

Delta-Suisun Bay Biogeochemical Modeling: Year 1 Progress

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Executive Summary

Processed-based numerical models are an essential tool for understanding how systems function, forecasting how they may respond to new conditions, and enriching the interpretation of observational data. Through this project we are developing a coupled hydrodynamic-biogeochemical model of Suisun Bay and the Sacramento-San Joaquin Delta. As the first step of biogeochemical model development for the Delta and Suisun Bay, we focused our effort on resolving nitrification and denitrification processes, using a finite volume biogeochemical transport and cycling model DWAQ (Deltares Water Quality) and three-dimensional hydrodynamic output from DFM (Deltares Flexible Mesh) for water year 2011 (WY2011). The modelling results show that the model predictions of dissolved nitrate and ammonia match well broadly with the discrete sampled data across the Delta, even though at this stage processes associated with organic nitrogen (production, grazing and mineralization) have not been implemented. A rough estimation of production, mineralization, and denitrification rates from the observational data revealed that the error associated with ignoring organic nitrogen processes for WY2011 is likely small, because of the balance between two relatively large terms: production and system respiration, resulting in a small residual term. However, when ambient chlorophyll-a concentrations are much greater, such as in WY2016, the balance between the two terms may be violated and the impact of phytoplankton dynamics on nitrogen cycling can be important. Therefore, to fully understand the vulnerability of the system and the risk of high ambient nutrient condition to the ecosystem, it is important for us to further implement the full biogeochemical cycling processes in the model. We also show that the model can be used as a powerful tool to run future and management scenarios to investigate the outcome of certain management actions such as the ongoing Sacramento Regional Wastewater Treatment Plant (SRWTP) upgrade or hypothetically removing discharge from Central Contra Costa Sanitary District (Central San) completely.

1. Introduction

The northern San Francisco Estuary (nSFE), including the Sacramento-San Joaquin Delta and Suisun Bay, receives large inputs of anthropogenic nutrient loads, resulting in ambient N and P concentrations that exceed levels linked to adverse impacts in other freshwater and estuarine systems (*Dahm et al.* 2016; *Paerl*, 2009). Regulators and stakeholders have collaboratively identified goals for informing nutrient management decisions, which include identifying protective nutrient loads to the nSFE and evaluating the potential effectiveness of various nutrient management actions (*CVRWQCB*, 2018; *SFBRWQCB*, 2012).

The development and application of coupled hydrodynamic-biogeochemical models have been identified as essential components of the scientific work needed to achieve those goals. This report describes work on the first stage of biogeochemical model development for Suisun Bay and the Delta and is organized as follows:

- Background
- Objectives
- Methods: data preparation, model structure, and techniques used to set up tracer runs;
- Results and Discussion: performance of the stage 1 model (comparing model output with observations); and examples of potential model applications;
- Recent progress since last progress report meeting: data preparation and biogeochemical model structure including full biogeochemical cycling processes;
- Overview of on-going and anticipated future work.

2. Background

Development of the biogeochemical model has been motivated by the broad needs of regulators, stakeholders, and the scientific community to reach science-based answers to Bay-Delta nutrient management questions. Topics such as the potential role of anthropogenic nutrient loads on ecosystem responses, the effect of planned reduction in nutrient loads from SRWTP, the conditions (hydrological, biological, meteorological, or biogeochemical) that lead to water quality issues, and the management actions that may help address or ameliorate the nutrient-related issues, are central to informing effective decision-making in this system. In order to make progress on

these topics, a holistic understanding of the mechanisms and pathways spanning complex biogeochemical processes is required (*see CVRWQCB, 2018*).

Nutrients and phytoplankton undergo complex biogeochemical transformations (*SFEI, 2014*) as they are transported, mixed, and dispersed through the Delta and Suisun Bay. The rates of these transformations can be strongly influenced by physical, hydrological, atmospheric and biological conditions, such as bathymetry, river discharge, light availability, winds, tides, surface waves, turbidity, water temperature, salinity, primary production and higher trophic levels, which can all vary greatly in space and time. Thus, nutrient concentrations, including relative abundance of different forms (e.g., ammonium vs. nitrate), and indicators of response (e.g., phytoplankton biomass) exhibit strong spatial, seasonal, and inter-annual variability (e.g., *Jassby, 2008; SFEI, 2015*). In addition, major changes in some important forcings have occurred in the Delta and Suisun Bay over the past ~40 years, resulting in sudden shifts or gradual changes in the balance among ecosystem processes. The invasion of *Potamocorbula amurensis* around 1987 resulted in abrupt drop in phytoplankton production and biomass in Suisun Bay and the western Delta (*Cloern and Jassby, 2012; Jassby, 2008*). In addition, there is anecdotal evidence that abundances of *Potamocorbula* (the salty-region invasive clam) decreased substantially in Suisun after WY2017's extremely wet winter and spring, which could again alter the balance of important processes. Recent analyses (*Cloern and Jassby, 2012; Schoellhamer, 2011*) found that suspended sediment concentrations in Suisun Bay have decreased by ~50% since 1975, meaning that light levels available to support phytoplankton growth have essentially doubled. In addition, Regional San's 2010 National Pollution Discharge Elimination System (NPDES) permit sets May 2021 as the operational date for an upgrade to an ammonia limit of 1.7 mg-N/L (April-October) and 3 mg-N/L (November-March), and sets an interim ammonia limit of 47 mg-N/L year-round prior to the completion of the upgrade (*NPDES Permit, 2010*). Relative to the typical performance of the current treatment plant, the upgrade is anticipated to result in a >95% reduction in effluent dissolved ammonia concentration and a >65% reduction in effluent total inorganic nitrogen concentration (pers. comm., Lisa Thompson, Regional San). All these changes may influence primary production, phytoplankton biomass, and nutrient concentration in the system.

The complexity of processes affecting nutrient pathways and the numerous spatiotemporally-varying environmental factors that influence nutrient dynamics in the Delta and Suisun Bay call

for the use of spatially explicit process-based models. State-of-art coupled hydrodynamic-biogeochemical models enable us to take advantage of existing data, integrate complex biogeochemical cycling, and incorporate our knowledge and insight of the system. The process-based biogeochemical model will serve as a useful tool for:

- developing the quantitative understanding necessary to accurately characterize conditions and infer causal factors under current conditions,
- untangle the respective influence of each process that affects nutrient dynamics, identifying important drivers for observed processes and substances, and
- forecast ecological responses to future natural or management scenarios, including climate change or altered nutrient loads.

For the next two and a half years, we will focus our efforts on Stage 2 and 3 of the model development, building a biogeochemical model with the complexity needed to resolve nitrogen cycling, phytoplankton dynamics, organic matter/detritus mineralization, benthic fluxes, and zooplankton/benthic grazer dynamics, and validate the biogeochemical model for one particular year (WY2011). The stages of modeling development are as follows:

- Stage 1 (6/2017-5/2018): Gather data on and develop boundary conditions for biogeochemical simulations, for WY2011 and other years (from 2000 to 2016); Conduct conservative tracer and age tracer runs to test basic model performance and extract informative transport output; simulate nutrient concentrations for WY2011 using a limited set of processes (nitrification and denitrification);
- Stage 2 (2/2018-5/2019): Integrate additional important processes and perform preliminary model runs with these processes. Prepare model input data, including atmospheric data, high frequency sampling data, turbidity, zooplankton, and benthic grazer data. Expand the biogeochemical model to include nitrogen cycling, phytoplankton dynamics, grazing behavior, mineralization, and benthic processes. Perform test runs with the model and input data, identify dominant processes, and prioritize refinements to input data or model structure related to current processes.
- Stage 3 (2/2019-2/2021): Iteratively improve model performance, and apply model to explore management-relevant scenarios. Specific priorities will be determined based on Stage 2 model status, stakeholder priorities, input from technical advisors, and include

some or all of the following: tuning biogeochemical model coefficients; adding spatial and/or temporal variations in coefficients or important data fields (e.g., suspended sediment concentrations or clam grazing rates); incorporating additional biogeochemical processes or variables or adjusting how processes are implemented; setting up and running additional time periods when rich observational records are available or when noteworthy events occurred (e.g., blooms, distinctly different nutrient concentrations); extend and refine model to resolve dissolved oxygen (DO) dynamics and validate DO across the Delta. During this stage, model status and findings will also be described in a final report.

3. Objectives

The objective of this project is to develop and calibrate a three-dimensional finite-volume biogeochemical model (DWAQ) offline coupled to an unstructured-grid hydrodynamic model (DFM) for WY 2011 in the Delta and Suisun Bay. The model results will be calibrated against measured nitrogen, chlorophyll-a, and dissolved oxygen across the Delta and Suisun Bay. The objective of this report is to describe the first stage of the model development in which we have modeled nitrification and denitrification processes, validated the model against the observed dissolved nitrate and ammonia, and developed proof-of-concept approaches to addressing management questions.

4. Methods

In this section, we will first introduce the modelling framework, the structure of the biogeochemical model, and our approach to managing the data for model input and validation. We will then focus on using the model to derive useful information, such as source water composition and water age by applying different types of conservative tracers in the model. The information derived from these tracer runs can assist in investigating management questions detailed in the Discussion section.

4.1 Modelling framework

We used a process-based, spatially-explicit, coupled hydrodynamic-biogeochemical modelling approach to model water quality in the Delta/Suisun Bay. We selected the Deltares Flexible Mesh (DFM) model and the Deltares Water Quality model (DWAQ) as our primary platforms for coupled hydrodynamic and biogeochemical modeling. This modeling platform was suggested by the San Francisco Bay Nutrient Management Strategy (NMS) based on an extensive review of modeling options and input from modeling experts (*SFEI*, 2014)¹. This choice of model framework allows us to apply our existing experiences from San Francisco Bay to the Delta/Suisun Bay, since both efforts utilize the same platform. Working in the DFM-DWAQ platform for this project also allowed us to build upon the existing multi-year CASCade project², where extensive effort has been invested into the hydrodynamic calibration for Suisun Bay and the Delta.

DWAQ has been widely used and steadily refined since the 1980s for applications in freshwater, estuarine, and coastal ocean systems, and is thus well-suited for simulating processes across that continuum for the Bay-Delta. DWAQ contains an extensive library of biogeochemical processes and modules³ that can be selectively enabled, allowing the flexibility to include various levels of model complexity. DWAQ recently (2014) became freely-available and open-source, and is well-documented, maintained and supported by Deltares. Furthermore, our ongoing collaboration with Deltares (including a project supported with Deltares in-kind funds) will ensure that we will receive the technical support required to refine the biogeochemical model, as needed, to include features unique to the Delta and Suisun Bay.

DFM is the most recent iteration of hydrodynamic model developed by Deltares, distinguished from the previous Delft3D model by its support for unstructured grids. The support for unstructured grids and compatibility with DWAQ make it an effective hydrodynamic model for

¹ The criteria for model platform selection included: broad user base and well-maintained model, with technical support; open-source and well-established peer-reviewed model platform, especially, in this, case with regards to the biogeochemical model; ease of direct coupling of hydrodynamics and biogeochemistry; potential for use with a GUI for model set-up and analyzing simulation output.

² USGS-led project, partially funded by the Delta Science Program. Collaborators: Deltares, UNESCO-IHE, and SFEI.

³ e.g., benthic nutrient cycling/fluxes with multiple sediment compartments; multiple multi-species algae growth and mortality, including size-selective grazing; planktonic and benthic grazers; dynamic energy budget model for grazer-phytoplankton coupling; oxygen cycling.

the Bay-Delta system. For the present project we are using existing DFM simulations generated by the CASCaDE project. The DFM model from CASCaDE is driven by historical winds, tides, ocean salinity, river flows, and controlled water removal or discharge due to federal, state, and local freshwater withdrawals, and regional gate and barrier operations. The CASCaDE model has been calibrated for flow rate, water level, salinity and temperature for WY2011 and WY2012 (*Martyr-Koller et al. 2017*). We used the same computational domain (see Figure 1) as the CASCaDE project and used their model output flow field to drive the DWAQ offline. It has 10 vertical layers and 75019 horizontal cells. The resolution is higher in the Delta and Suisun Bay. Our modelling development effort for the current project will be focusing on WY2011 (August 2010 to October 2011).

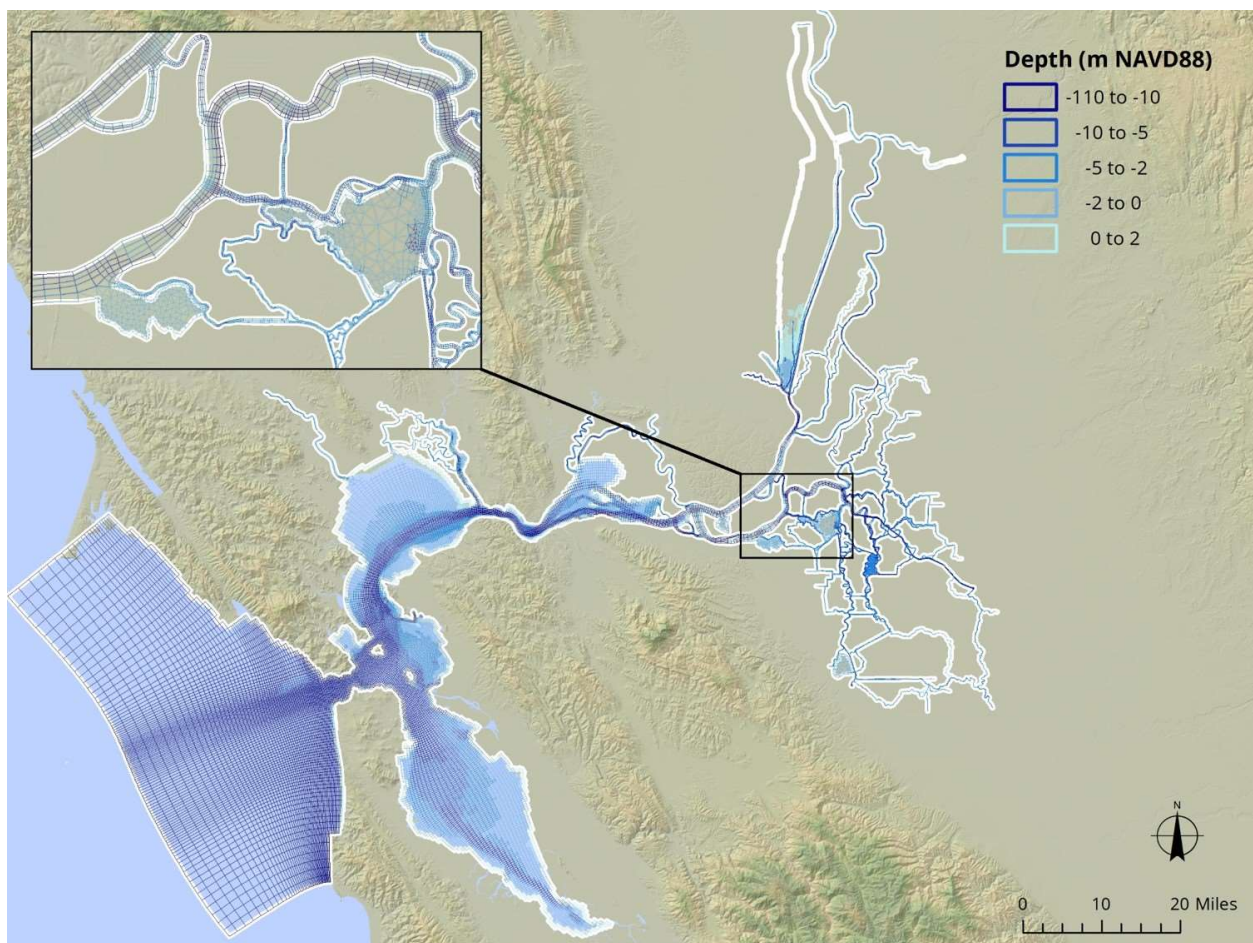


Figure 1 Computational domain and model grid from the CASCaDE project.

4.2 Biogeochemical model structure

The detailed biogeochemical processes we will implement in the current project are illustrated in Appendix A. However, as the first step of this development, we focused on nitrification and denitrification (Figure 2). The processes related to system metabolism (conversion of dissolved inorganic nitrogen (DIN) to organic nitrogen) were ignored in this phase. We made the assumption that the net contribution from primary production and mineralization (including autolysis, detrital mineralization, and sediment diagenesis) can be ignored based on our experience with open-bay biogeochemical modelling that, when the observed chlorophyll-a concentration was consistently low (less than 10 $\mu\text{g/l}$), the net contribution of processes related to organic nitrogen to the DIN pool is small.

