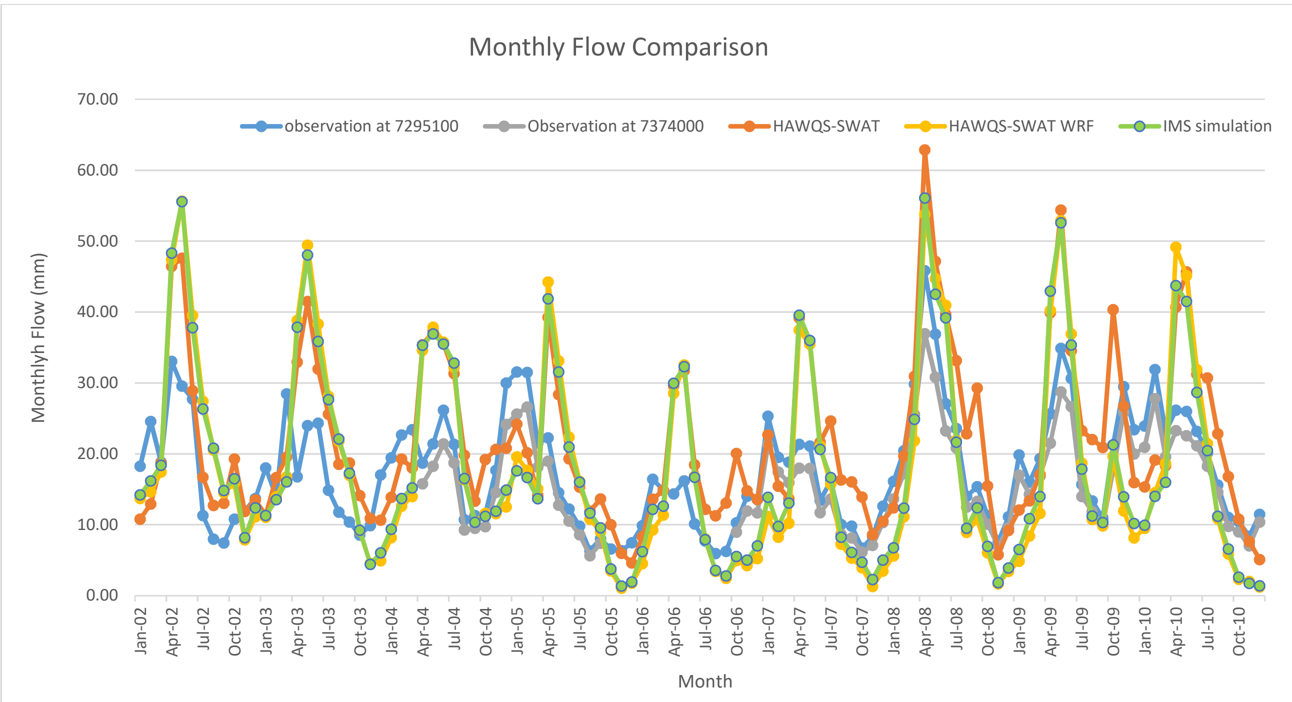

Fig. 3. Monthly streamflow evaluation at USGS gauges for IMS

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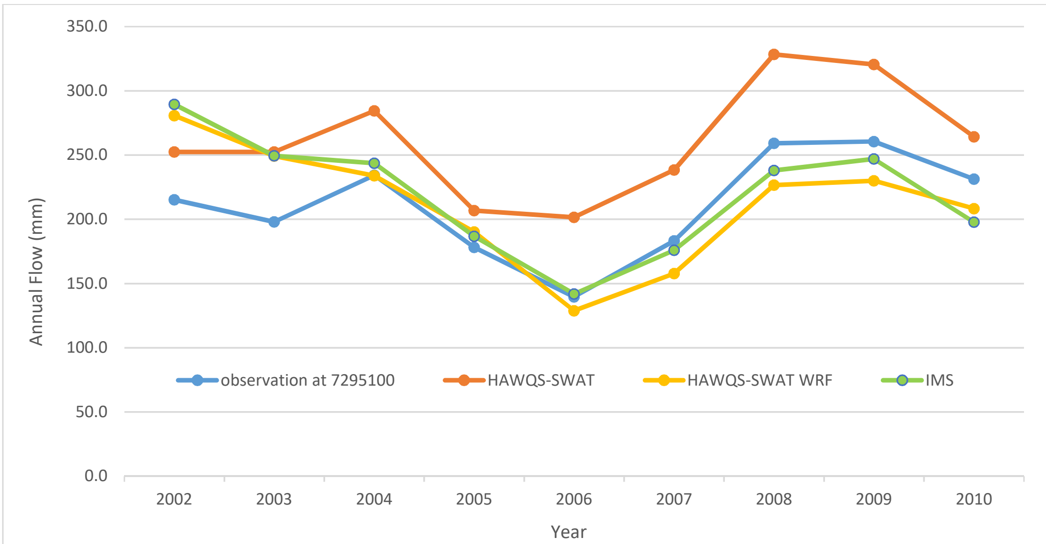

Fig. 4. Annual streamflow evaluation at USGS gauges

