

LakeN

Yoav Ben Dor

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Introduction

This model was written as a project for course 68806: Eco-hydrologic modelling with R, Hebrew University of Jerusalem.

The purpose of this model is to illustrate the annual N cycle in a lake in northern Israel, and to simulate the transitions between two dominant N species: Nitrate (NO_3) and Ammonium (NH_4^+)

Key terms

Nitrate



Nitrite



ammonia



ammonium



Hypolimnion

The lower layer of water in a stratified lake, typically cooler than the water above and relatively stagnant. develops anoxic condition due to limited interaction with the atmosphere

Epilimnion

The upper layer of water in a stratified lake, which remains oxygenated throughout the year.

Thermocline

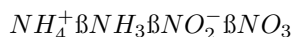
A steep temperature gradient in a body of water such as a lake, marked by a layer above and below which the water is at different temperatures. Because warmer water are less dense, the thermocline dictates the mixing depth of the lake, and therefore directly determine chemical properties of the lake's layers. In the studied lake, the developing thermocline closely coincides with the oxycline and chemocline.

Oxycline

The layer that encompasses a sharp gradient in oxygen concentration in the lake.

Nitrification

Nitrification includes the oxidation of ammonia into nitrite in a two-stage process, initiated by the nitrosomonas bacteria, and followed by the oxidation of nitrite by nitrobacteria. The process can be summarized as:



This process largely depends on oxygen availability, ambient conditions and the size of bacterial populations. The process has been documented to be carried quickly and directly into nitrate in some years, whereas in others the increase in nitrite preceded the transformation into nitrate by several days and up to a couple of weeks.

Nitrification takes place in oxic conditions, and largely depends on the mixing of the water column during the winter. It is halted in the hypolimnion during the well-stratified conditions that develop from spring to autumn, and reignites in winter, when the lake is fully mixed. Nitrification is however still possible in the interface of the hypolimnion with the epilimnion, where dissolved oxygen is present to some extent. Nitrate concentrations are highest at the end of January after a full mixing of the lake is achieved, in addition to riverborn nitrate that originates from fertilization and soils.

Ammonification

Ammonification is the process by which organic biomass nitrogen is recycled after creatures death. Ammonification is carried out by a diverse array of microorganisms that perform ecological decay services, and its product is ammonia or ammonium ion. Ammonium builds up during anoxic conditions that form in the developing hypolimnion between spring and autumn. Ammonium is a suitable source of nutrition for many species of algae, and is therefore readily consumed upon lake mixing and its injection into the photic zone during winter.

Background

Anthropogenic effects during recent years had largely affected the nitrogen cycle in the lake during the last decades. Increased N inputs, primarily as river-born nitrate, originating in soils and fertilization, strengthen eutrophication, anoxic conditions and blooms of harmful algae, thus interrupting the ecological cycle.

The nitrogen cycle includes several key processes, which include the cycling between several species which dictate its bioavailability and importance in biogeochemical processes. Rivers are efficient N sinks, but in its inorganic forms, it is removed from the water through assimilation and adsorption onto sediments.

In the studied lake, an N-fixing algae of the cyanobacteria phylum appeared for the first time during the autumn of 1994. It reappears every year since that time, and was recently accompanied by another cyanobacteria species since 2005. This dramatic change in lake ecology is the likely result of changes in the availability of water-soluble nutrients, which provided the N-fixing species with a relative ecological advantage.

It is important to remember that the measurement process provides a “snapshot” of lake conditions in a specific time, and that all cooccurring processes form interchanging fluxes of nitrogen between the various nitrogen pools. While the modelling of the molecular process is difficult to configure, because it involves complex biological processes, the net transformation of species between pools can be modelled through a “net-gross” approach, where molecular transformations are summed into simplistic, time-dependent processes, that are arithmetically disconnected. If each of these processes can be adequately modelled following simplistic

time-dependant equations, the N cycle can be modelled in terms of net fluxes, without taking into account all possible processes and their complexities.

The N cycle

Several key process dominate the N cycle of the studied lake. These include nitrification, denitrification, the fixation of atmospheric nitrogen by cyanobacteria and N recycling through consumption of primary producer up the food chain. Nitrate and ammonium are constantly consumed by primary producers that are consequently consumed by grazers. The following ecological food chain serves as an endless conveyor that recycles nitrogen through the lake.

These processes are inherently biologically mediated, and their relative role in the transformation of one specie to another greatly depends on ambient conditions such as radiation and temperature, as well as other chemical properties, and oxygen content in particular, which are largely dependent on its limnological cycle. The consideration of these parameters in a limnological perspective is essential for the consideration of the dominant processes and their ecological impact.

References

Nitrogen Cycle - Ammonification And Nitrification - Ammonium, Bacteria, Nitrate, and Acidic - JRank Articles
<http://science.jrank.org/pages/4690/Nitrogen-Cycle-Ammonification-nitrification.html#ixzz4U1Rm3S3A>

About thist model

In this model I examine the possibility to model the transition between oxydized and reduced species in the lake using a very simplistic approach. Due to the complexity of the processes, and the plethora of available data, the simplistic approach in this model relies on four key processes to model the nitrate-ammonium transitions:

1. Nitrate buildup during lake stratification in the epilimnion
2. Ammonification buildup during lake stratification in the hypolimnion
3. Lake mixing
4. Nitrate consumption following lake mixing
5. Ammonium consumption following lake mixing

This model provides the opportunity to examine whether these processes suffice to model the dominant segments of the N cycle, or should a more complex, biologically-oriented approach be adopted to configure the N cycle properly.

Due to the time consuming nature of this process and the difficulties to model several coupled processes, only NH_4 is modelled here

Data preparation

The data is provided in discrete form of concentration measurements. The depths of the measurements are not constant, and the time intervals between measurements are also not constant, and range from several days to several weeks.