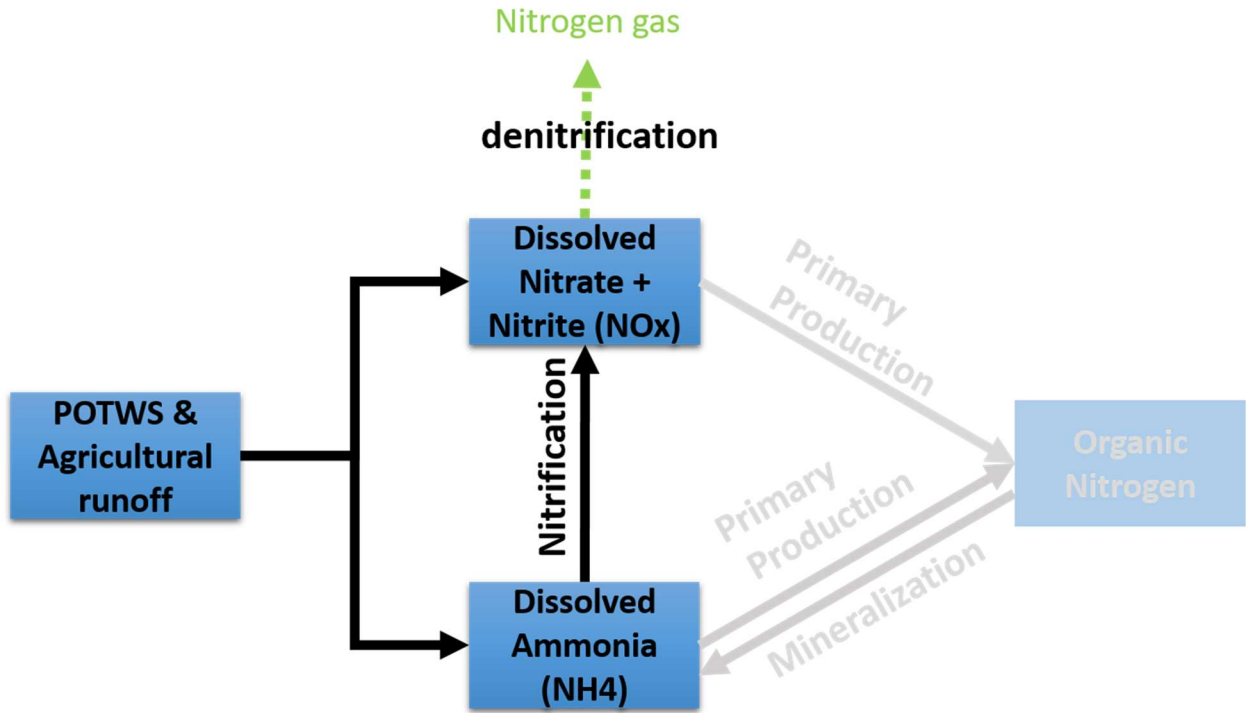


Figure 2 Nitrogen cycling processes implemented in the current model. The gray texts, arrows and boxes represent the processes and variables not yet implemented at this stage.

The equations describing nitrification and denitrification processes are as follows:

$$\text{nitrification rate} = \text{RcNit} \frac{NH_4}{K_{NH_4} + NH_4} \frac{DO}{K_{DO} + DO} \text{TcNit}^{T-20^\circ C}$$

$$\text{denitrification rate} = \text{RcDenSed} * \text{TcDen}^{T-20^{\circ}\text{C}} / \text{depth}$$

where RcNit and RcDenSed are the 1st order nitrification rate and sediment denitrification rate, respectively; K_{sub} represents the half-saturation coefficients for substances (NH₄ or DO); and TcNit and TcDen are temperature-dependency constants for nitrification and denitrification, respectively. We used the model default values for half saturation coefficients and tuned RcNit, RcDenSed, TcNit and TcDen until the model results matched well with the observations.

4.3 A project database that grows with the project

Being a heavily-studied system, the Delta and Suisun Bay have extensive datasets with wide spatial and temporal coverage across the region through multiple sampling efforts, providing a valuable record of the present and historical nutrient conditions. The long-term observational analytes relevant to the model development include dissolved nutrients (N, P, Si), dissolved oxygen, turbidity, chlorophyll-a, zooplankton density, and benthic grazer biomass and grazing rate. To compile existing data from multiple sources and make sure that they are consistent, non-redundant and compatible, a project database is required.

To promote a community modelling framework philosophy, we chose the open-source software SQLite (<https://www.sqlite.org/>) as our database management tool. It is a compact, self-contained, serverless, zero-configuration, transactional SQL database engine. It supports data queries like more sophisticated databases, yet it does not require an external server or database administration. The database – a single file – can be shared online and is accessible across different platforms, including desktops (Windows, Linux, Mac) and portable devices (Android, iOS). The data tables in the database can also be easily exported to a csv file and imported by a more advanced relational database, such as PostgreSQL, if the need arises. The data in the database can be conveniently queried using SQL directly, via most popular programming languages (e.g. R, Python, Matlab, and Java). The database can also connect with ArcGIS or QGIS to display geospatial information.

The data we have compiled so far in the Delta-Suisun database include only historical discrete nutrient sampling data. Zooplankton and benthic grazer data will be added as the project progresses. The data sources were based on a summary of existing nutrient monitoring programs in the Delta

from the *Delta RMP* (2016) post-workshop report. A list of monitoring programs and the websites available for downloading the data is provided in Table 1. We only downloaded data from 2000-01-01 to 2016-12-31, but further updates to the database to include additional years are possible.

Table 1. The sampling programs and downloading links for discrete nutrient data compiled in the Delta/Suisun database.

Program	Link
DWR-EMP	http://www.water.ca.gov/bdma/meta/
DWR-MWQI	http://www.water.ca.gov/waterdatalibrary/
DWR-NCRO	http://www.water.ca.gov/waterdatalibrary/
USGS-NWQAP	https://www.waterqualitydata.us/portal/
Irrigated Lands Regulatory Program	CEDEN
USGS Water Quality Cruise San Francisco Bay	https://sfbay.wr.usgs.gov/access/wqdata/

4.4 Biogeochemical Model Set-up: Boundary Conditions and Forcings

To prepare the boundary condition files and nutrient load data for the model, we collected, cleaned, and synthesized point source nutrient load data from the Delta and northern Bay (25 WWTPs, 2 refineries) and 4 river loads (Sacramento River at Verona, American River, San Joaquin at Vernalis, and the Fremont Weir above the Yolo Bypass). For each WWTP, nutrient loads ($= \text{flow rate} \times \text{nutrient concentration}$) were added to the bottom cell closest to its outfall. At river boundaries nutrient concentrations were taken from measurements at a nearby sampling site, and applied across the entire river cross-section. Original data have been checked for consistent metadata and units. Generally, observations are only available for intermittent periods and at irregular intervals. To generate continuous daily time series data required by the model, temporal interpolation was required. A synthesis procedure has been applied to extract seasonal cycles and long-term trends, which was then been used to fill gaps in the original data. Although the primary focus for model set-up for this Stage 1 work was on WY2011 (including final QA-QC), it was also efficient to, in parallel, compile and develop the same input data files for WY2000-WY2016, to streamline future model setup for other years. The compiled nutrient loads, the scripts for data quality check and interpolation, and the documentation of the data sources can be downloaded from: https://github.com/rustychris/sfbay_potw.

An overview map with the sampling locations as well as POTWs in the Delta and Suisun Bay is shown in Figure 3.

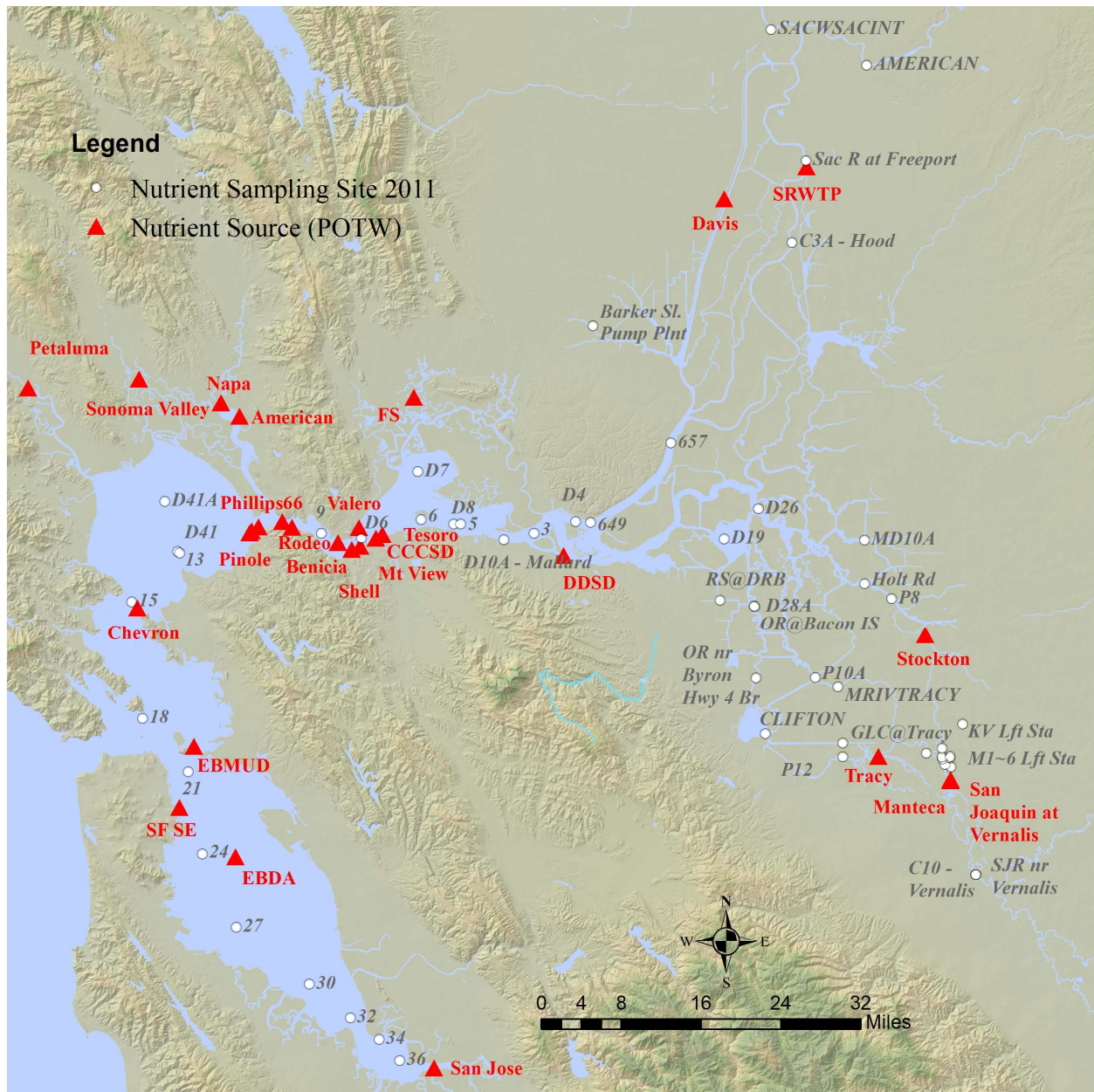


Figure 3 POTWs and Nutrient sampling sites from Delta/Suisun database for WY2011.

4.5 Volumetric source water calculation

To model the composition of the water (in percentage) from different source locations, we released three types of conservative tracers, each at one of the three major freshwater input boundaries (Sacramento River at both Verona and American River, San Joaquin River at Vernalis, and the Fremont Weir above the Yolo Bypass), to tag their respective origin. The concentrations of the tracers were set to one at their respective source boundaries. The sum of all three tracer concentrations should be close to one if the water mass was from one or a combination of the above three sources. However, when the sum of tracer concentrations was above one, some water mass was lost along the way due to evaporation and a correction was applied to the tracer concentrations by normalizing each concentration with the sum. When the sum was significantly less than one, the system was gaining water from sources other than the above assigned river boundaries (for instance, the open ocean) and no correction was applied in this case.

4.6 Water age calculation

Water age is defined by the time it takes for a water parcel to travel from the source to a particular location. Particles released from one source location can end up at the destination at different times, resulting in a statistical distribution rather than one scalar value for the water age. The calculated water age should therefore be an ensemble mean of all possible travel time for particles released at the given location and time. We released an impulse conservative tracer at the source location (in our application, the source location is the SRWTP discharge point) and tracked its evolution downstream. The advantage of the impulse tracer method is that, at each location (x), the modelled concentration (C) as a function of time constitutes a statistical distribution of travel time (t), from which we can conveniently calculate water age as:

$$\text{water age } (x) = \frac{\int C(x, t) t dt}{\int C(x) dt}$$

This method is particularly suitable for water systems that branch and meander, where a proportion of particles released at the source take a different path and merge downstream with particles taking the main path, resulting in drastically different water ages due to various particle pathways.

5. Results and Discussion

The flow condition from August 2010 to October 2011 shows that WY2011 is a wetter than normal year; the corresponding chlorophyll-a was generally on the low side (less than 10 $\mu\text{g/l}$) and remained low for most regions, except the South Delta. Within the South Delta, high chlorophyll-a was advected into the system from the San Joaquin River, rather than generated within the system. The collapse of phytoplankton biomass as the water enters the system may potentially cause a low DO issue when the dead organic material becomes remineralized within the South Delta. Currently, the natural runoff from Sacramento and San Joaquin River constitutes $\frac{3}{4}$ of the total nitrate load and only 4% of the total ammonium load into the Suisun Bay-Delta system. On average, Sacramento River contributes 17% and San Joaquin River contributes 20% to the total DIN load into the system.

5.1 Model validation

To tune the model, we started with the optimized set of coefficients for nitrification and denitrification from the San Francisco Bay nutrient modeling project, and gradually adjusted the coefficients until the model results matched well with the observations (see Table 2). Our final set of coefficients agreed with the range of coefficients reported for previous Delta biogeochemical modelling project by Delta Simulation Model II (DSM2), however, we did not assign different sets of coefficients for different regions in the model as in DSM2. Note also that DSM2 did not model denitrification (*SFEI*, 2015).

Table 2: The coefficients for nitrification and denitrification used in the current project compared to those used in other related projects.

Coefficient	RcNit (/day)	RcDenSed (m/day)	TcNit	TcDen
Current Project	0.18	0.12	1.10	1.10
San Francisco Bay optimized	0.09	0.12	1.05	1.00
DSM2	0.2~0.6	NA	1.08	NA

The half-saturation coefficients for ammonium and DO were taken directly from the default settings of DWAQ, with $K_{NH_4} = 36 \mu MN$ and $K_{DO} = 1 mg/l$.

The comparison between modeled and measured time series of dissolved nitrate and ammonia shows that our model was performing well at multiple locations across the Delta (see Figure 4). The detailed validation for each sampling site can also be found in Appendix B.

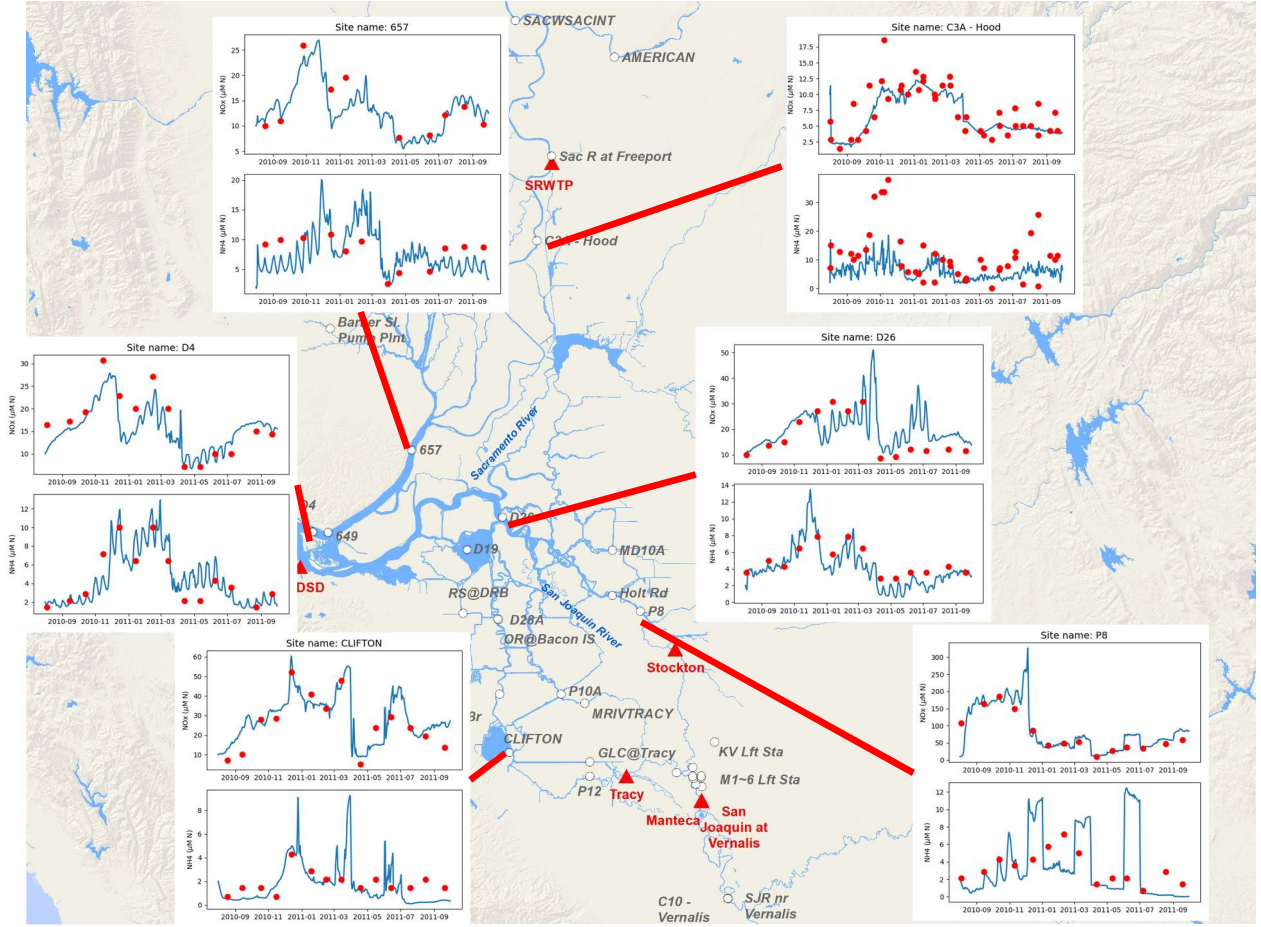


Figure 4 Comparison between the modeled (blue line) vs. measured (red circle) dissolved nitrate and ammonia at select sampling sites in the Delta and Suisun Bay.