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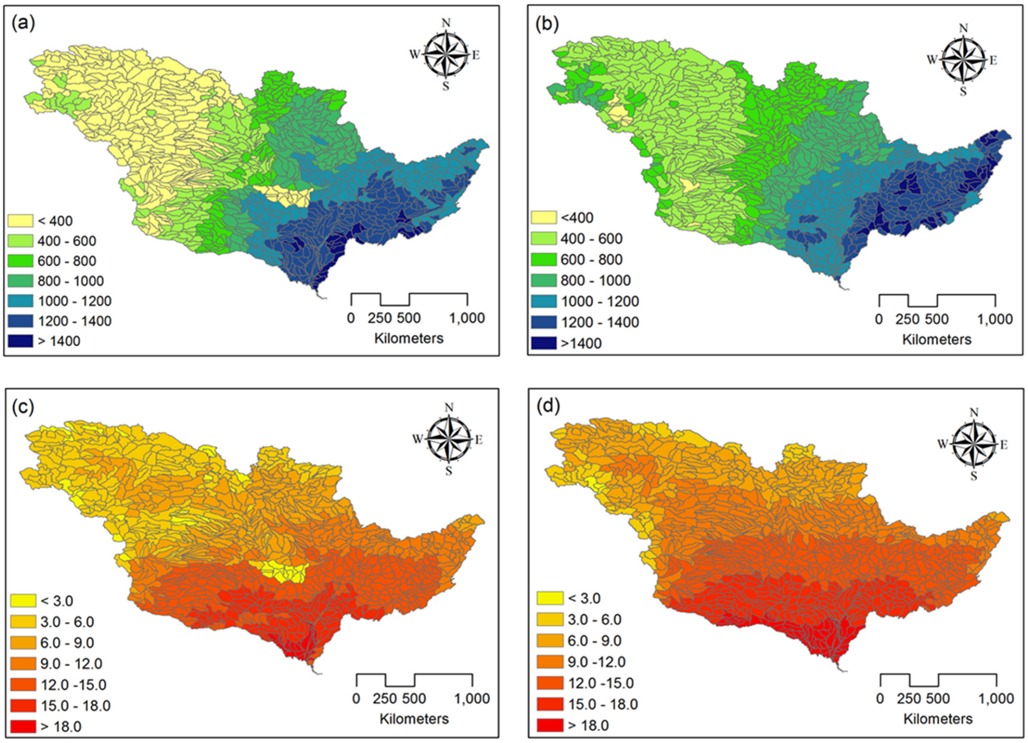

Fig. 5. Comparison of average annual precipitation (mm) and temperature (^{0}C) (2002-2010) between HAWQS and WRF climate at HUC8 level: a) HAWQS precipitation; b) WRF precipitation; c) HAWQS temperature; and d) WRF temperature