| ## | Date | Depth | NH4 | Nitrit |
|----|----------------|---------------|----------------|-----------------|
| ## | 2012-06-03: 13 | Min. : 1.00 | Min. :0.0030 | Min. :0.00200 |
| ## | 2012-06-24: 13 | 1st Qu.: 5.00 | 1st Qu.:0.0210 | 1st Qu.:0.00200 |

```

## 2012-07-08: 13 Median :16.00 Median :0.0850 Median :0.00300
## 2012-09-23: 13 Mean :16.91 Mean :0.2125 Mean :0.01409
## 2013-06-02: 13 3rd Qu.:25.00 3rd Qu.:0.2447 3rd Qu.:0.01400
## 2013-06-23: 13 Max. :40.00 Max. :2.5400 Max. :0.27300
## (Other) :1565 NA's :1 NA's :1
## Nitrate Norg_par Norg_dis Ntot
## Min. :0.0000 Min. :0.00000 Min. :0.0000 Min. :0.1100
## 1st Qu.:0.0140 1st Qu.:0.02000 1st Qu.:0.1230 1st Qu.:0.3800
## Median :0.0660 Median :0.06000 Median :0.1695 Median :0.5500
## Mean :0.1435 Mean :0.08667 Mean :0.1739 Mean :0.5979
## 3rd Qu.:0.2395 3rd Qu.:0.11000 3rd Qu.:0.2190 3rd Qu.:0.7200
## Max. :0.6200 Max. :1.74000 Max. :0.9300 Max. :2.9700
## NA's :360 NA's :11 NA's :11 NA's :1
## Oxygen
## Min. : 0.000
## 1st Qu.: 0.700
## Median : 6.300
## Mean : 5.087
## 3rd Qu.: 7.700
## Max. :17.800
## NA's :29

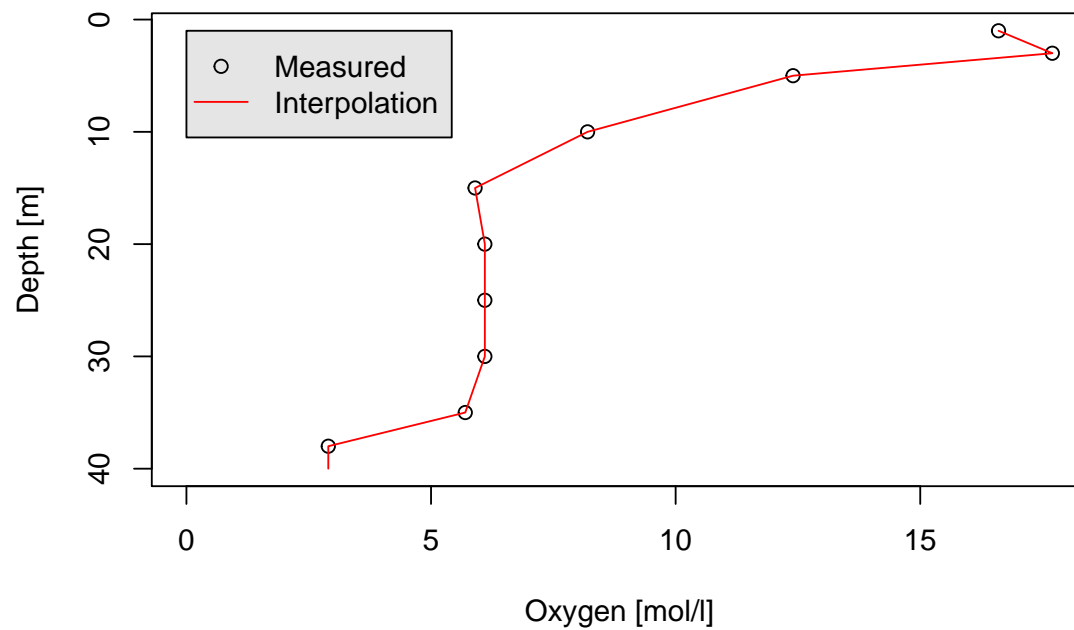
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Data interpolation into 1 m Intervals

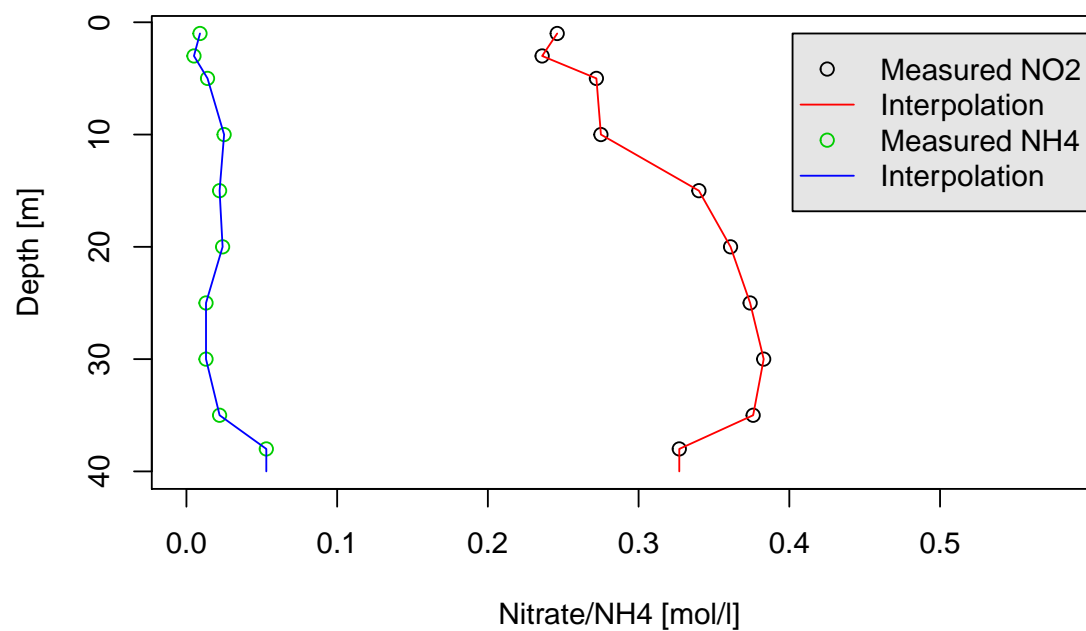
Use the function “depthinterp” to interpolate the data into uniform length for every 1 m. This is essential for later calculating the volume of each depth interval and the mass of each N specie measured in this depth.