To summarize the model performance, we quantify the errors using correlation coefficient (R), normalized Root Mean Square Error (RMSE), and Bias at each site. When these error statistics for all the sampling sites were plotted on the same map, we obtain a validation map (Figure 5). The model was generally performing well at most sampling sites except C3A – Hood and two sampling sites in San Pablo Bay. The reason our model seems to under-predict DIN at C3A – Hood was

because that the sampling site was so close to the SRWTP discharge point that the effluent was not given enough time to become homogenized across the cross section of the river basin. The measured concentration can thus be very sensitive to the exact depth and location from which the measurements were taken. San Pablo bay water was generally strongly influenced by the ocean, where the nutrient boundary condition was unknown. It is also noticeable, though generally low in amplitude, that our modeling results show positive bias (over-prediction) in Central-South Delta and negative bias (under-prediction) in North Delta and Suisun Bay. This may imply that either benthic nutrient flux, mineralization rate, or denitrification rate in these two regions were drastically different. Tuning the coefficients to improve the performance at one region will result in worsening performance at the other. We may therefore need to tune two separate sets of coefficients for each of these regions to further improve the overall performance of the model.

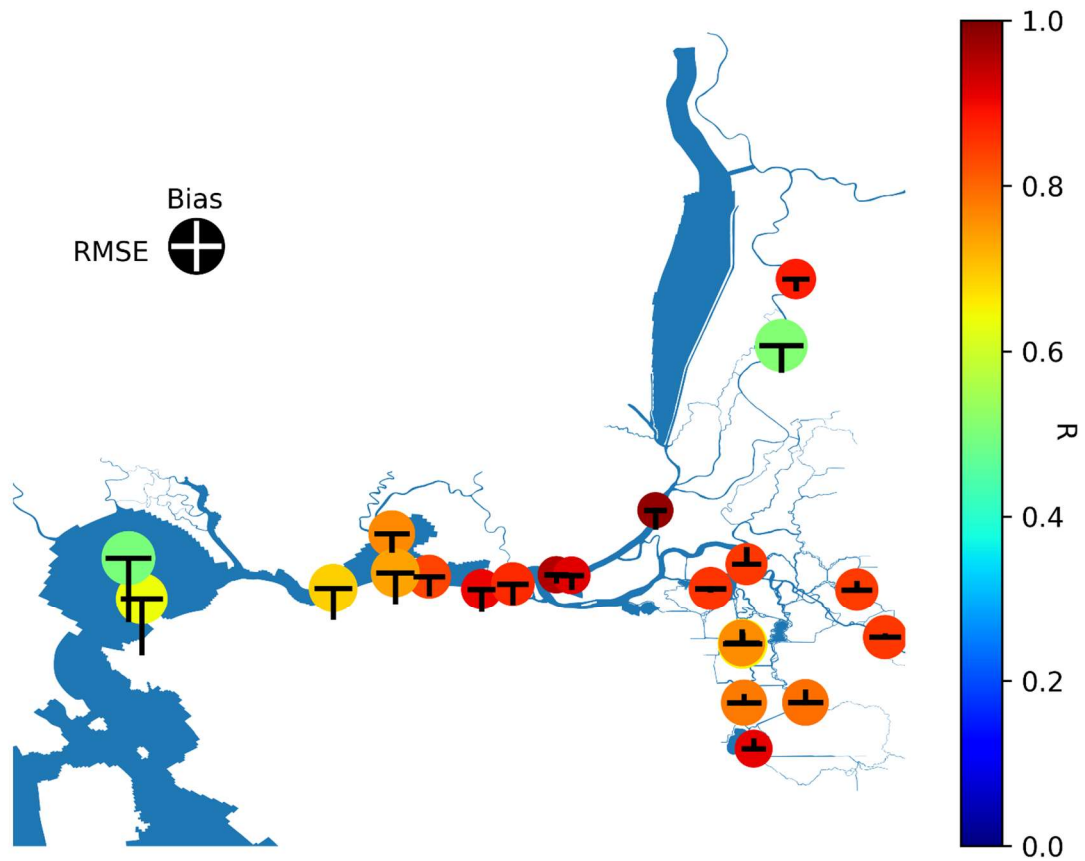


Figure 5 Validation map for Dissolved Inorganic Nitrogen (DIN). The color represents the correlation coefficient (R); the size represents the Root-Mean-Square-Error (RMSE) normalized

by the standard deviation; and the lengths of the horizontal or vertical white lines in the legend represent the magnitude of normalized RMSE or Bias equal to 1.

5.2 Example Scenarios

This section presents model results in ways that aim to highlight eventual model applications or scenarios. It should be noted, though, that the model output described below is based on an early-stage model, and substantial model development and validation are still required before we can properly answer these questions.

Management Question 1: Which sources are contributing water (and nutrients) to specific locations or regions, and how does this vary over time?

In order to identify nutrient management actions that have the potential to be effective for some region of the Delta or Suisun Bay, determining the nutrient sources (source proportion) is essential. Releasing conservative volumetric tracers from different river sources and calculating their respective percentage contribution (see details in Section 4.5) can provide useful information on the dominant source water during a particular time and at a specific location. As an example, we released tracers to tag water coming from the Sacramento River, San Joaquin River, and Yolo Bypass, which are the three major freshwater inputs into the system for WY2011. Figure 6 shows time snapshots of water composition from these three different sources, and illustrates the strong spatial heterogeneity in water sources and temporal variability.

Management Question 2: What can we do to improve a water quality issue

Model scenario runs can be performed to investigate the effectiveness of certain management actions. As an example, we did two hypothetical scenario runs: 1) shutting off Central San discharge completely; 2) reducing nutrient release from SRWTP due to a hypothetical wastewater treatment process upgrade. For this second scenario, we used an ammonia limit of 1.7 mg-N/l during April to October, 3 mg-N/l during November to March, and a nitrate limit of 10 mg-N/l to represent the effluent nutrient condition after the upgrade to SRWTP (*NPDES Permit*, 2010).

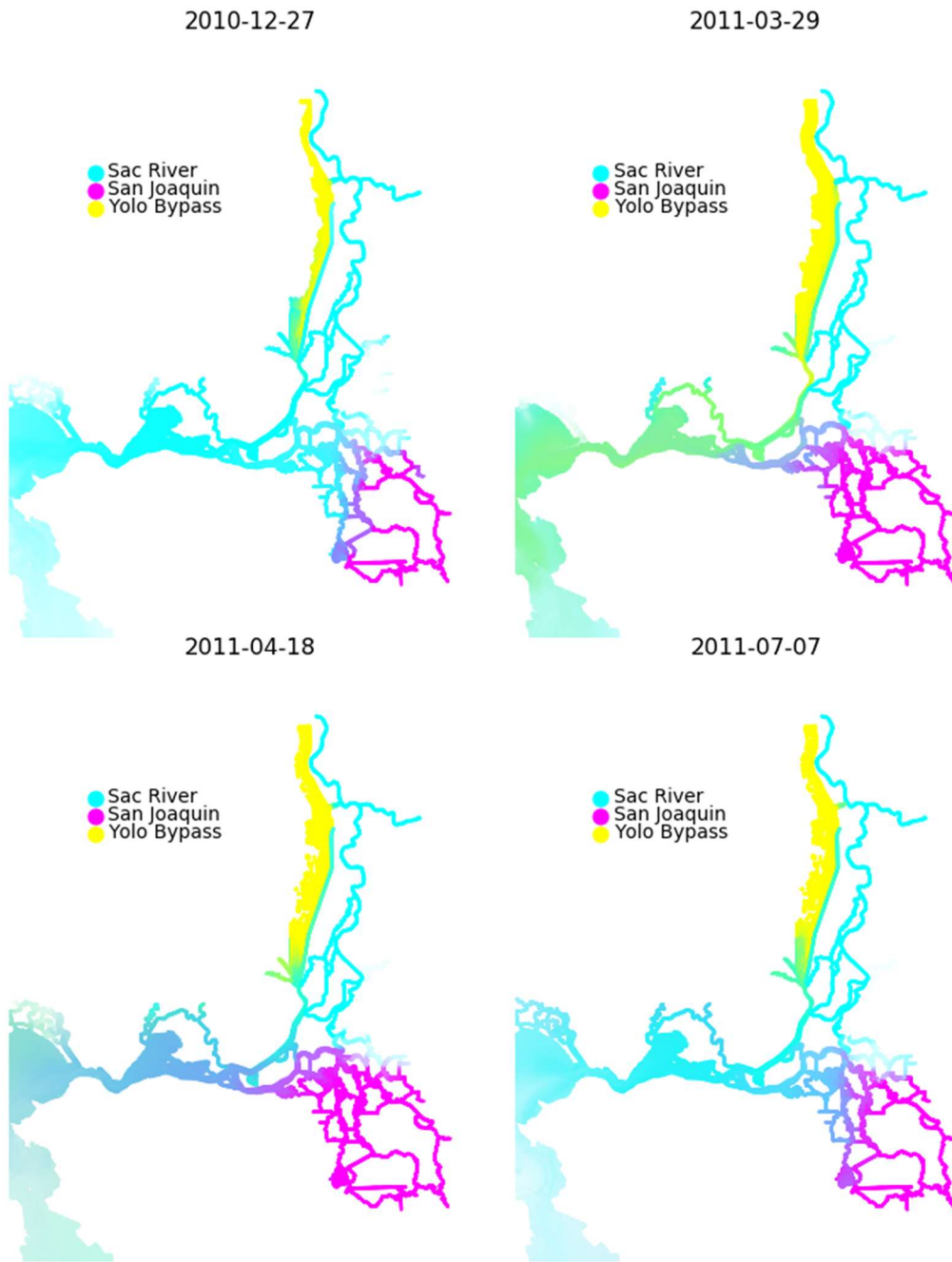


Figure 6 Snapshots of conservative tracers from the Sacramento River, San Joaquin River, and Yolo Bypass.

A comparison between the current condition and the scenario of hypothetically removing discharge from Central San can be found in the attached Movie 1. Snapshots of the modeled DIN before and after SRWTP upgrade, and the difference between the two are shown in Figure 7 and more detailed comparisons between before and after the SRWTP upgrade can be found in the attached Movie 2.

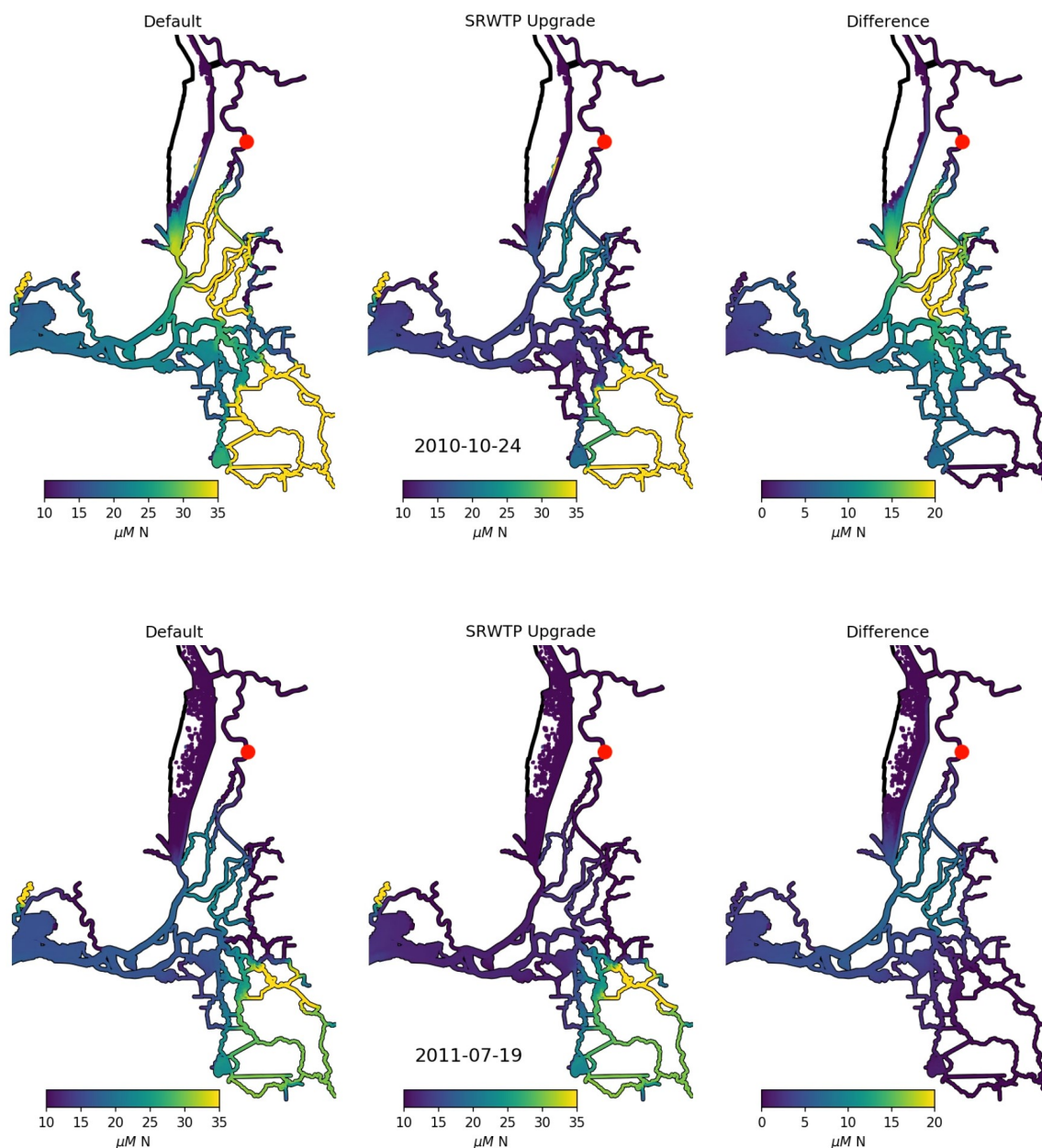


Figure 7 Snapshots of the modeled DIN before (left) and after SRWTP upgrade (middle), and the difference between the two (right).

Management Question 3: Which biogeochemical processes are important, why and when?

A biogeochemical process is considered to be important when it causes substantial change in the concentration of a substance, such as nutrients. Water age provides an estimation of how long the substance is subject to the same condition and processes, and thus the chance it can be altered by a biogeochemical process, i.e., longer water age can augment the impact of a biogeochemical process in an aquatic system and vice versa. We calculated water age of effluent from SRWTP under two different flow conditions during WY2011: one from August to November, representing low flow condition (flow rate $\sim 400 \text{ m}^3/\text{s}$) and the other from December to February, representing high flow condition (flow rate $\sim 1200 \text{ m}^3/\text{s}$). The water age exhibits great spatial variations and substantial difference between the two flow conditions (Figure 8). The water age during high flow condition ranged from a few days to 10 days, whereas it ranged from a few days to 30 days during the low flow condition.

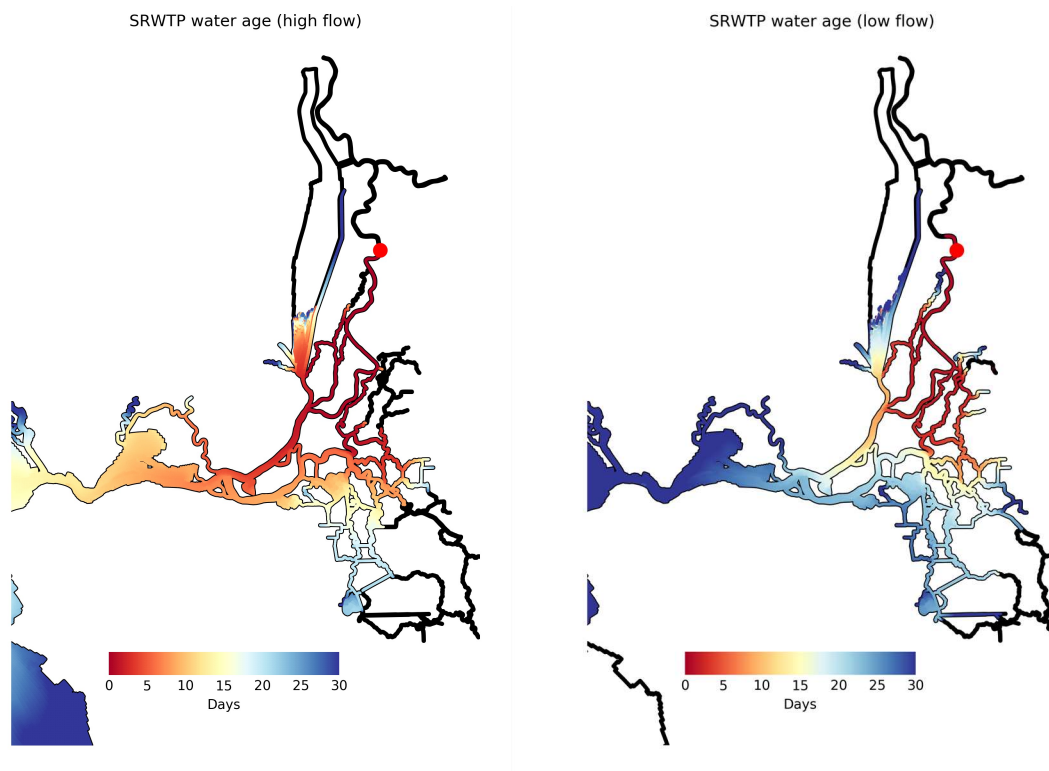


Figure 8 The water age of effluent from SRWTP (location indicated by the red circle) under high flow and low flow conditions during WY2011.