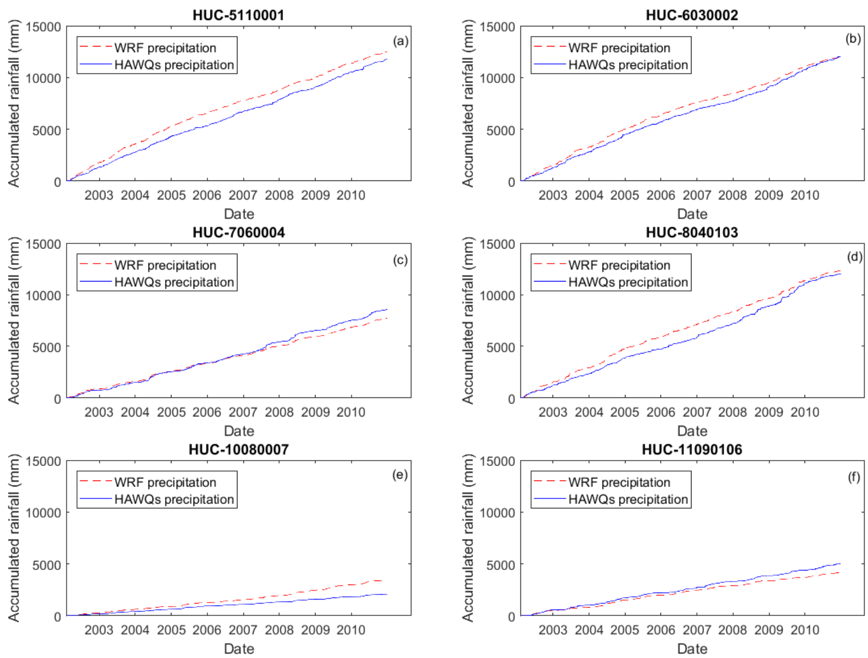

Fig. 6. Rainfall accumulation curve comparison between NOAA-NCEI for HAWQS and WRF climate at randomly selected 8-digit HUCs: a) Ohio River Basin; b) Tennessee River Basin; c) Upper Mississippi River Basin; d) Lower Mississippi River Basin; e) Missouri River Basin; and f) Arkansas-Red-White River Basin

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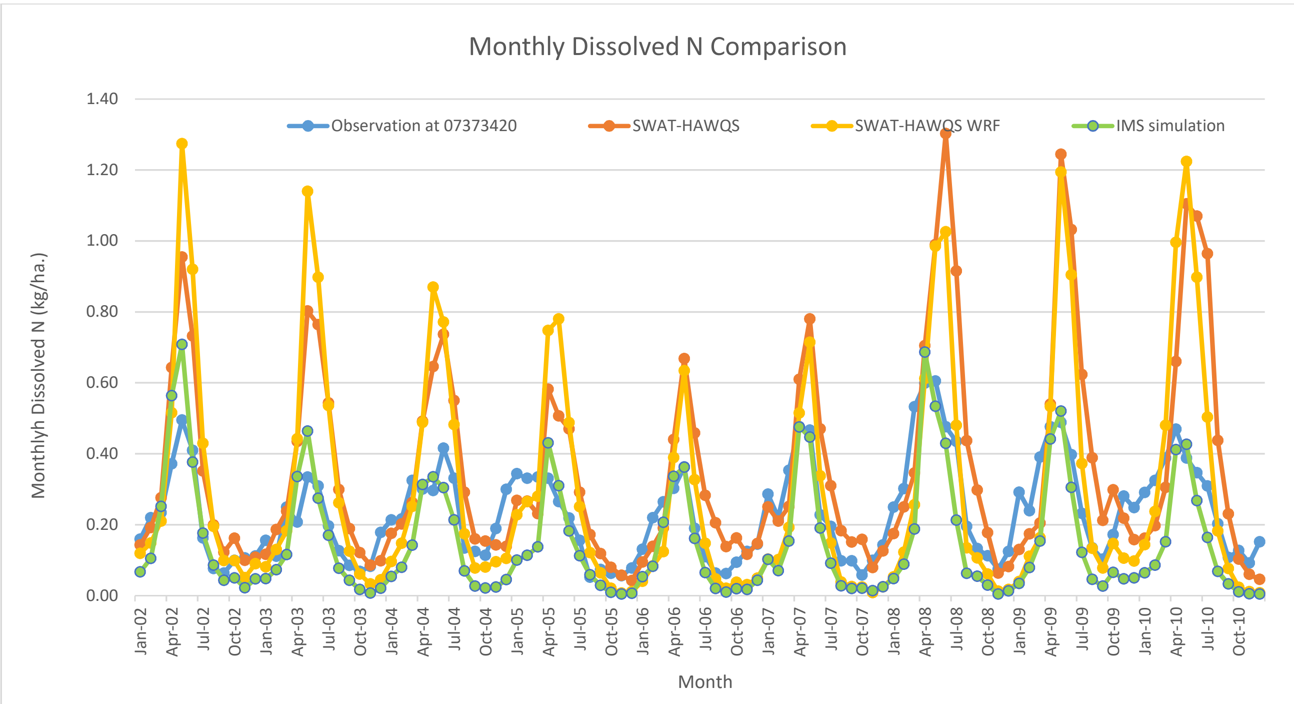