Demonstrate interpolations of randomly selected data

Oxygen interpolation 2012-04-15



N species interpolation 2012-04-15

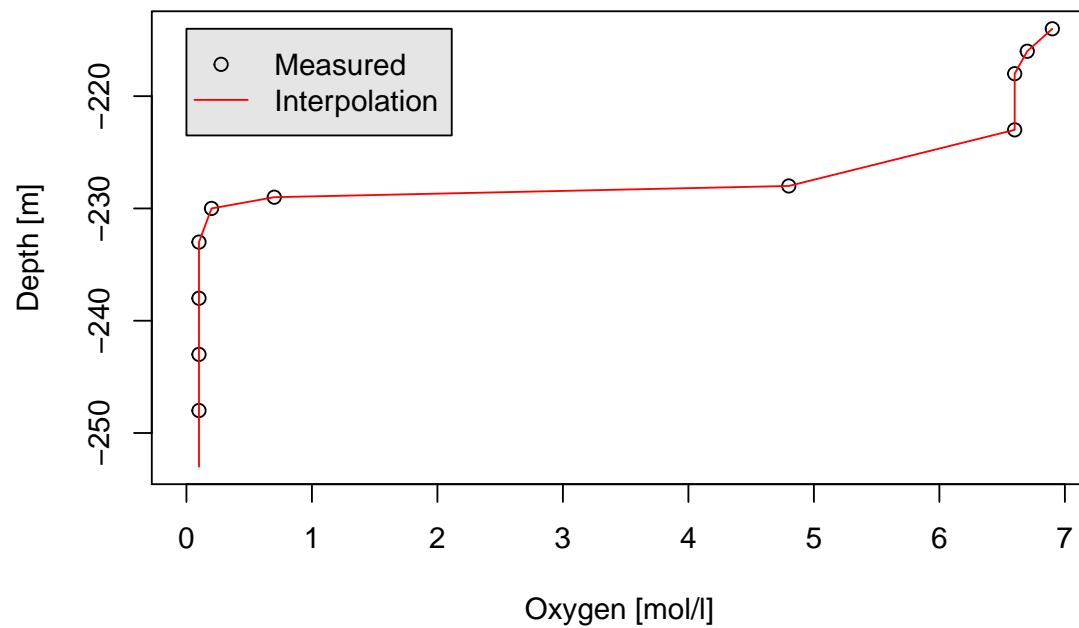


Depth-Level Corrections

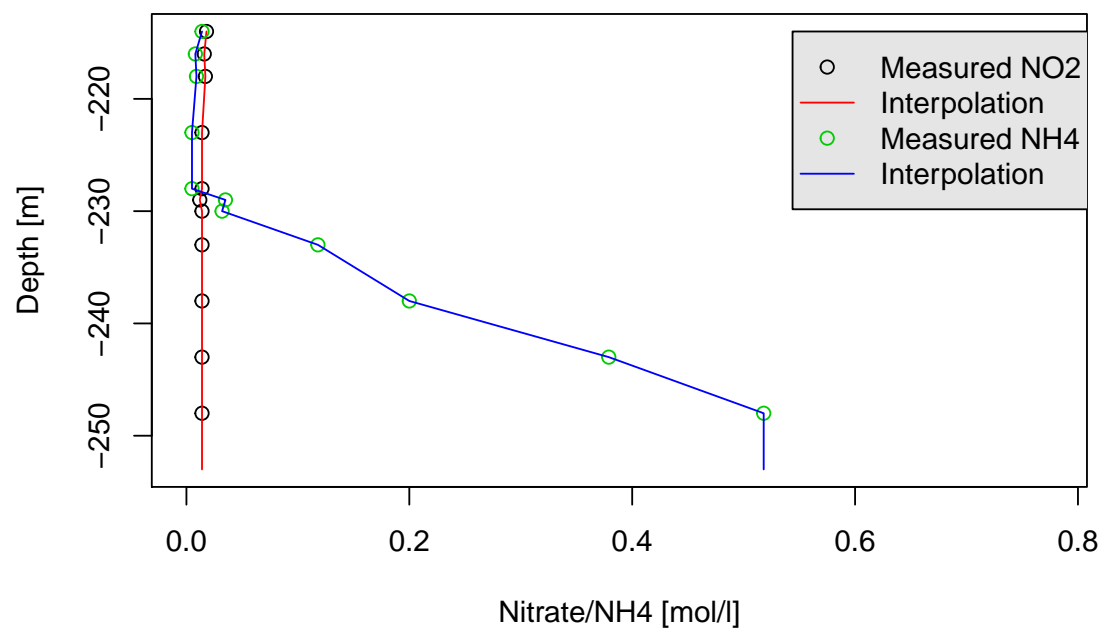
Calculate the appropriate depth for each measurement using available daily level measurements. Use function “realdepth” and use closest day if no level measurement of that day is available. This correction is essential for later calculation of depth to volume and concentration quantification of N species in the lake.

Demonstrate the results of randomly selected data according to the new depth scale