To estimate the impact of system metabolism, we used the method introduced in *Smith et al.* (1991) and *Smith and Hollibaugh*, (2006). We chose to perform the estimation of system metabolism along the Sacramento River and Suisun Bay (from C3A – Hood all the way to D6) during a low-flow warm period (Aug to Oct 2010) when the impact of system metabolism was the strongest. The observed N, P, turbidity, light, and chlorophyll-a for the above sampling sites were seasonally averaged to derive denitrification, production and mineralization rates (Table 3). The combination of all three processes resulted in a small change in DIN (~1% per day), however, the contribution from each individual terms was not trivial (2~5% per day). The combination of production and mineralization resulted in a residual term almost balanced by the denitrification. Note that to optimize the model performance, the 1st order denitrification rate used in the model (0.24~0.36 $\mu\text{M}/\text{day}$) was smaller than the estimated denitrification rate (0.53 $\mu\text{M}/\text{day}$) to compensate for the fact that the net metabolism term was not modelled.

Table 3 The estimated rates comparing the relative importance of various processes for nitrogen cycling.

Units	Denitrification rate	Net metabolism	Production rate	Mineralization rate (calculated)	Net metabolism & denitrification (calculated)
μM per day	-0.53	0.77	-1.26	0.49	0.23

The estimated denitrification rate (0.53 $\mu\text{MN}/\text{day}$) is compatible with the benthic denitrification rate of 0.6-1.0/Depth $\mu\text{MN}/\text{day}$ range measured by *Cornwell et al.* (2014). It is unclear if mineralization mainly happened in the water column or in the sediment (as benthic flux), or it could be a mix between the two. Compared with previously measured maximum DIN benthic flux rates (*Cornwell et al. 2014*) of 2.4/Depth $\mu\text{MN}/\text{day}$, if we assume an average depth of 5m along the transect, the maximum measured benthic flux rate for the water column would be 0.48 $\mu\text{MN}/\text{day}$, which matches the amplitude of net nitrogen increase rate of 0.23 $\mu\text{M}/\text{day}$.

So in WY2011, it is reasonable for us to assume that the net effect of system metabolism is small and we can still get reasonable simulation results that match well with the reality. However, if, for instance, some factors result in a sudden huge increase in either production or mineralization,

or if the amplitude of chlorophyll-a is large (such as in WY 2016, they got 10 times higher), we would expect that the combined effect of organic processes (phytoplankton, zooplankton, and detritus) will play a significant role in nitrogen cycling.

6. Recent Progress

The progress we have made since January 30th 2018 includes: data preparation for model input and validation; and building biogeochemical models capable of simulating full biogeochemical cycling processes.

6.1 Model data preparation

To compile data needed for model input and validation, two types of data were added to our databases. The discrete sampling data were added to the SQLite database (see Section 4.3), whereas the continuous data were added to the existing San Francisco Bay Nutrients visualization tool (with a backend PostgreSQL database) hosted on www.enviz.org, which can handle large datasets more efficiently than the SQLite database. The additional discrete data we brought in the database include: zooplankton density, categorized as micro- and meso-zooplankton, as well as bivalve density, biomass, mean size, and grazing rate for both *Potamocorbula* and *Corbicula*. The high-frequency data we brought in ENVIZ include solar radiation, wind speed and wind direction. ENVIZ already has historical and recent high-frequency data from both DWR and USGS throughout the Delta, and it is updated on a bi-weekly basis. The high-frequency analytes relevant to the current project include turbidity, nitrate, Chlorophyll-a (measured by Fluorometers), dissolved oxygen, temperature, and specific conductivity.

6.2 Building the biogeochemical model

The additional processes included in the biogeochemical model were: nutrient uptake by phytoplankton, primary production, zooplankton grazing (Dynamic Energy Budget model), mineralization of dead organic matter in water column and sediment, settling and resuspension of detrital material, and sediment diagenesis model. A schematic diagram showing the connections among various biogeochemical processes and the DWAQ modules turned on is shown in Figure 9.

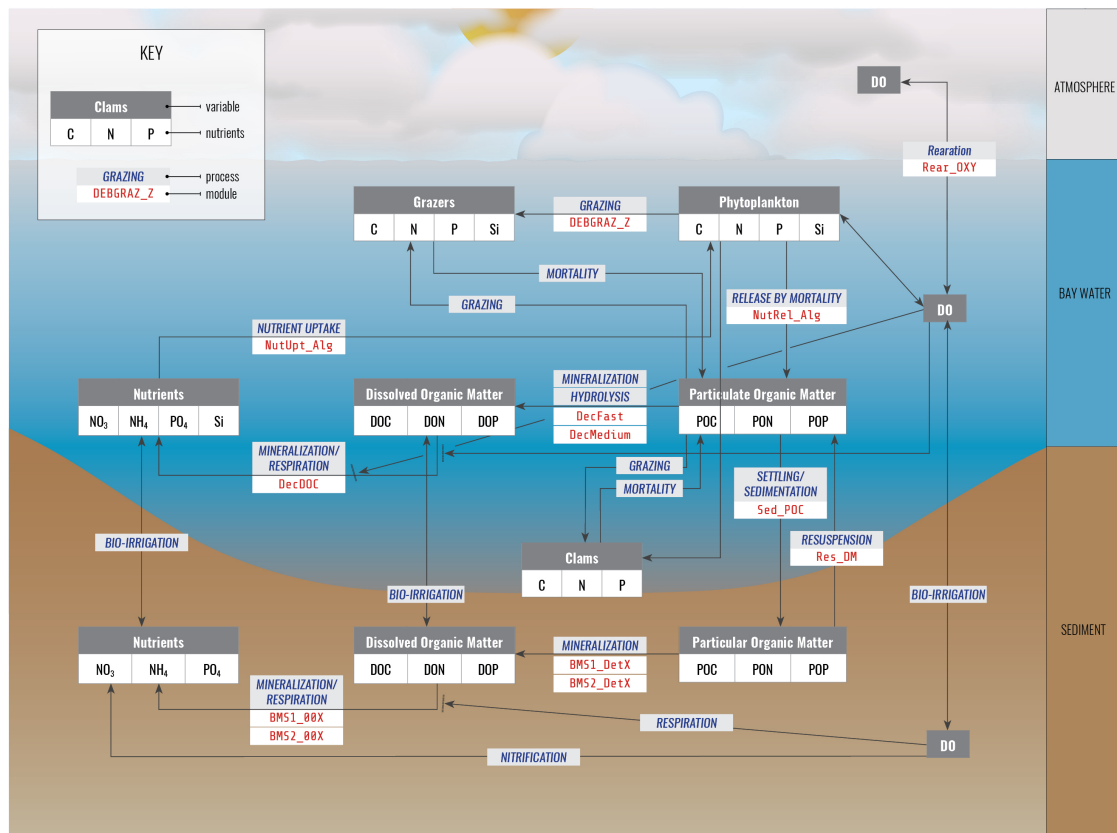


Figure 9 Schematic diagram showing the connections among various biogeochemical processes.

Detritus or particulate organic matter is released from algal predation, algal and zooplankton metabolism (death, maintenance, and faeces), and external input. Detritus both within the water column and in the sediment surface can be food sources for zooplankton, although zooplankton tend to preferentially graze on phytoplankton. Detritus is comprised of DOM (dissolved organic matter, C, N, P or S) and POM (particulate organic matter). POM will first be converted to DOM through hydrolysis before it can be mineralized. POM can also sink to the bottom and go through diagenesis in the sediment layers and return to water column as DOM or DIM (dissolved inorganic matter, such as DIN). The sinking and resuspension of POM is governed by bottom shear stress, which is determined by bottom roughness and a combination of benthic unidirectional flow and

wave-driven oscillatory flow. Both mineralization and diagenesis are a function of temperature and proportional to organic matter concentrations.

Sediment is composed of inorganic matter, detritus (POM), and algae. At this stage, only detritus is modeled in the sediment model. POM in the sediment is divided into labile (DetX) and refractory (OOX) substances. When POM in the water column sinks to the bottom, it becomes DetX. The sediment diagenesis model includes two layers of sediment: S1 and S2. S1 can be partially enriched with DO (aerobic), but S2 is depleted of DO (anaerobic). We assumed that the sediment had fixed porosities and fixed layer thicknesses, so all advection processes related to flow through the sediment-water interface (i.e., seepage) that affect the benthic geometry and porosity were turned off. One reason we decided to make these assumptions was that we had very little knowledge of parameters needed to model the impact of suspended sediment on the morphology of the sediment layers. However, what we were trying to model were the concentrations of substances in the sediment (organic matter composition) and their exchanges with the water column. The dispersion of dissolved substances (bio-irrigation) causes transport fluxes of dissolved matters across the sediment-water interface. These fluxes include the so-called return fluxes of nutrients to the water column and the sediment oxygen consumption flux. We also turned on bioturbation to represent dispersion of particular matters between the sediment layers and water column. Lastly, as a suspected first-order term that controls phytoplankton bloom in the Delta and Suisun bay, benthic grazing needs to be added to the biogeochemical model, which we are currently working on.

Future Work

In the next two years, we will focus on building a solid foundation for the biogeochemical model and validate it as well as possible for WY 2011. We will gather more data for initializing the model at the boundaries as well as plotting, analyzing and integrating the atmospheric, turbidity, DO, zooplankton and benthic grazer data into the Delta/Suisun database. Then we will focus on building all the components (see Appendix A) needed to model nitrogen cycling, phytoplankton dynamics, benthic and pelagic grazing, mineralization of organic matter (including detritus), sediment processes, and dissolved oxygen. The modeled nutrients, DO, and chlorophyll-a will be validated against the measured data pulled from the database for WY2011.

Once we gain some confidence in our modelling results, we will start to investigate some management questions that identified to be of high priority by the stake holders during the 1st semi-annual progress meeting on 30 Jan 2018, which are:

1. Relative importance of light and benthic grazers in controlling phytoplankton blooms;
2. Quantitatively identify data gaps needed to be filled to support further model development and validation;
3. Future scenario runs for SRWTP upgrade.

Beyond the scope of the current project, more biogeochemical modeling work will be needed. Model development is an iterative process; as we progress in getting more in-depth understanding of the system, we may come up with new insights: such as identifying additional data gaps, running additional years, particularly a dry year scenario, and deciding that more efforts need to be put into a process that we initially thought we could simplify. When that happens, we may need to collect more data, do additional model runs for different years, and revise some processes for the model. As we gain more confidence in the model by testing it under representative as well as extreme events, we will be able to start using the model to answer management/scientific questions. In addition to the questions listed above, we are also interested in exploring questions such as:

1. Contribution of nutrient loads from each POTW in space and time;
2. Relative importance of major drivers: hydrological, meteorological and biogeochemical;
3. Low dissolved oxygen resulting from excess primary production in some localized settings;
4. Future scenario runs: e.g., change of hydrodynamic, hydrological, meteorological conditions.