Fig. 7. Monthly dissolved N evaluation at the total outlet of MRB (USGS 07373420)

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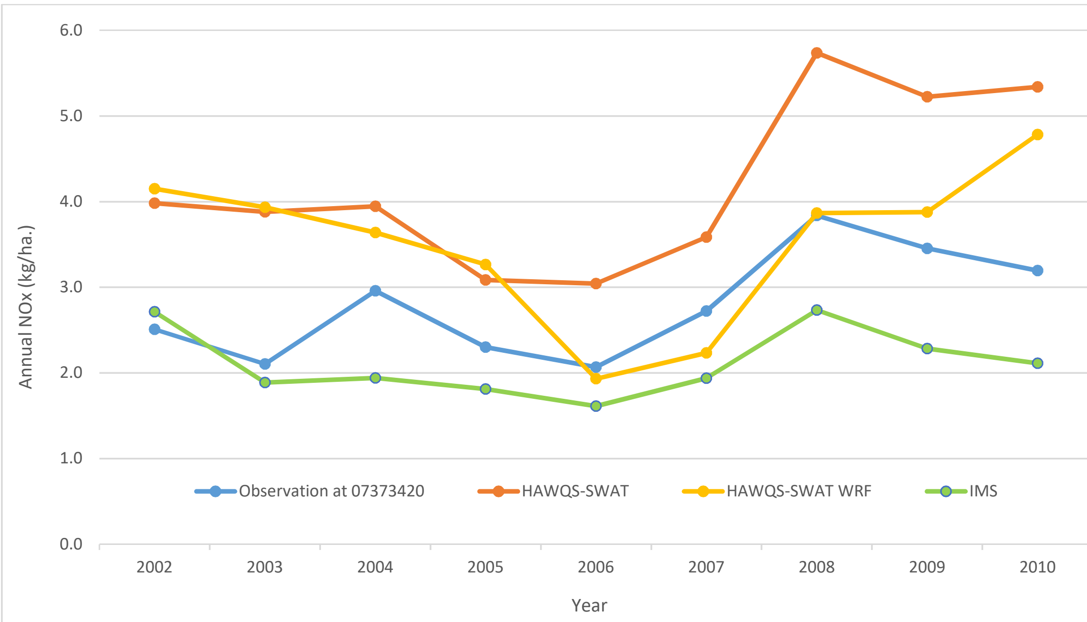

Fig. 8. Annual NOx evaluation at the total outlet of MRB (USGS 0737342