Oxygen interpolation 2010-08-29

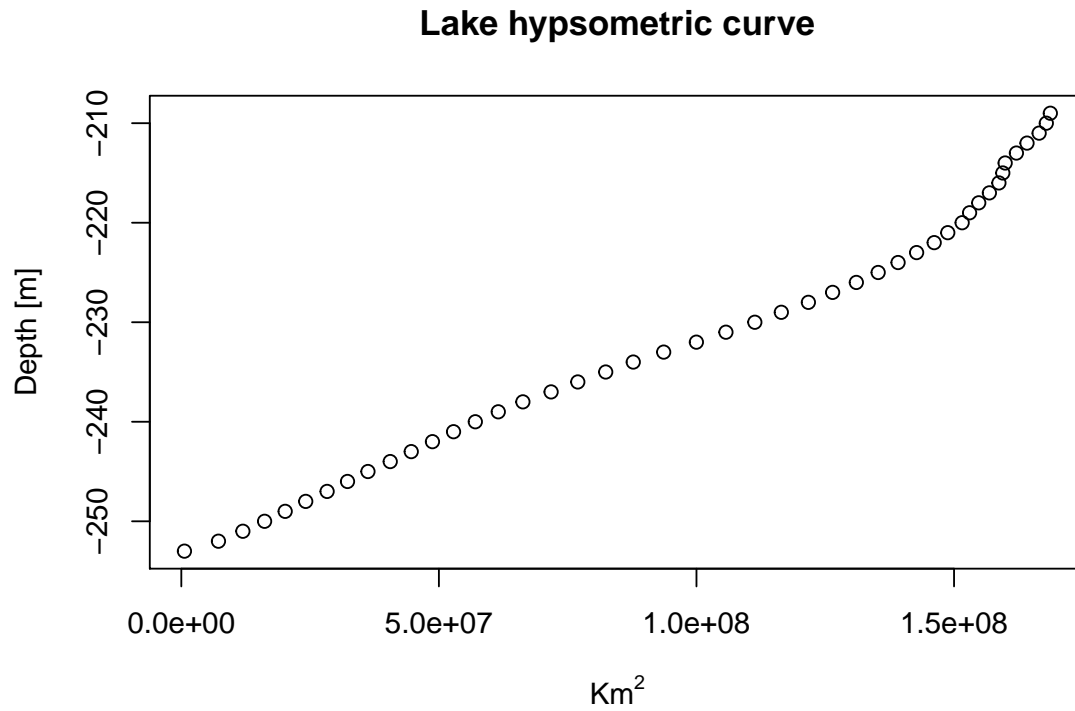


N species interpolation 2010-08-29



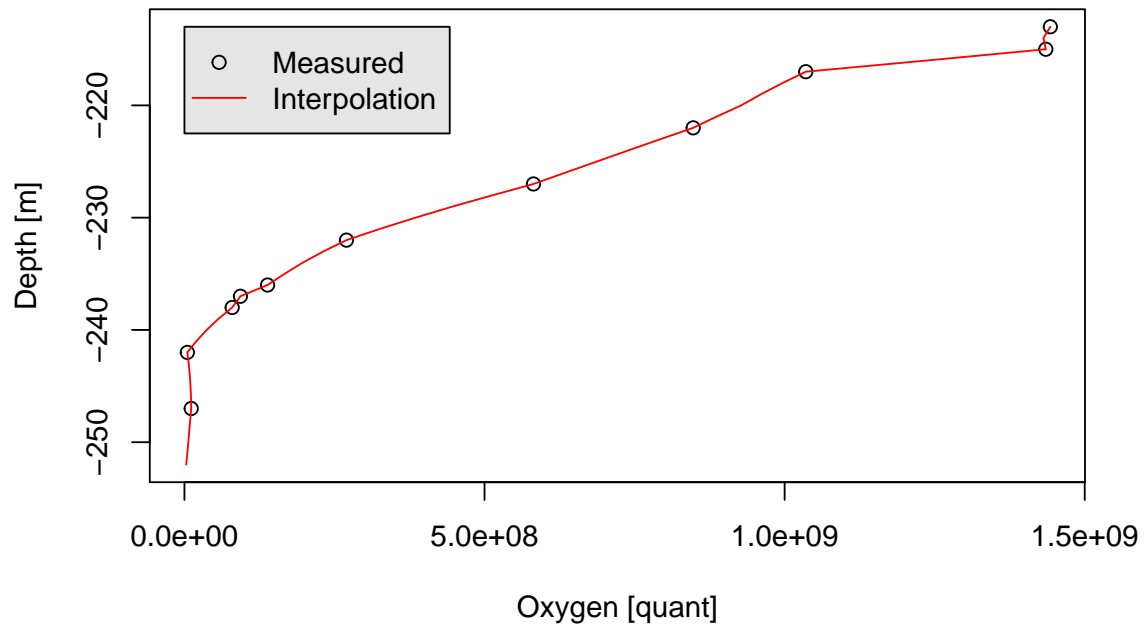
Quantification using lake hypsometric curve

The use of concentrations has limitations because it may enhance or demise processes that is inherently “mass-based”, and therefore limit our understanding of the process. In this section the data is quantified, and concentrations are transformed into amounts via multiplication of each concentration with its corresponding hypsometric curve value using function “conctoquant”.

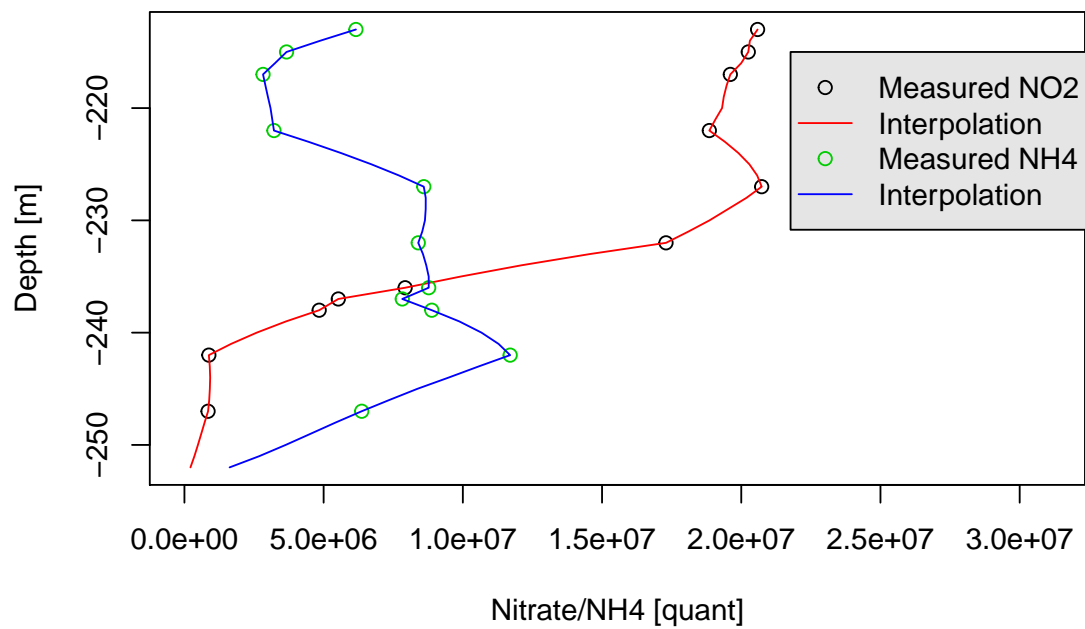


Demonstrate the results according to the new depth scale of randomly selected data