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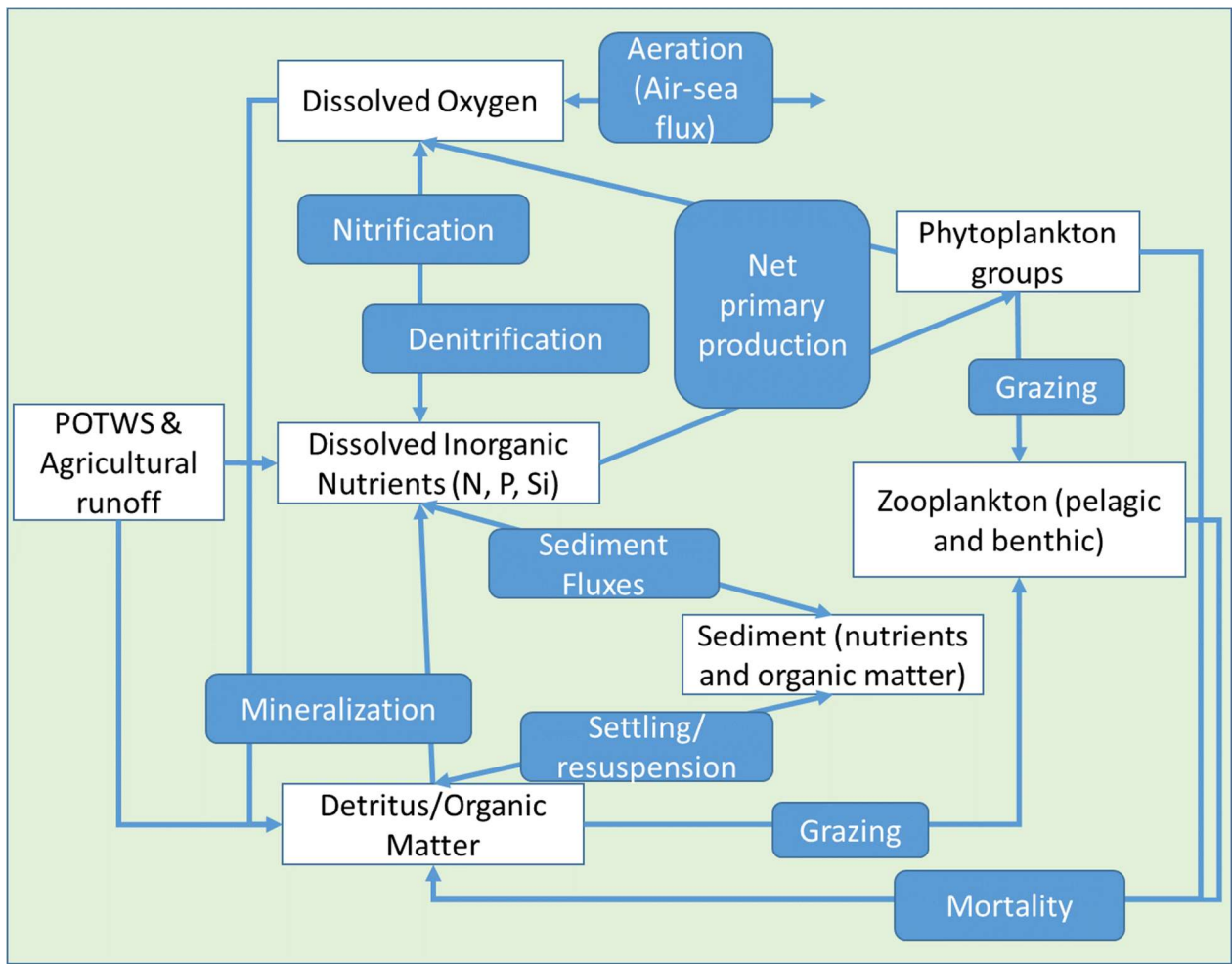
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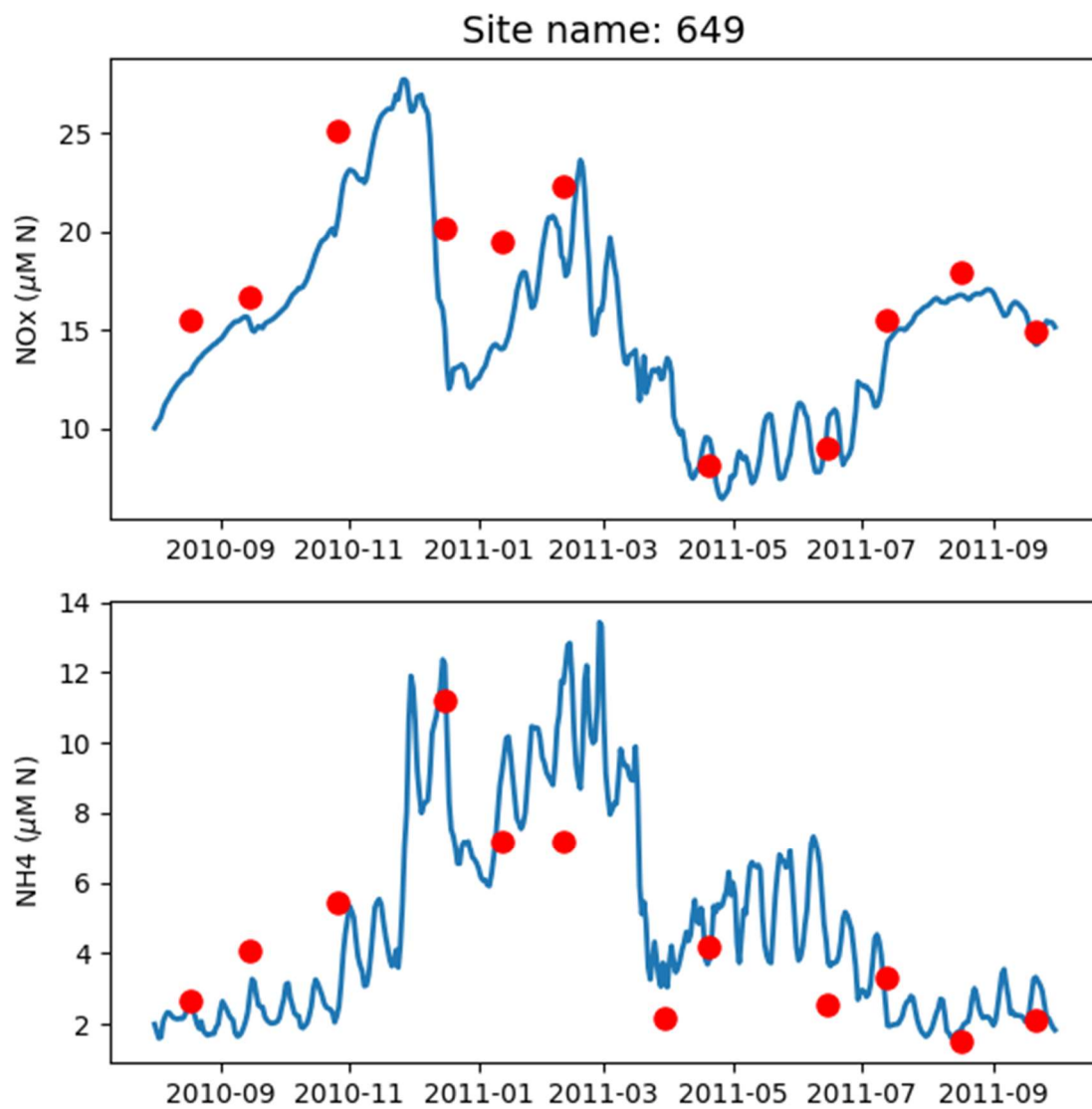
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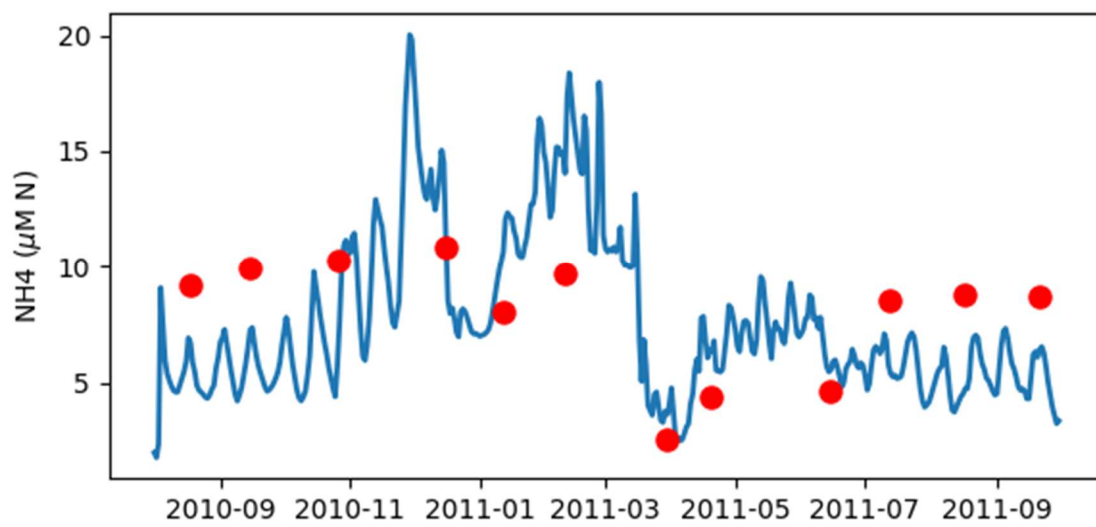
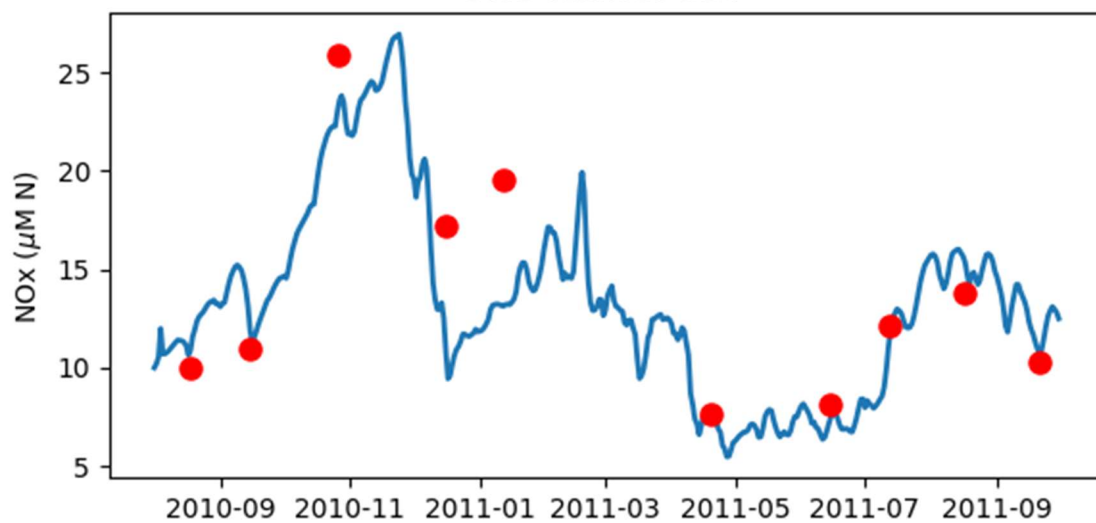
Appendix A: Biogeochemical model structure



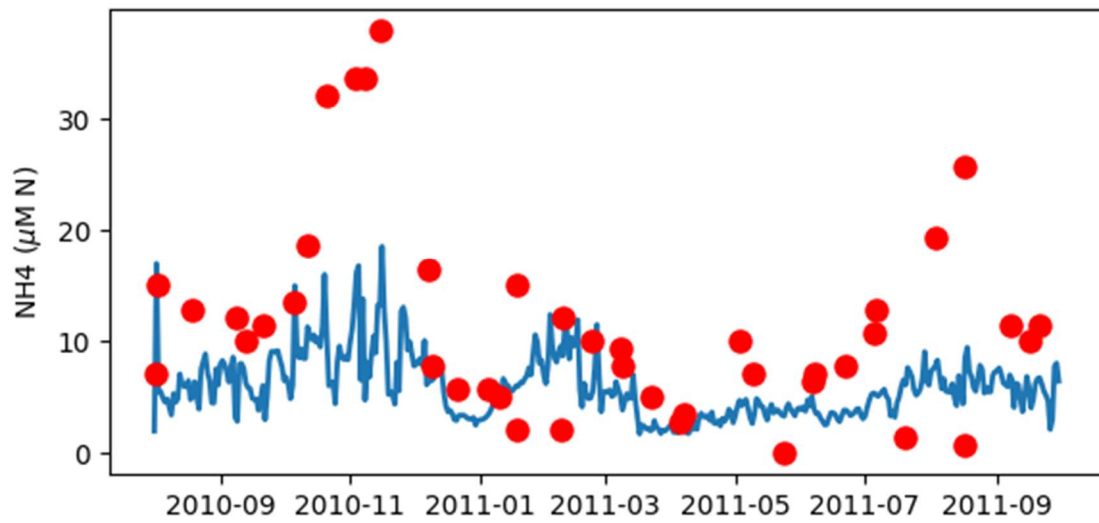
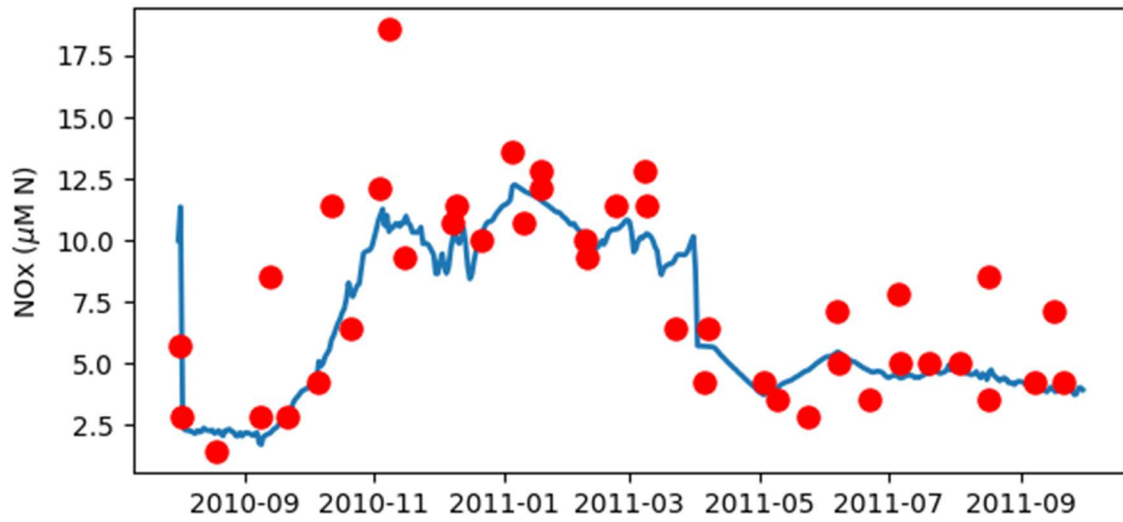
Appendix B: Nitrogen cycling validation results



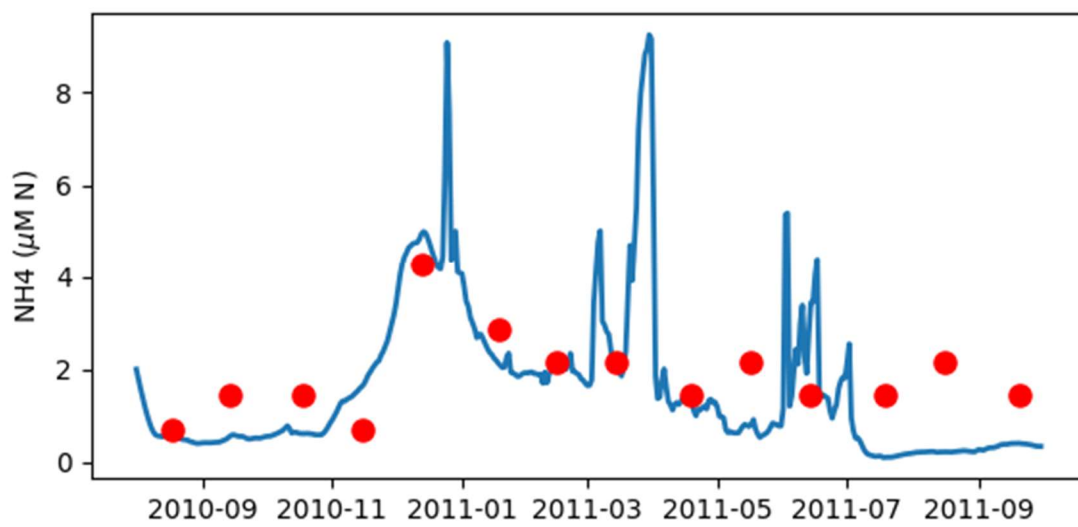
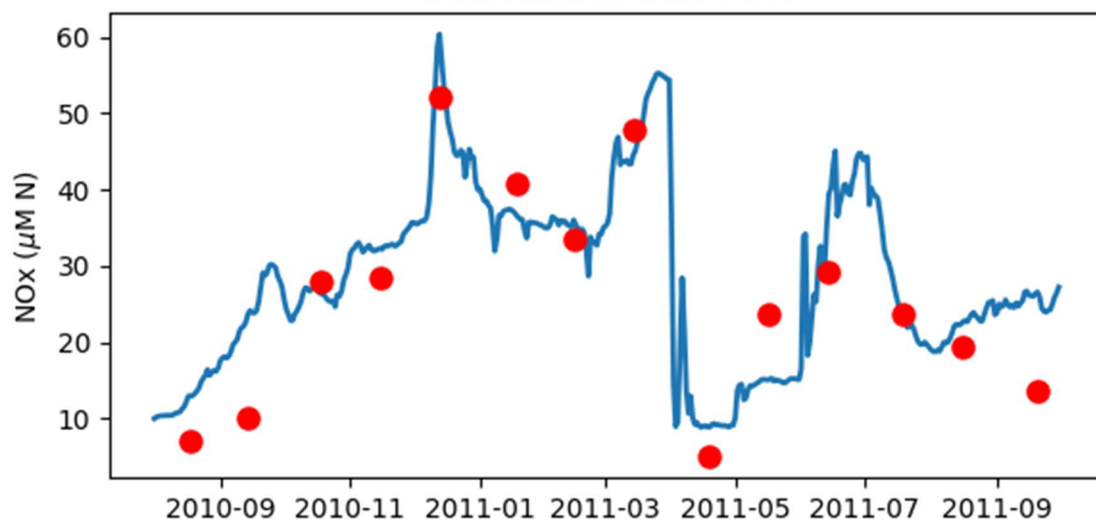
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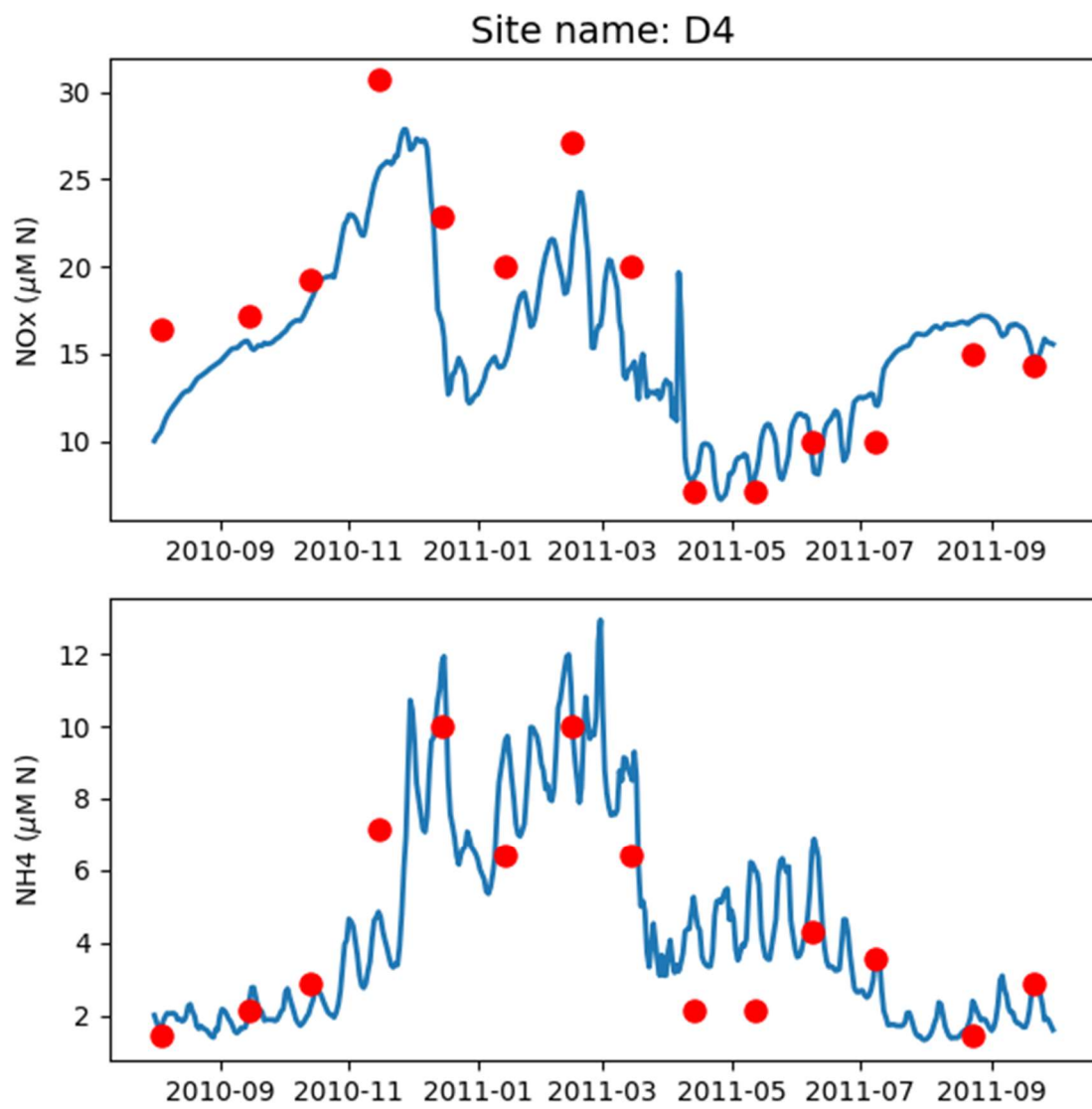


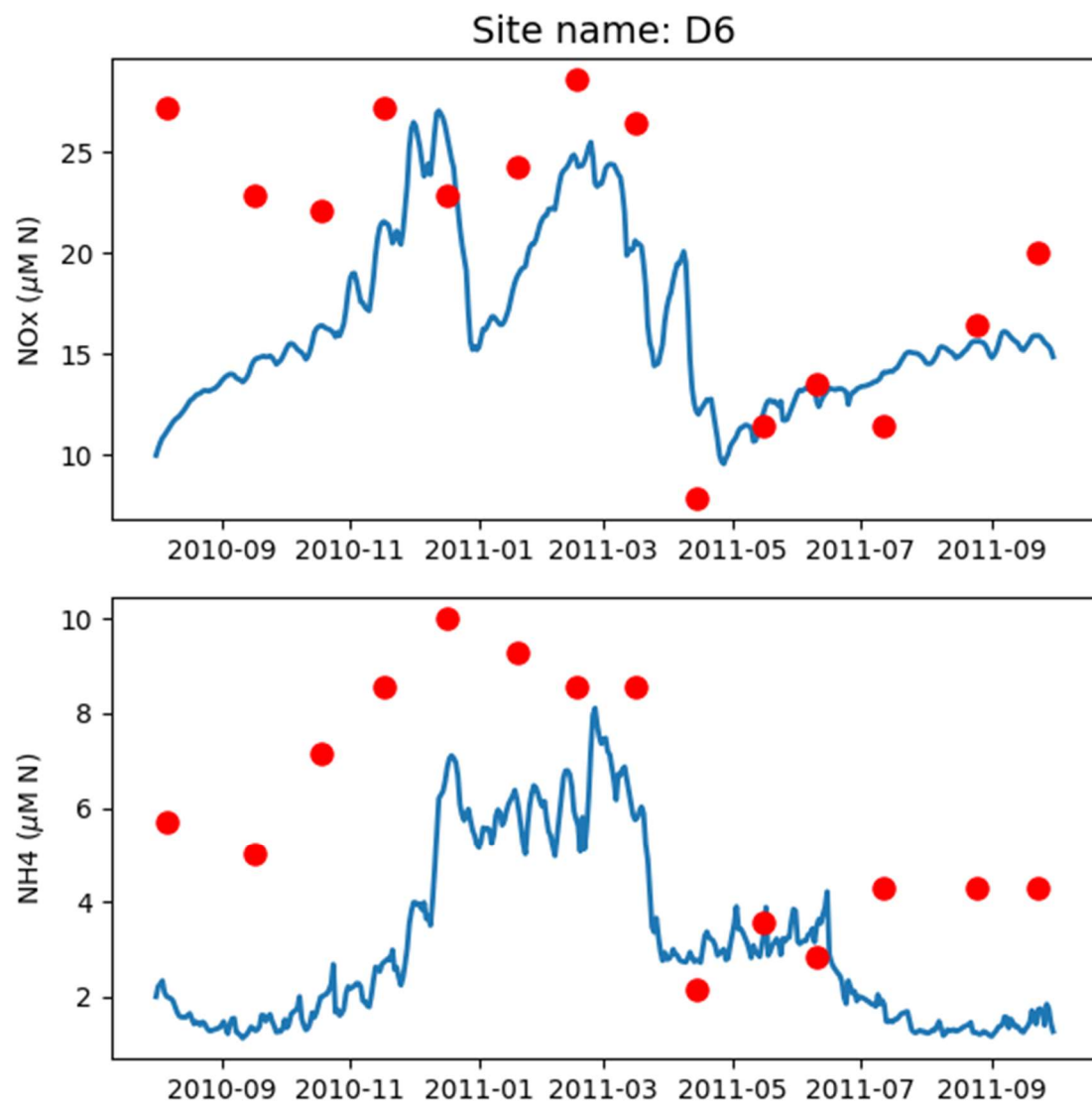
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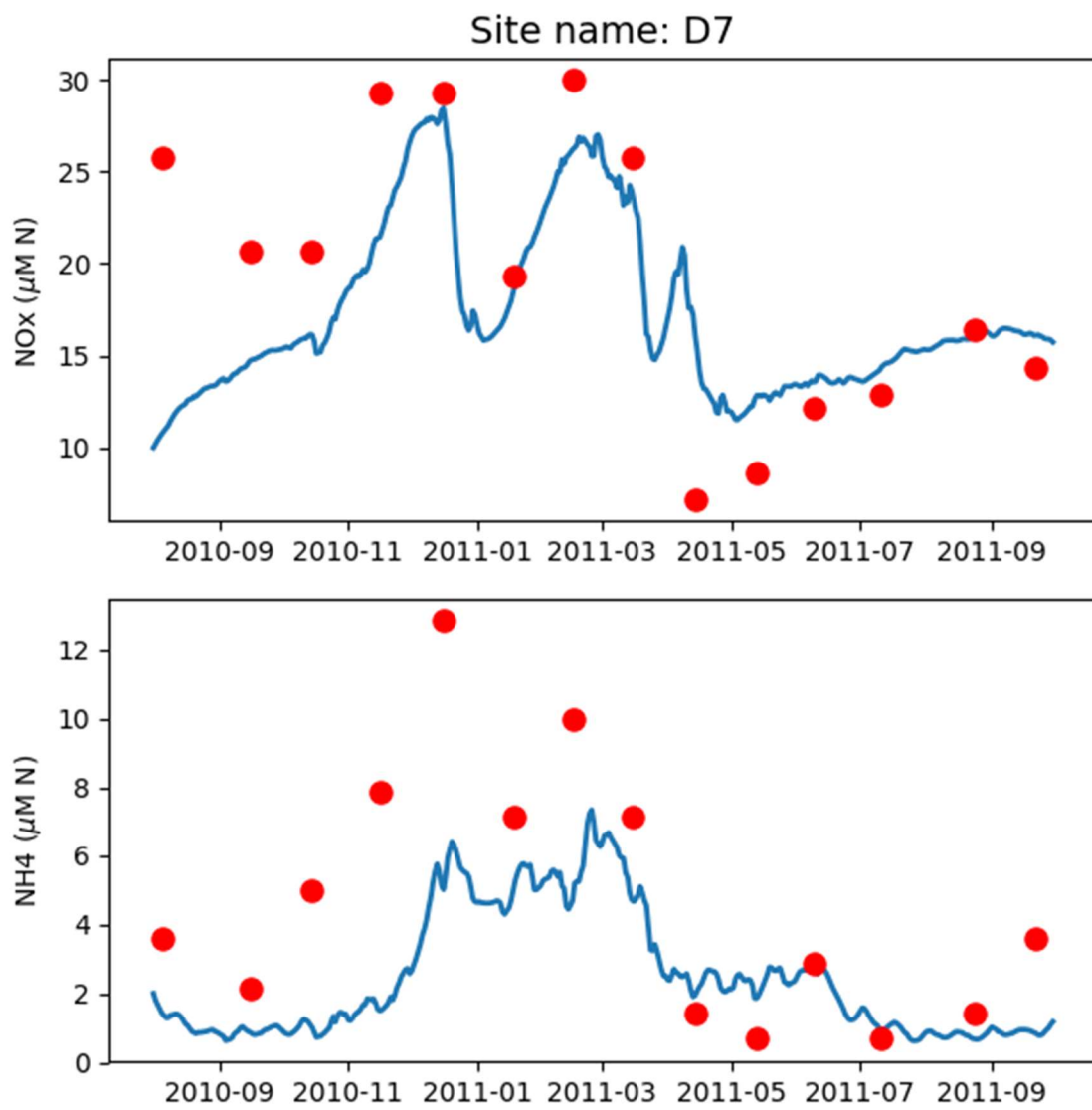


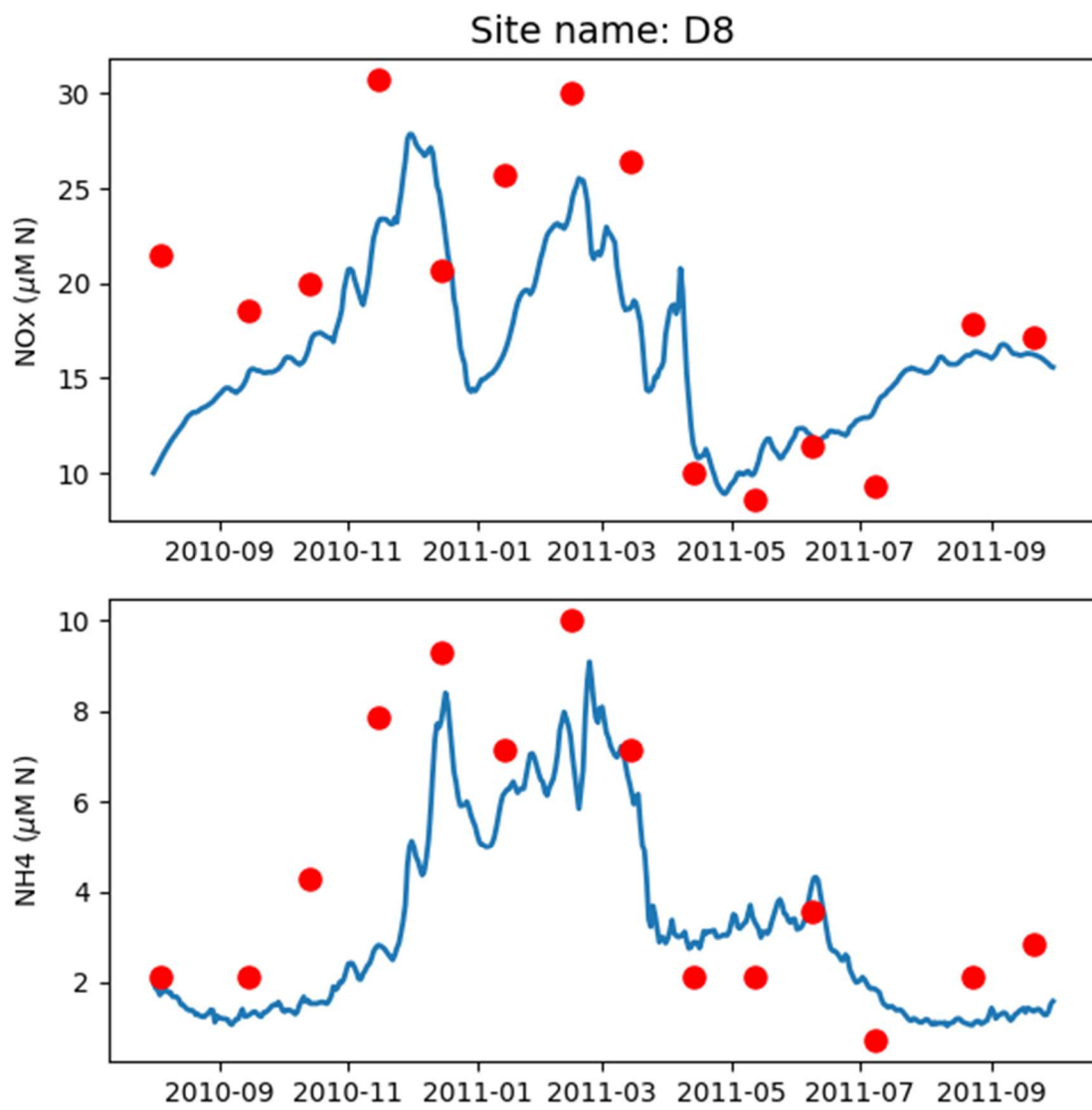
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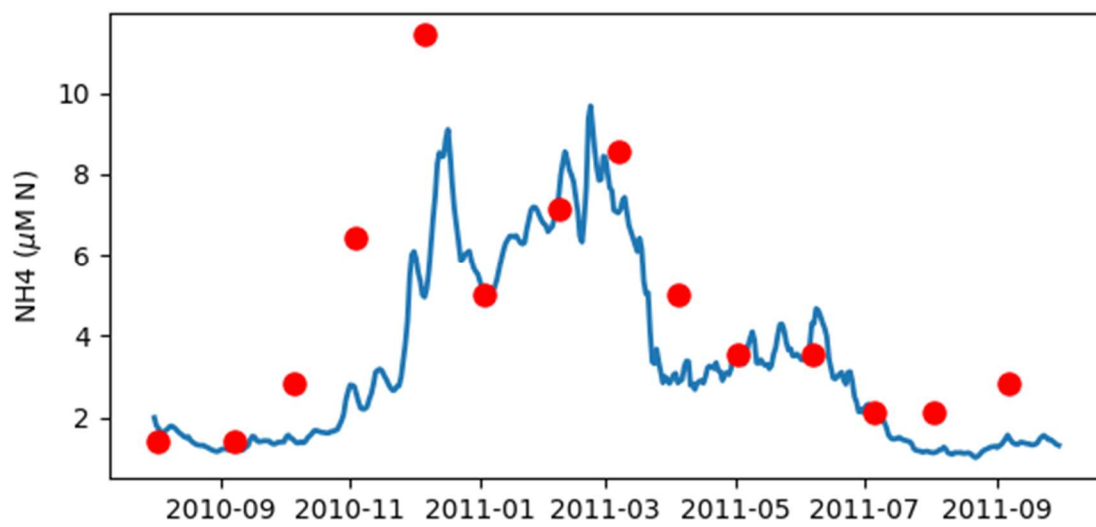
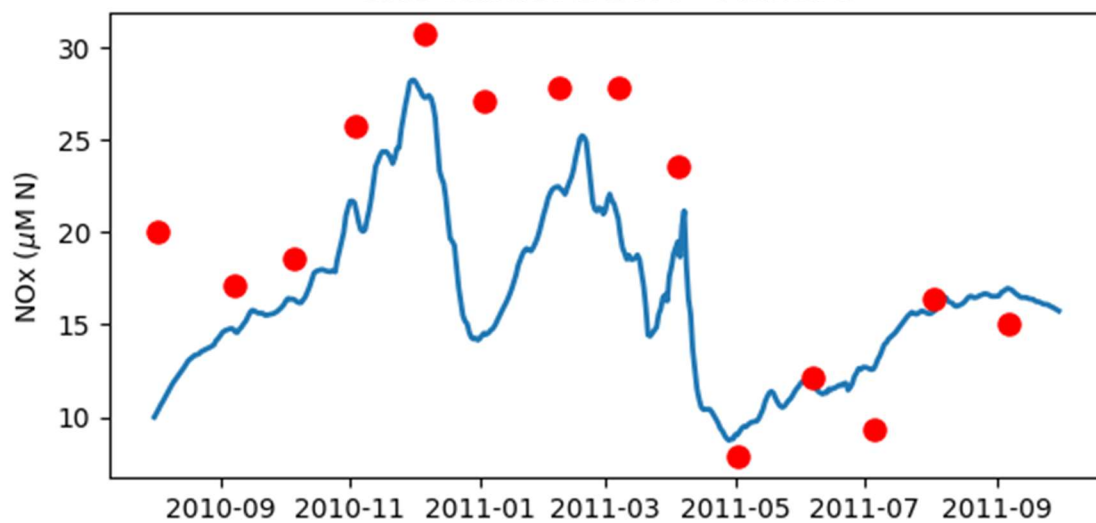




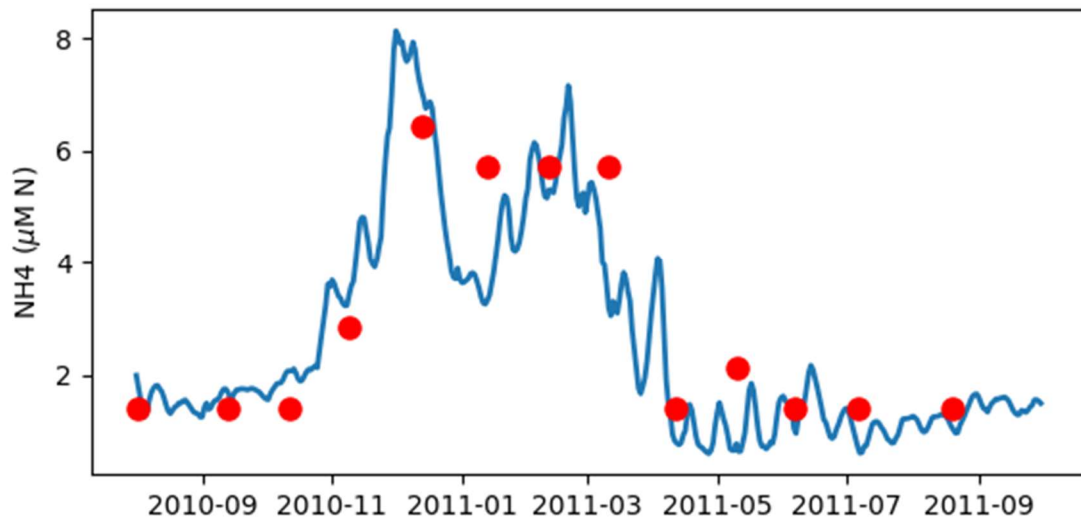
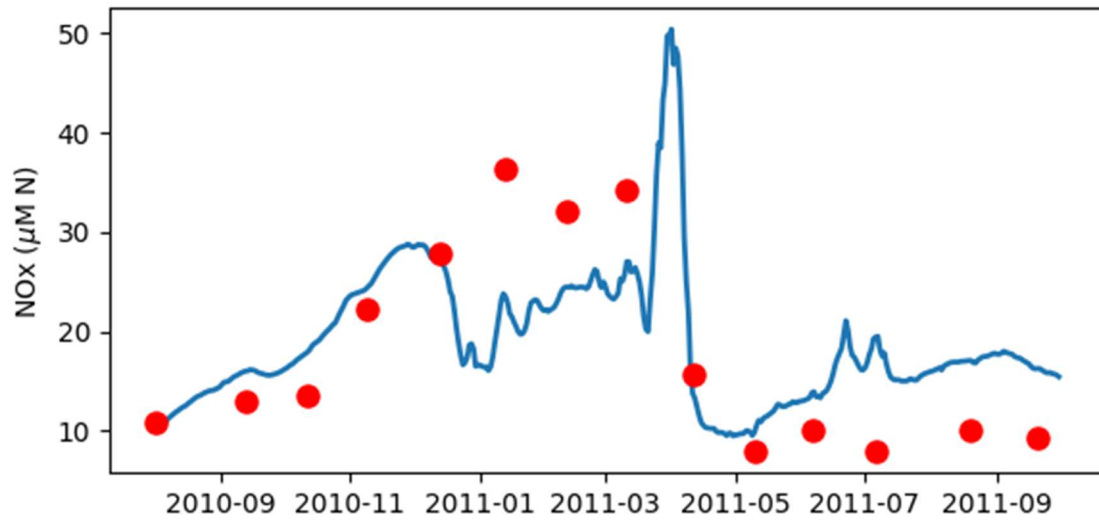