Oxygen interpolation 2011-06-12



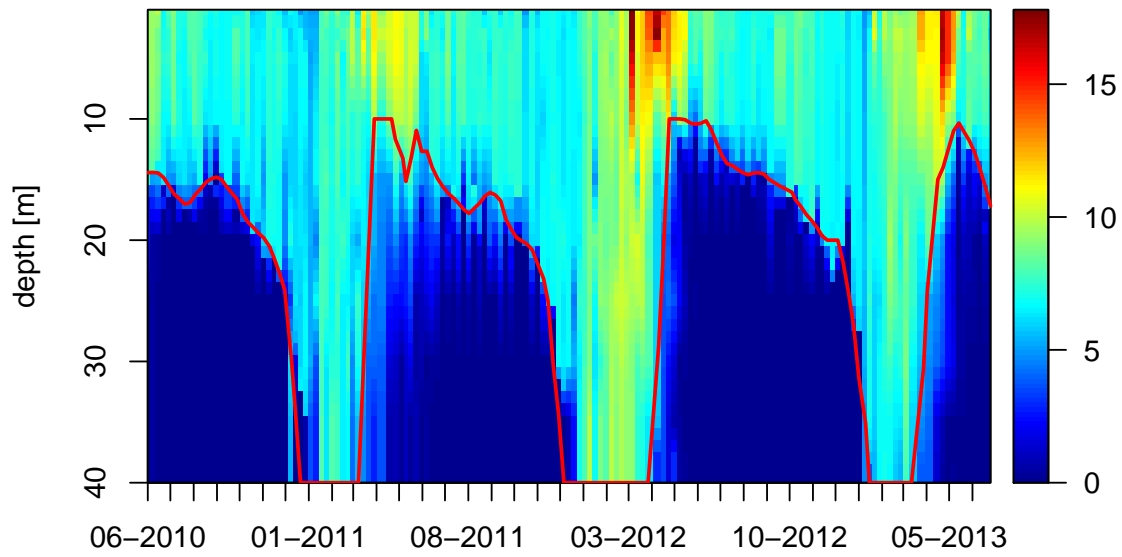
N species interpolation 2011-06-12



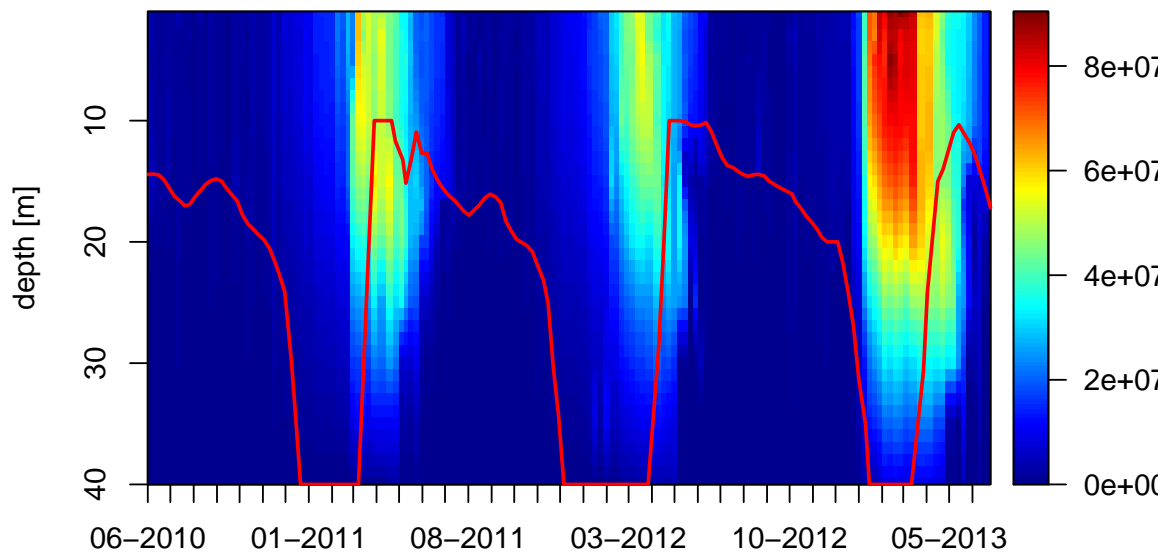
Time series plots

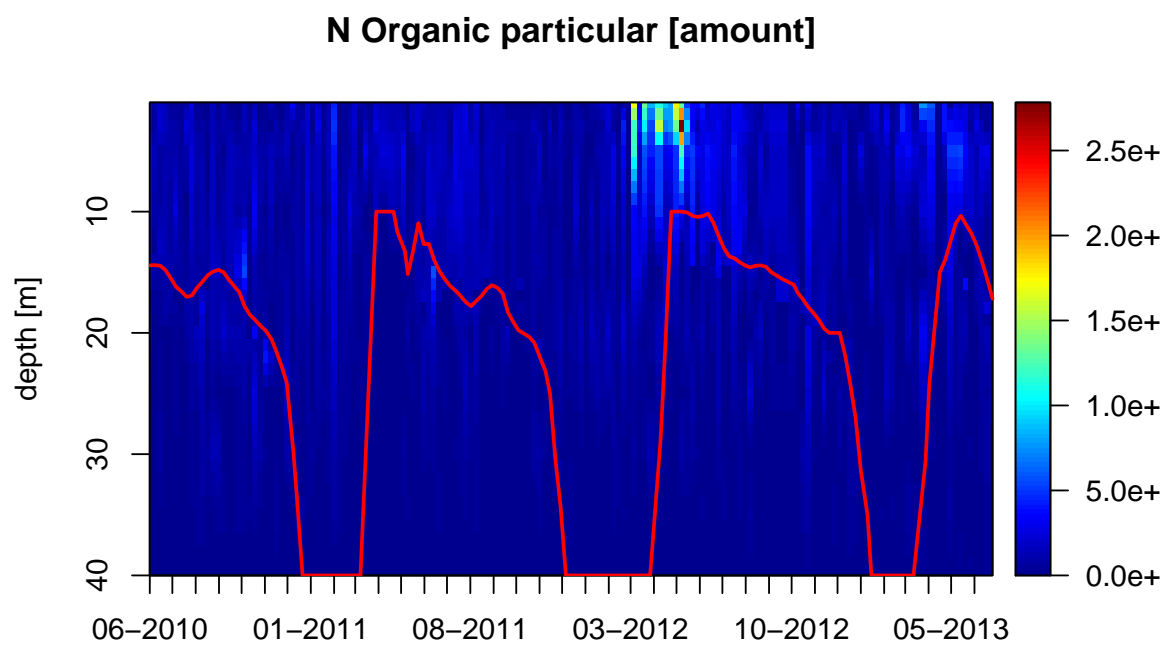
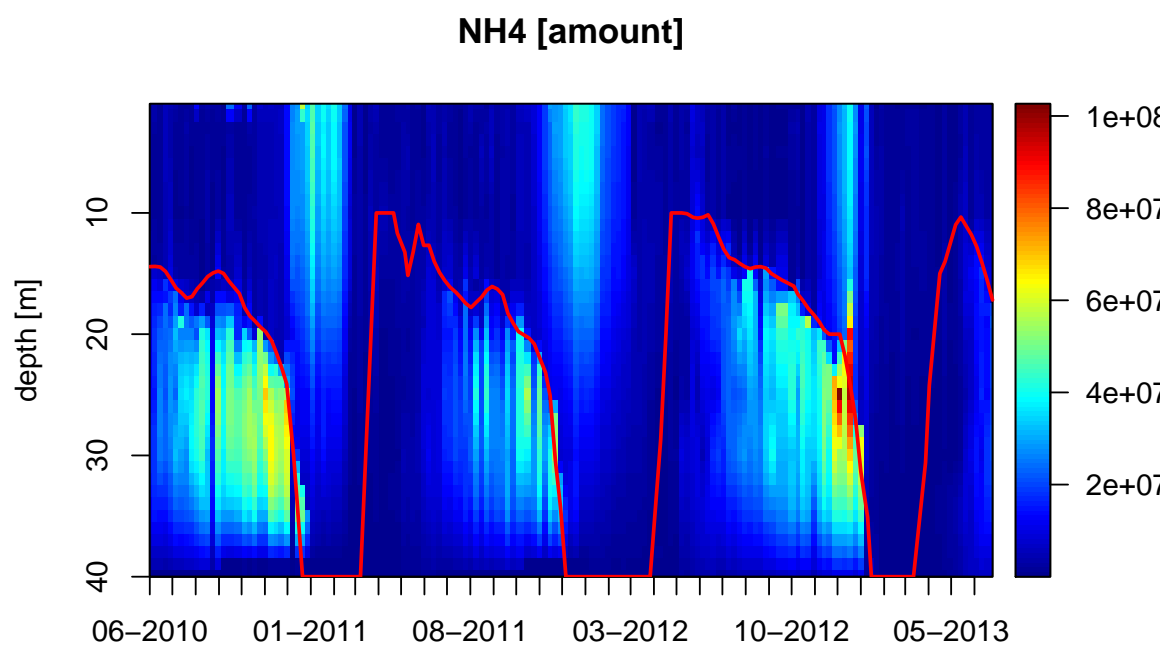
The following plots provide some visual estimation of the data to visualize time-depth processes for further considerations for the modelling of the processes. The depth of the Oxycline is inferred by looking for the steepest part of oxygen concentrations as well as the differences between the epilimnion and the hypolimnion, and is marked by a red line, this will be used to define the dominant process in each of the lake's parts according to its oxygen concentrations