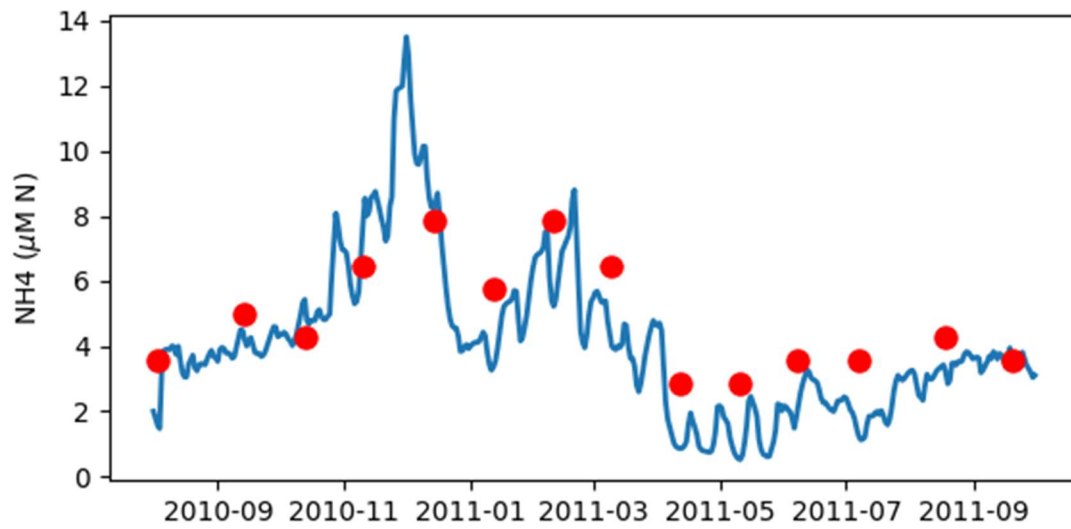
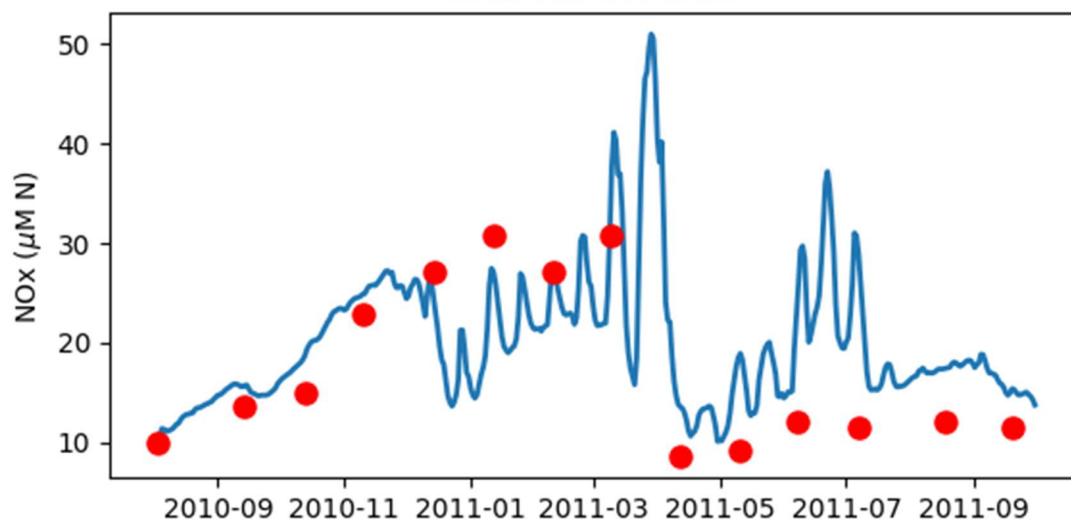
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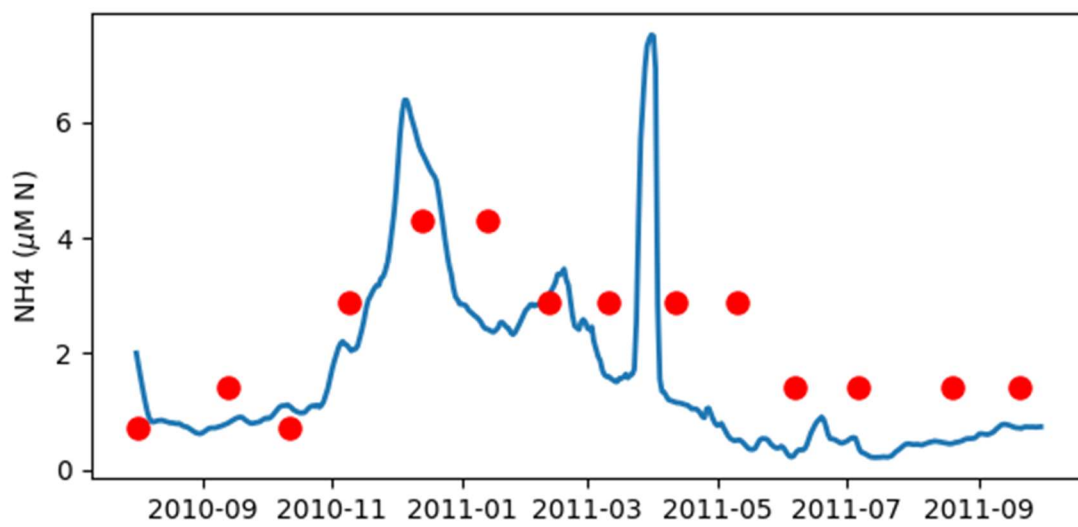
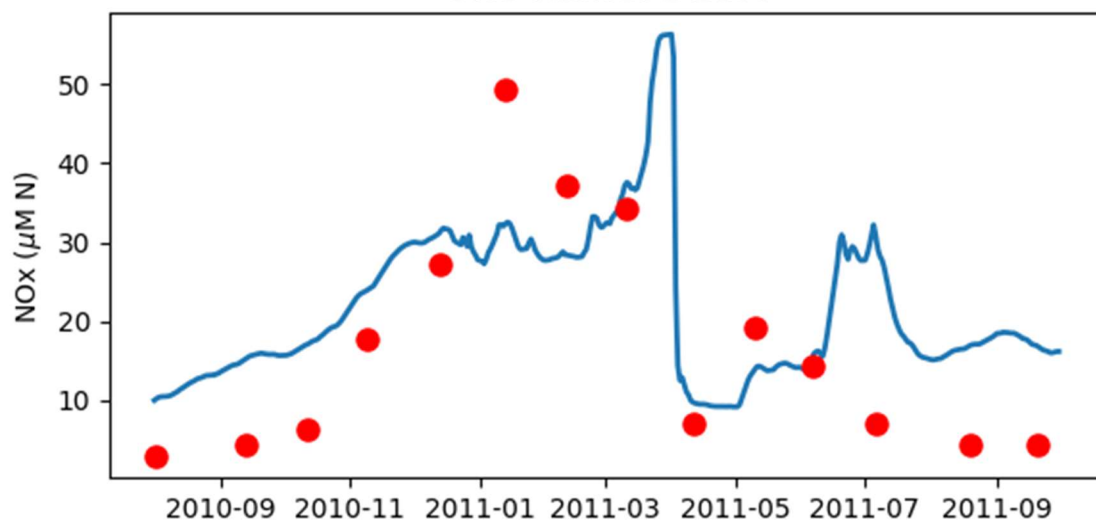
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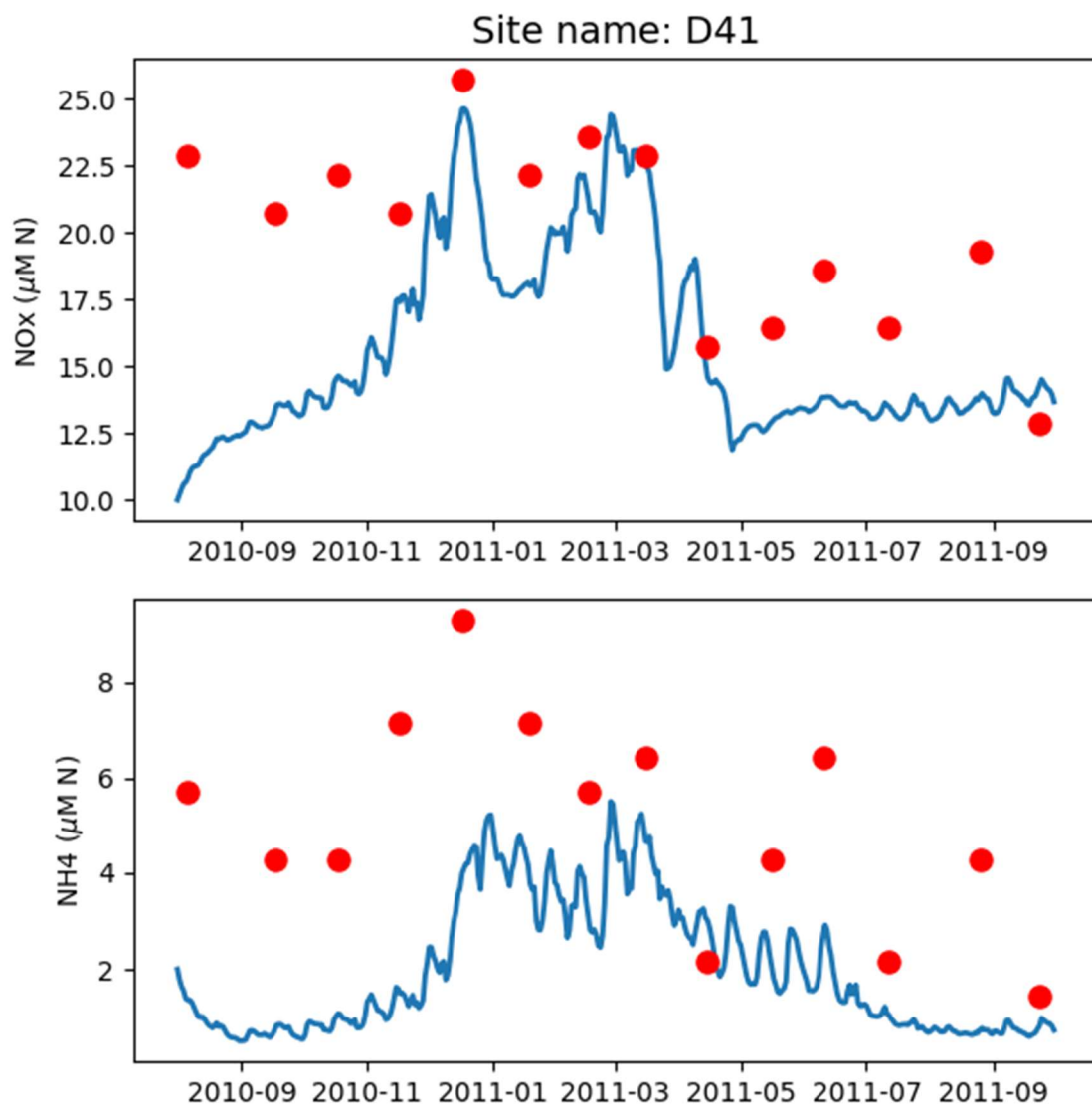


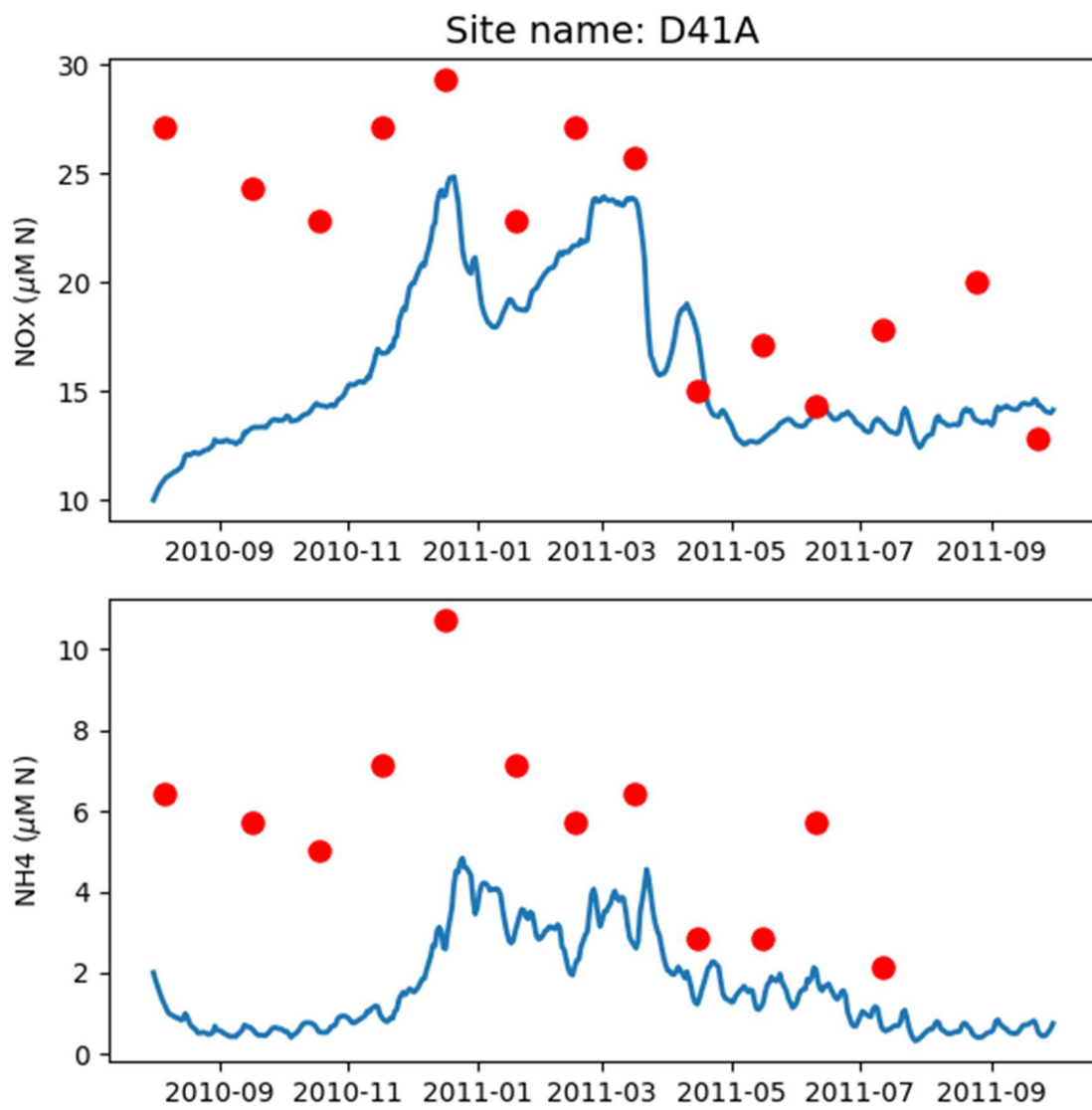
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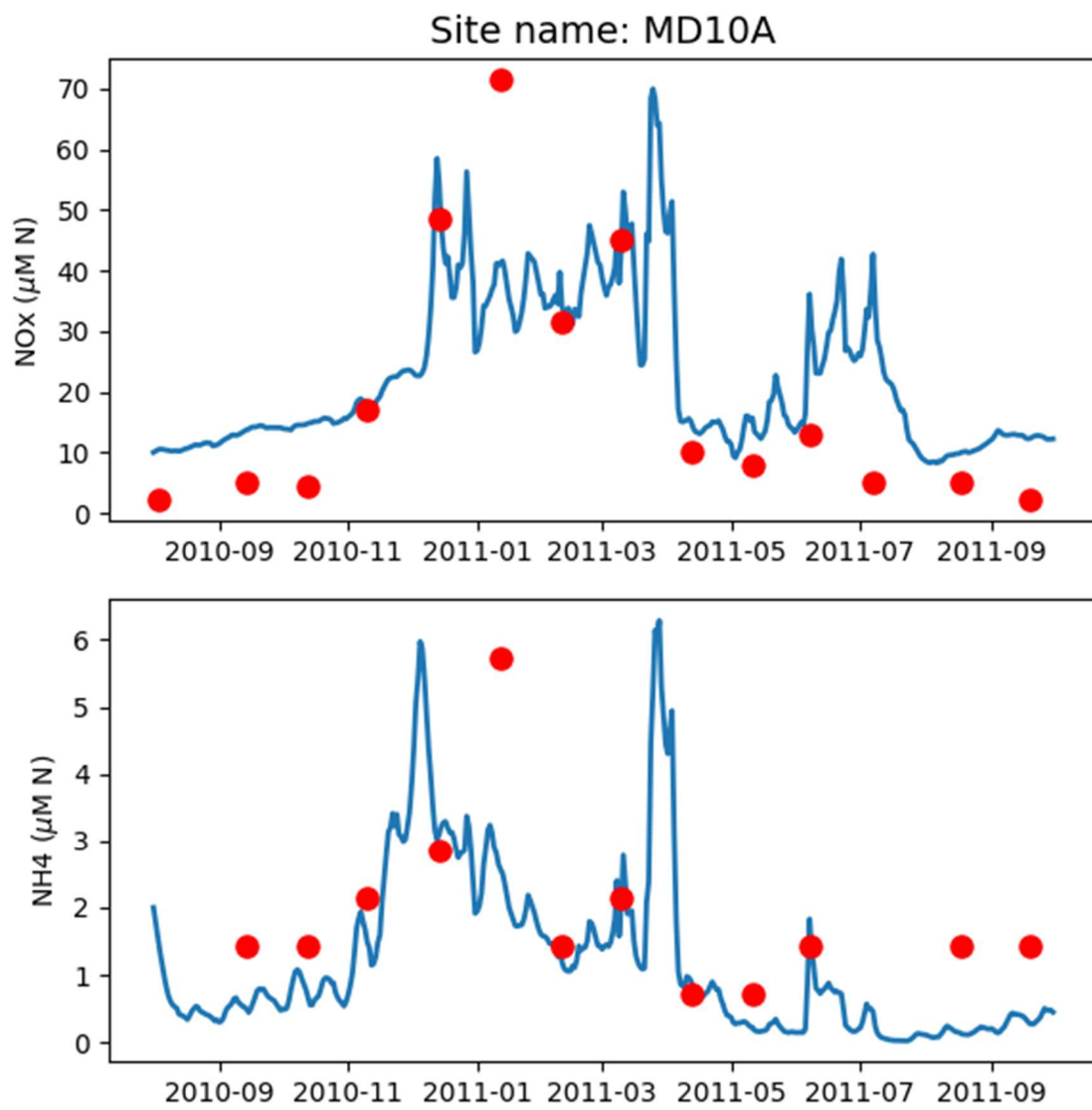