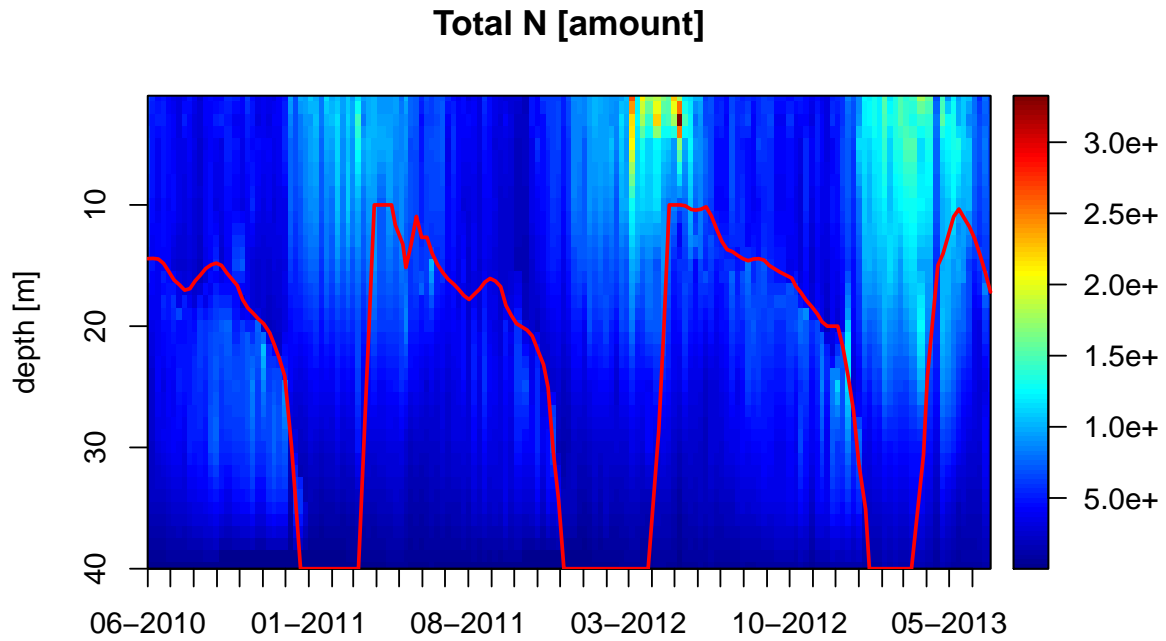
Oxygen [concentration] and Oxycline



Nitrate [amount]

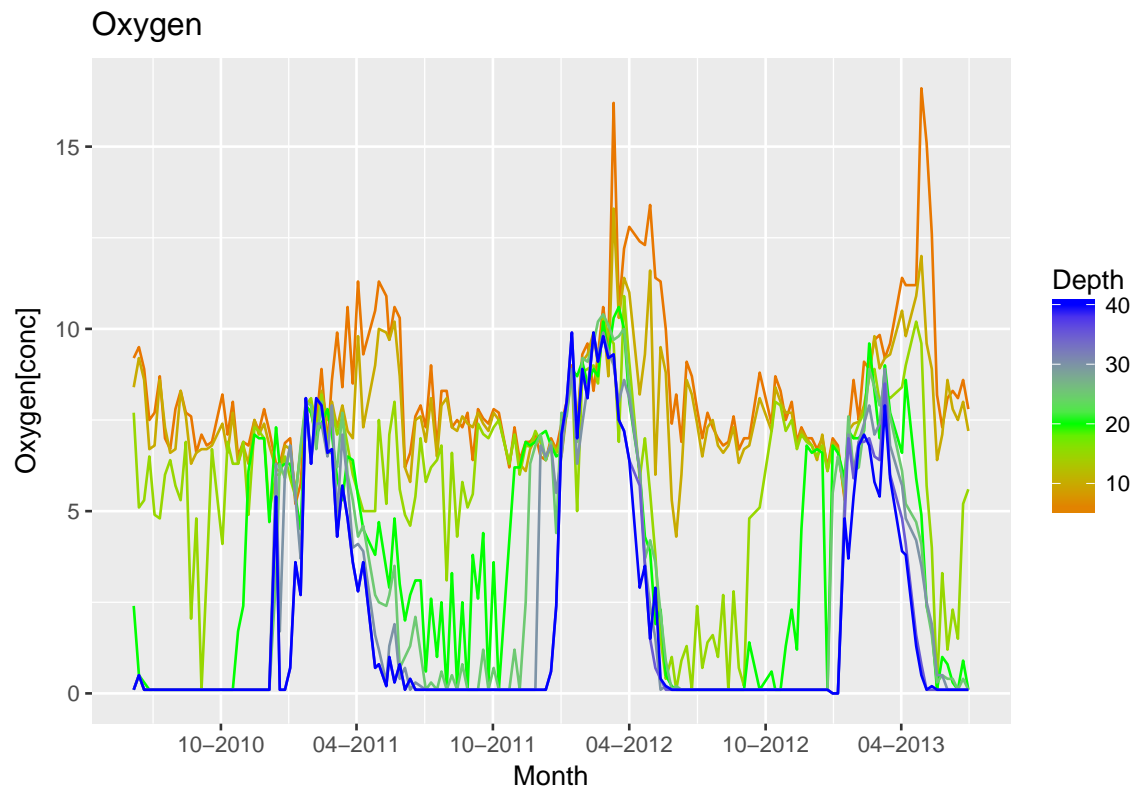
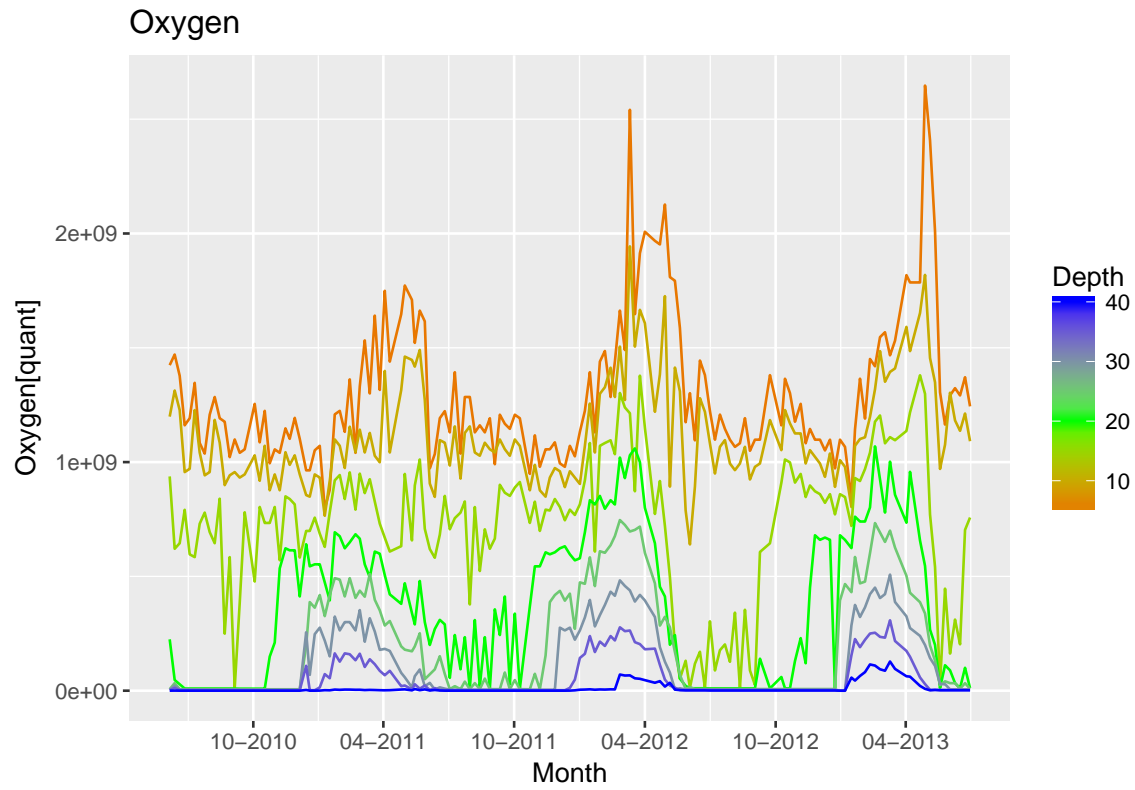


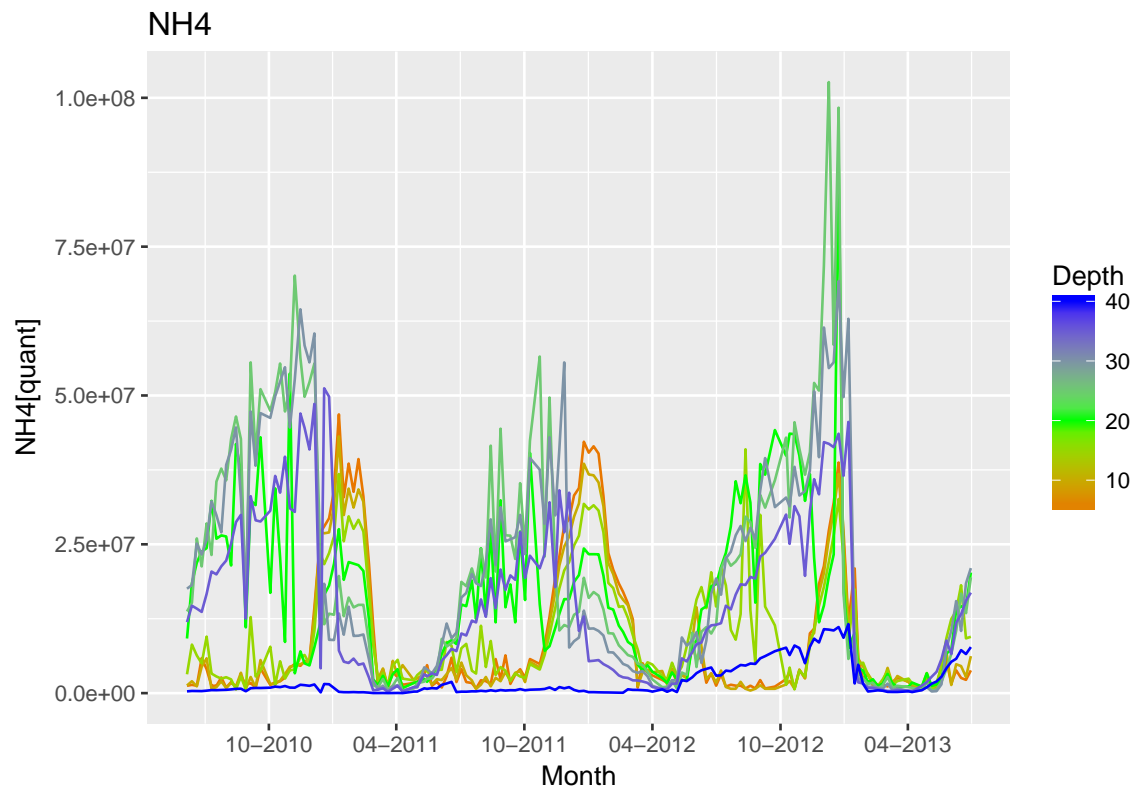
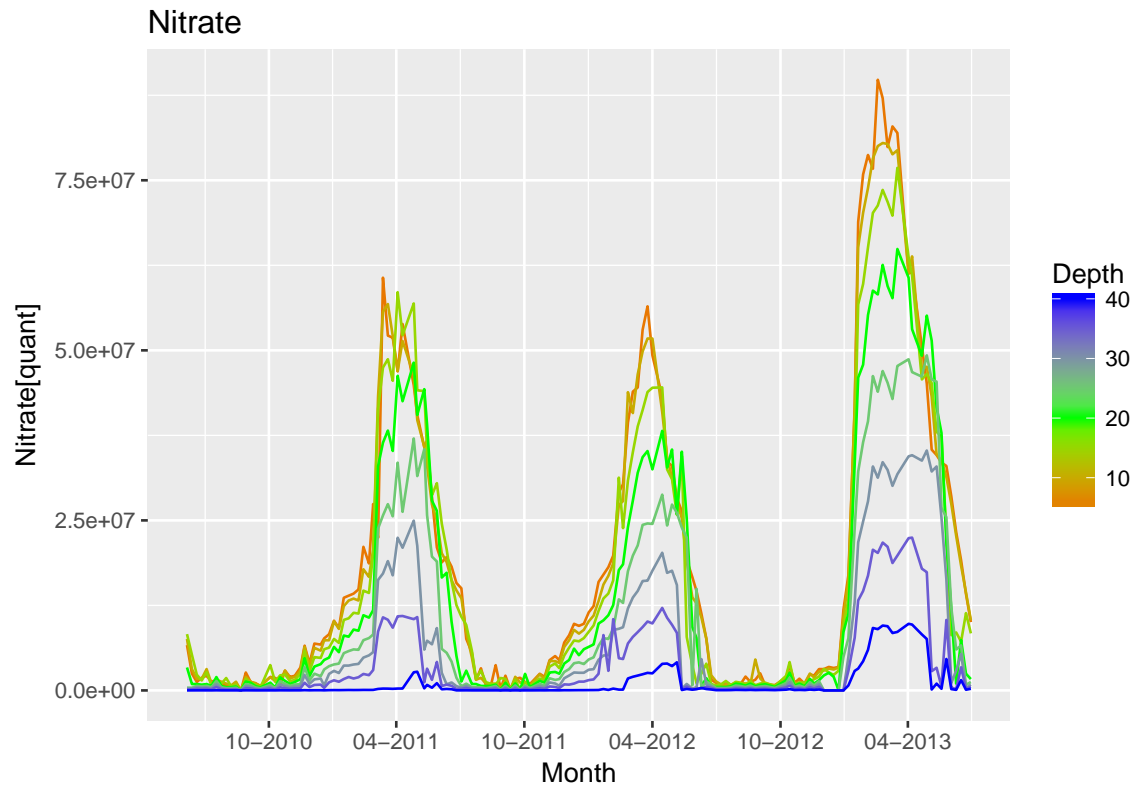




Time-depth cross sections

The following plots provide some basic illustration of the dominant processes in the lake. It can be observed that the concentrations of N species are dictated by mixing and stratification. The consumption and development of each species can be broken into several phases within the time domain. In other words, the processes can be broken down into phases of development, mixing and consumption of the elements.