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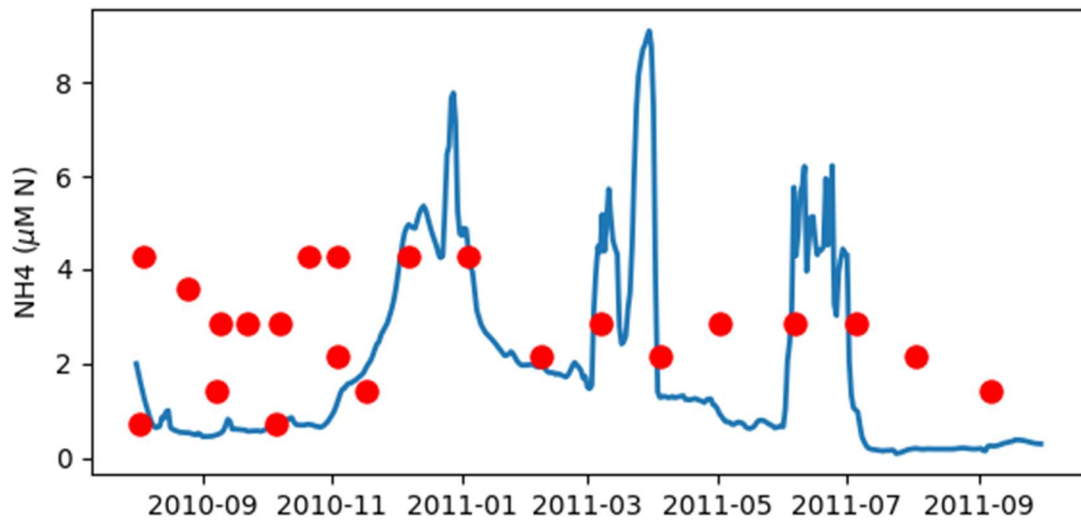
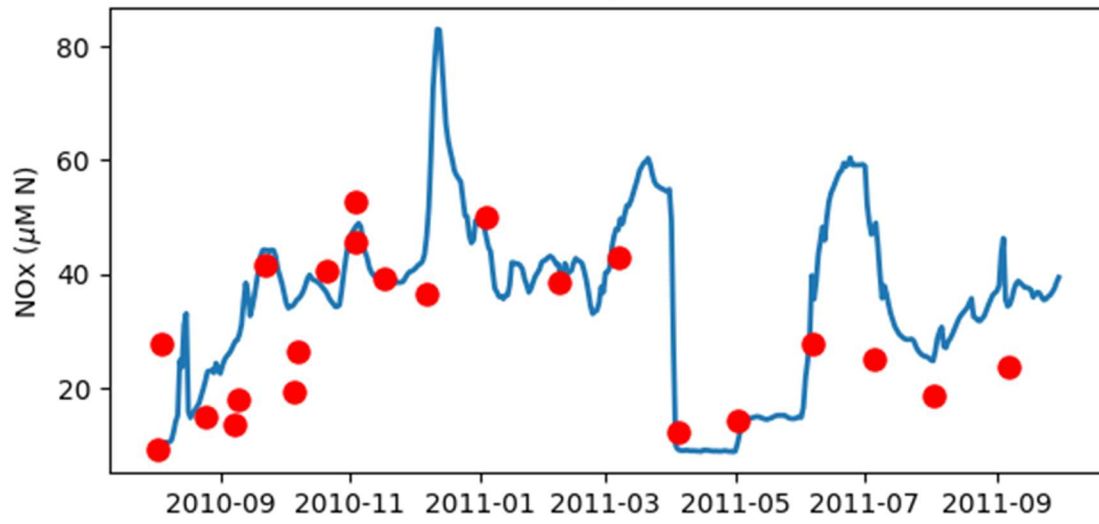


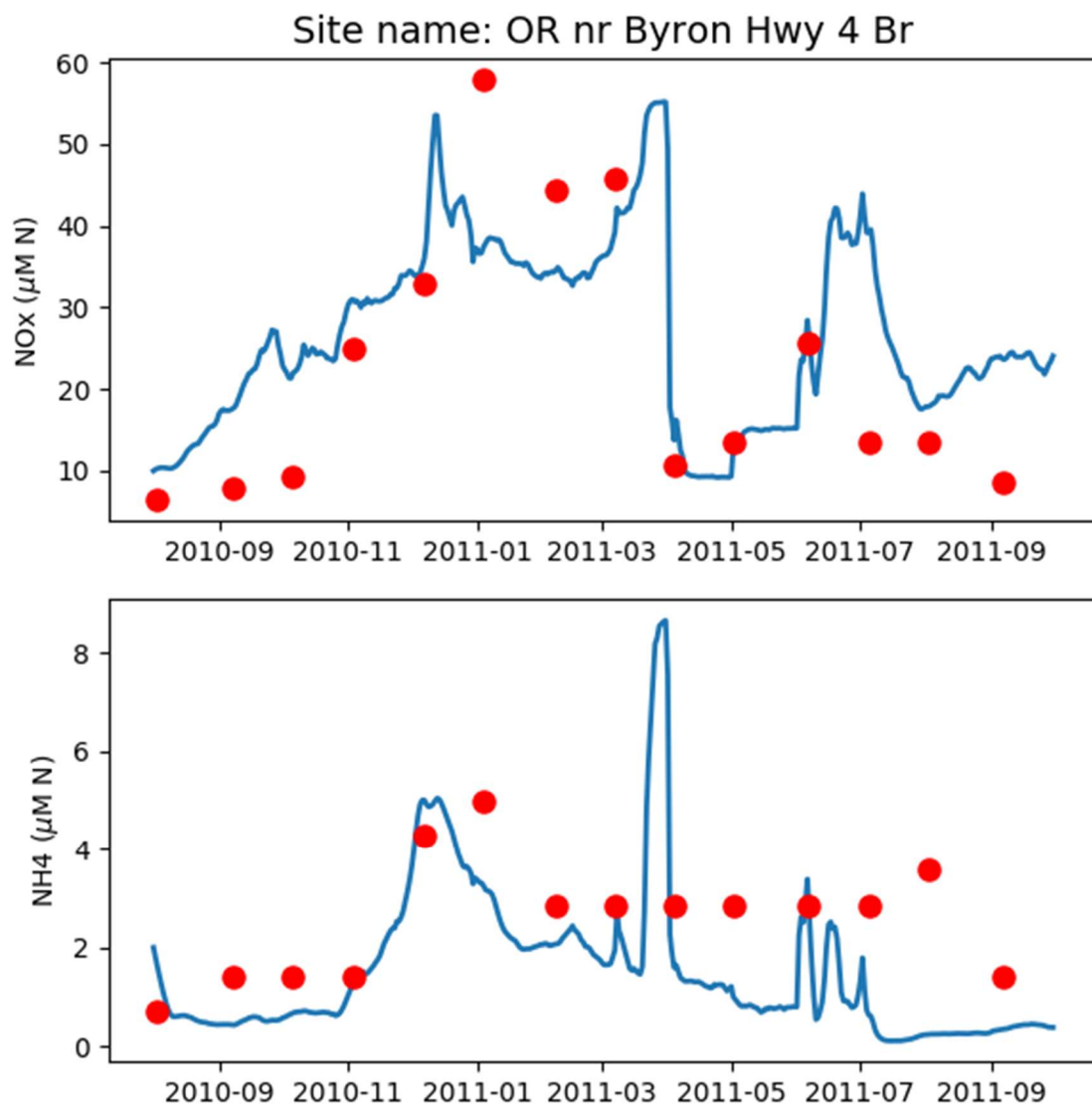




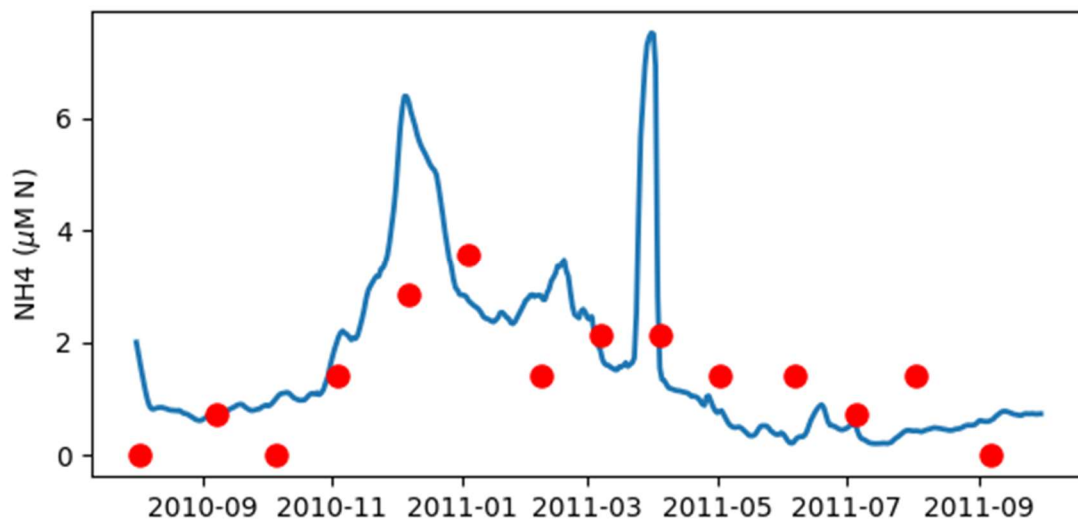
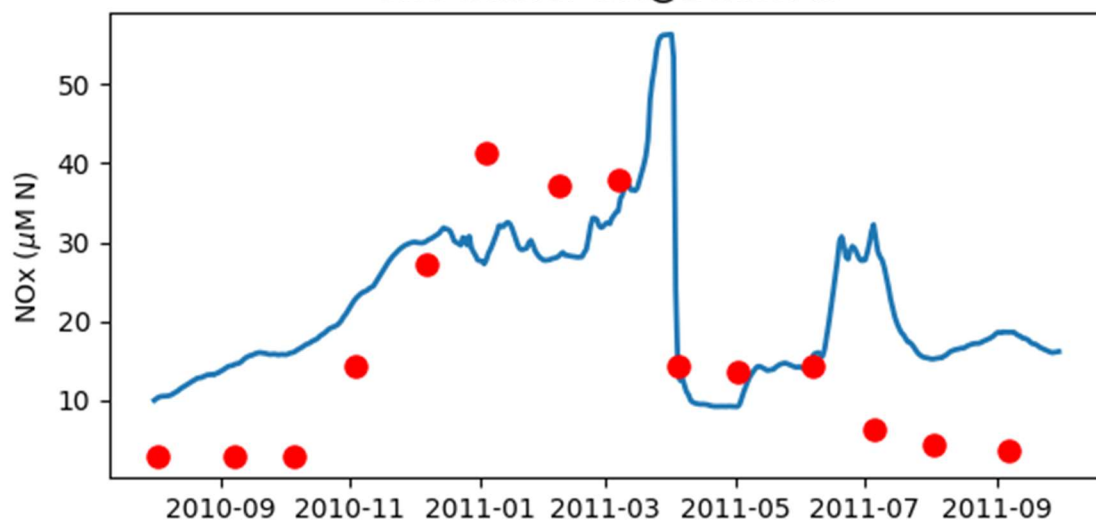


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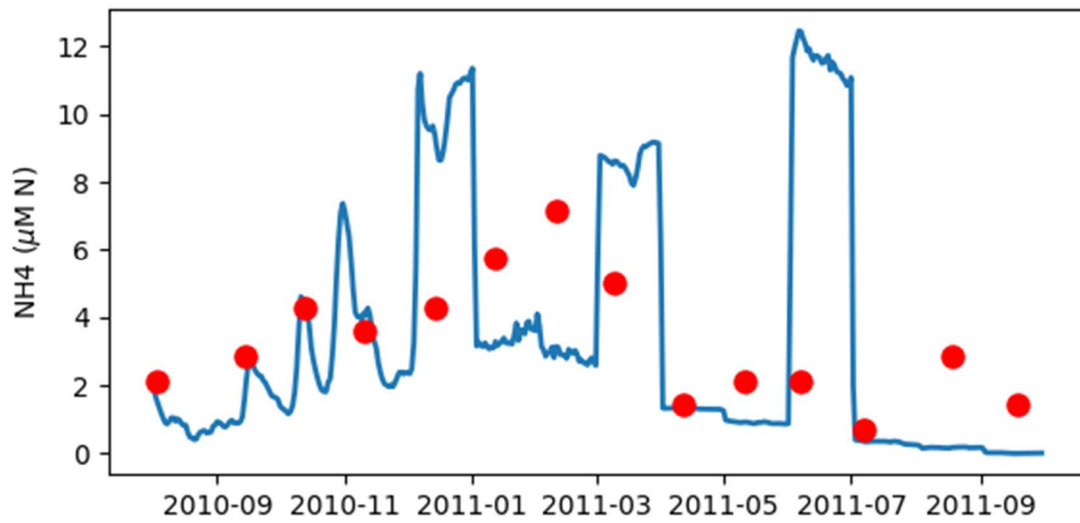
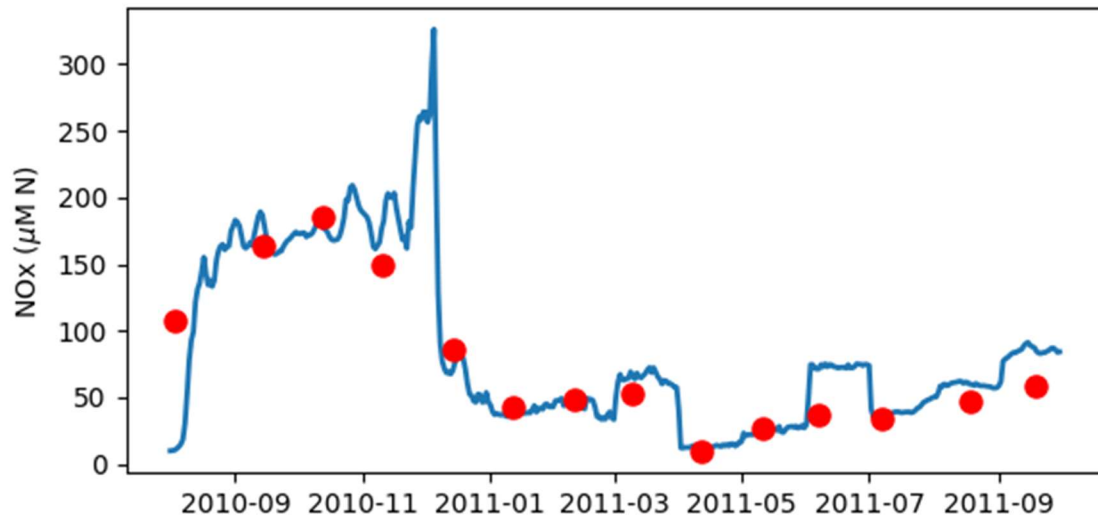




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