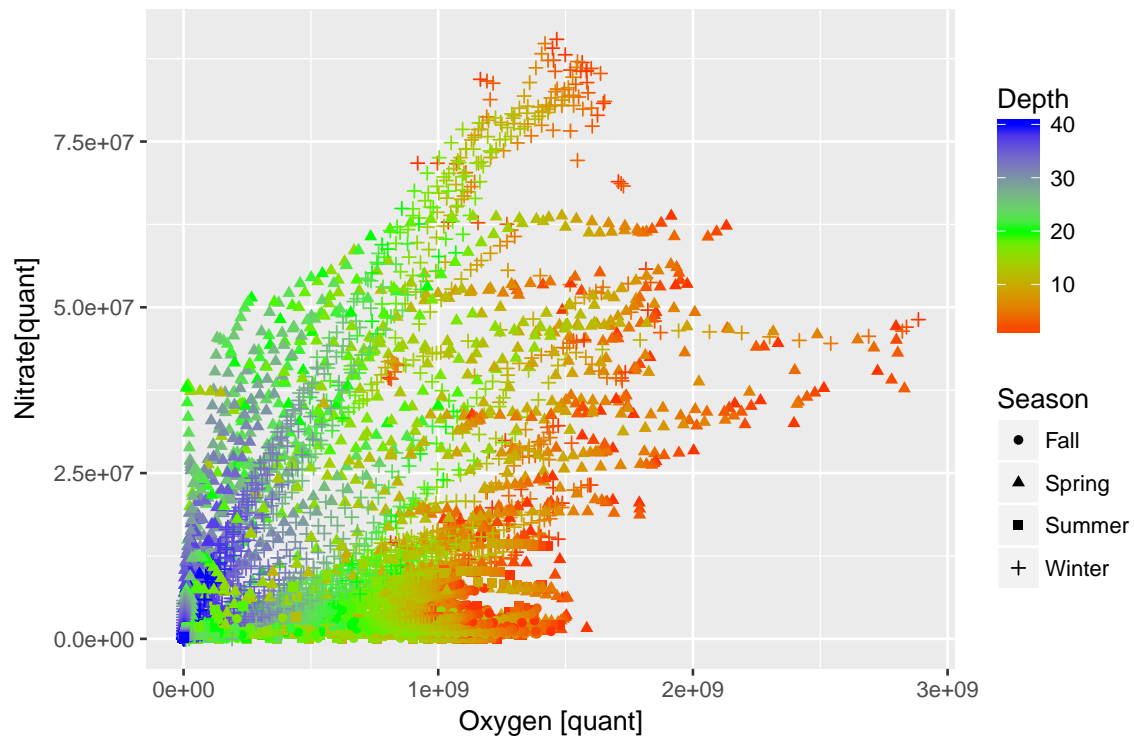




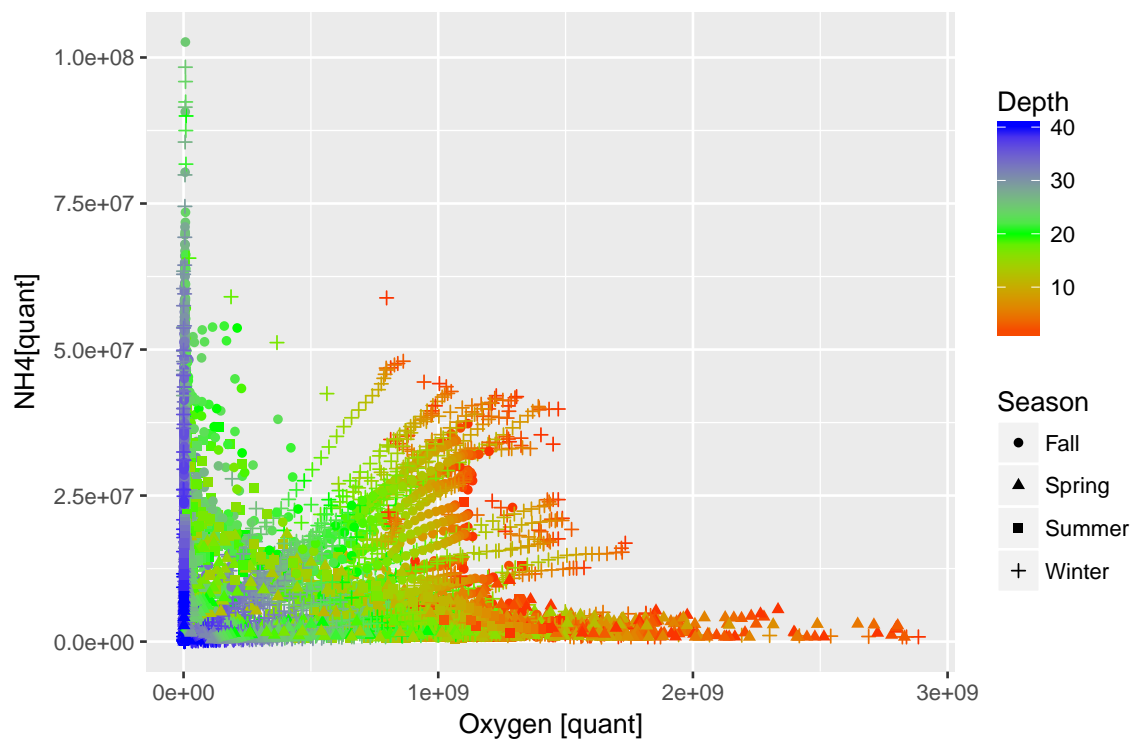
Correlation plots

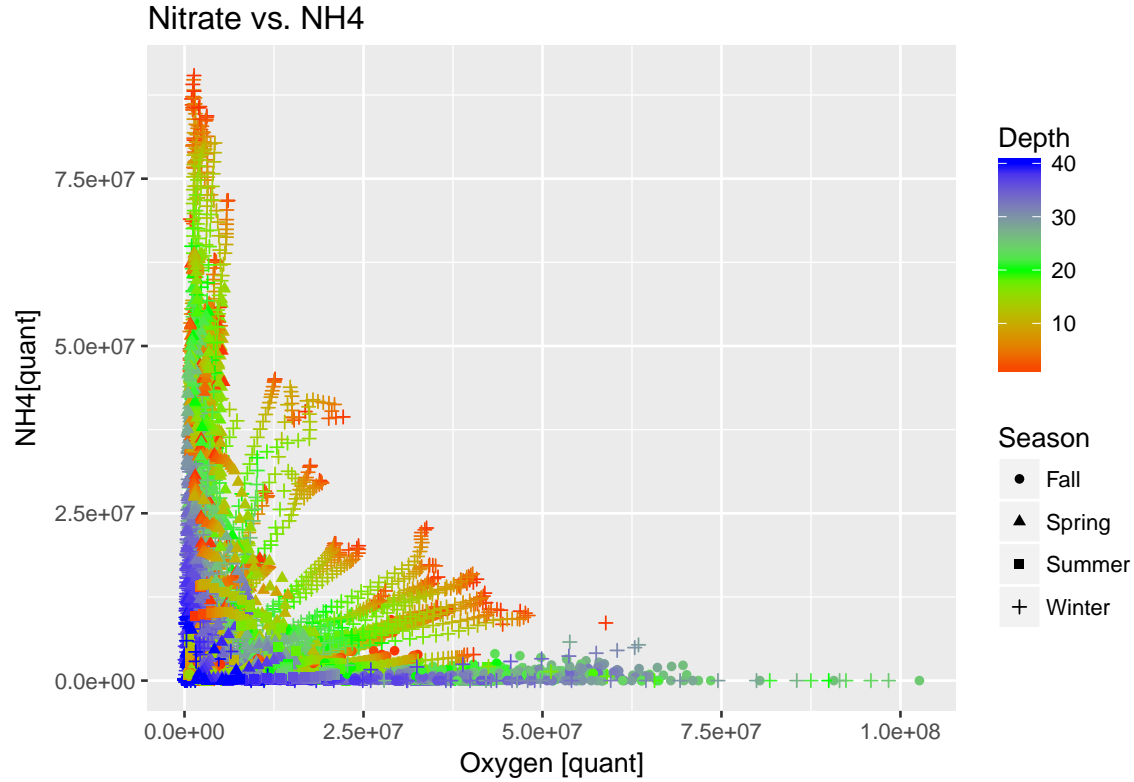
The following plots provide some visual estimation of data correlation and their significance. It can be observed that the dominant effect of oxygen concentration, which dictates the buildup of NH_4^+ and NO_3 . The additional process that dictates their distribution is the physical mixing of the lake, which follows an empirically fitted quadratic distribution in this model

Nitrate vs. Oxygen



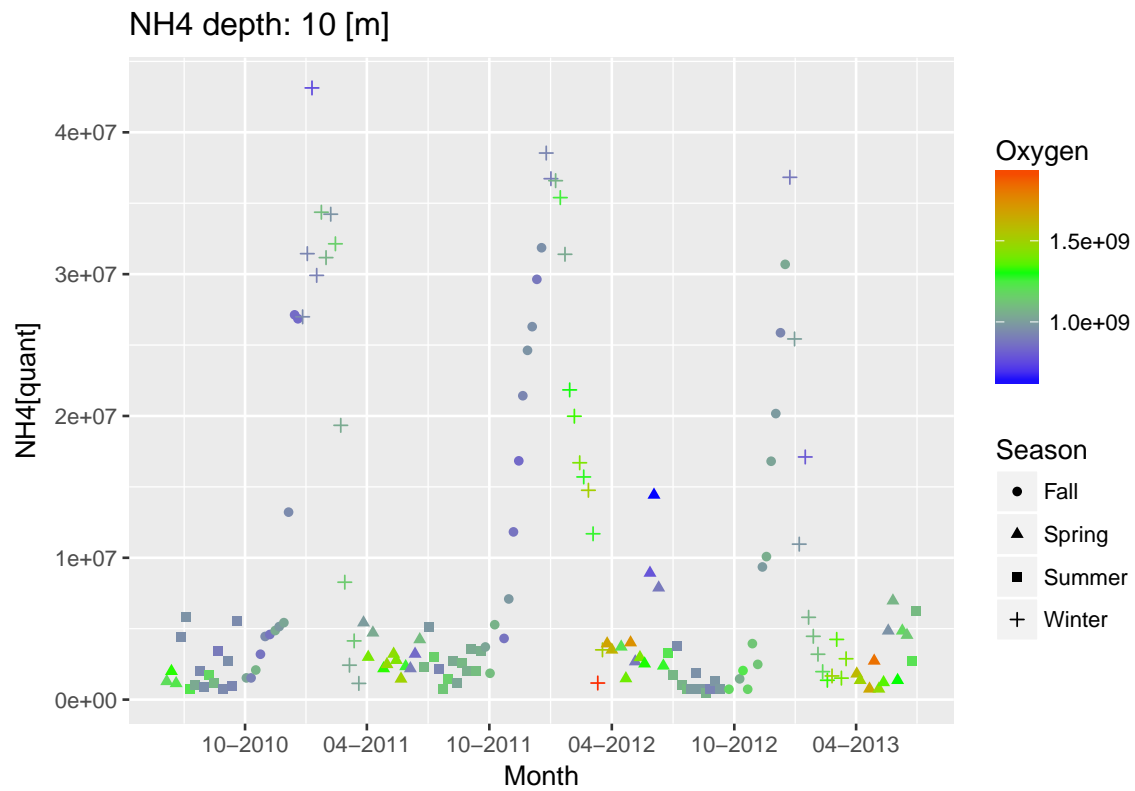
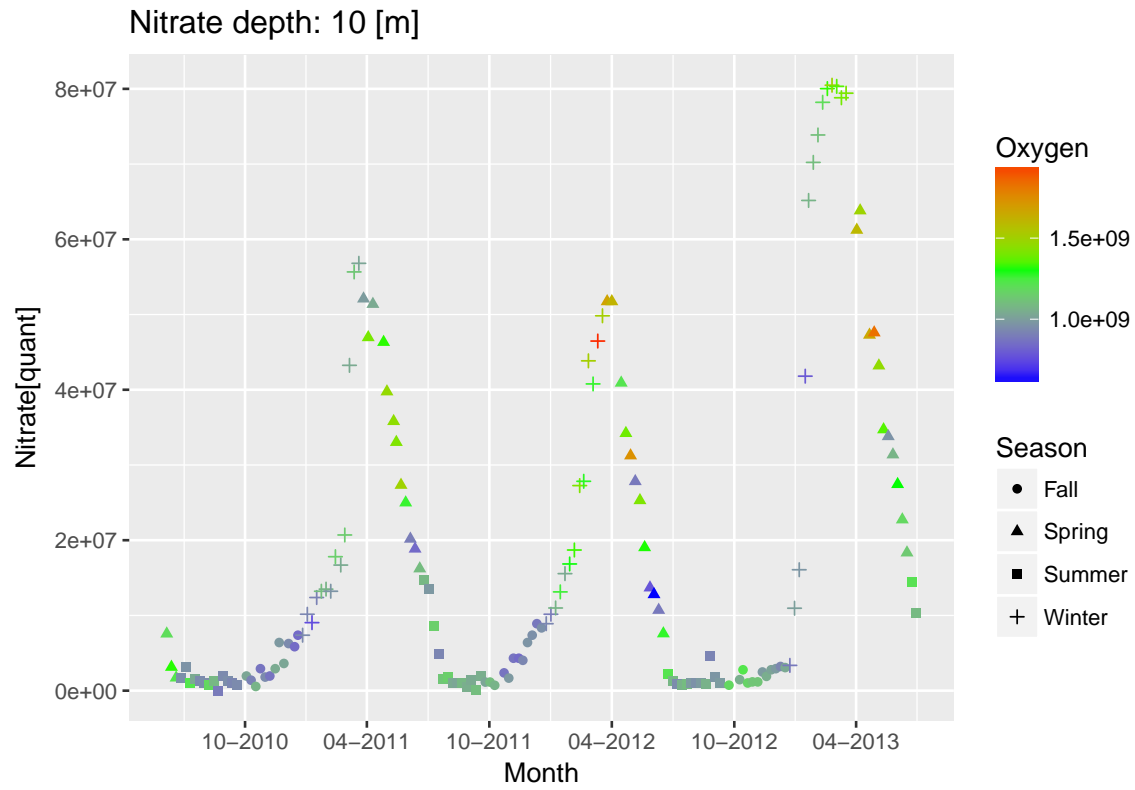
NH4 vs. Oxygen

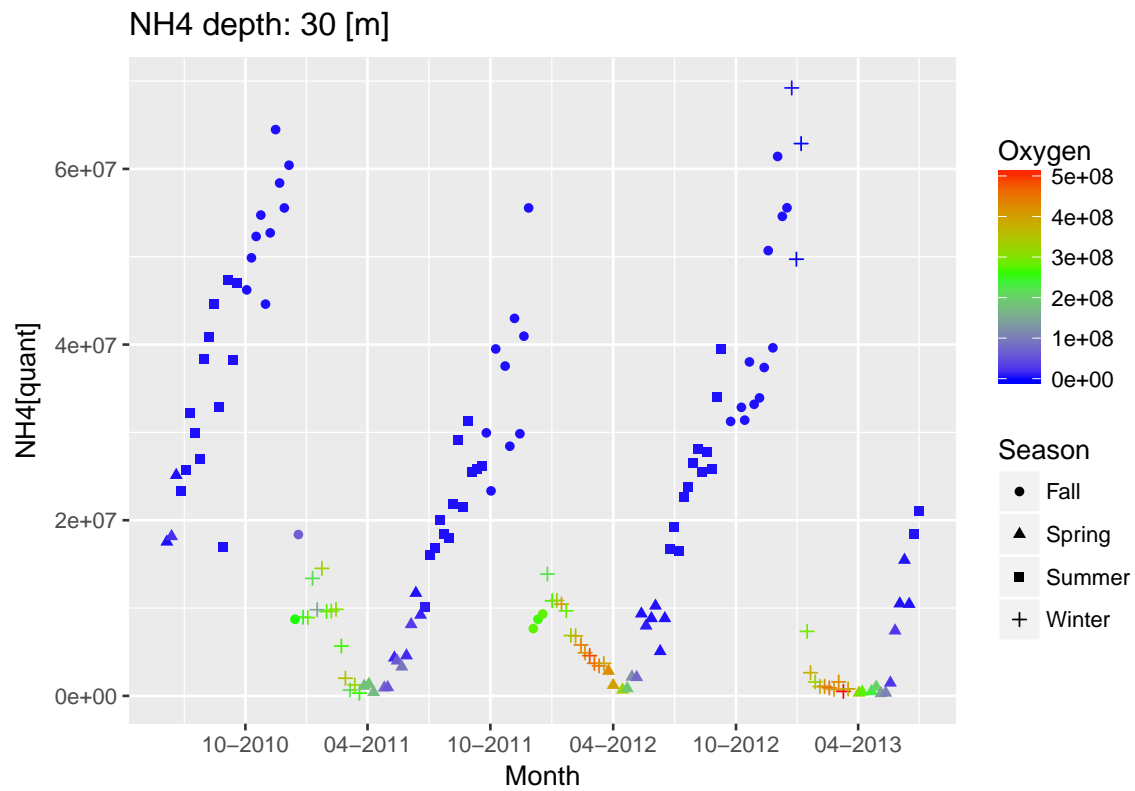
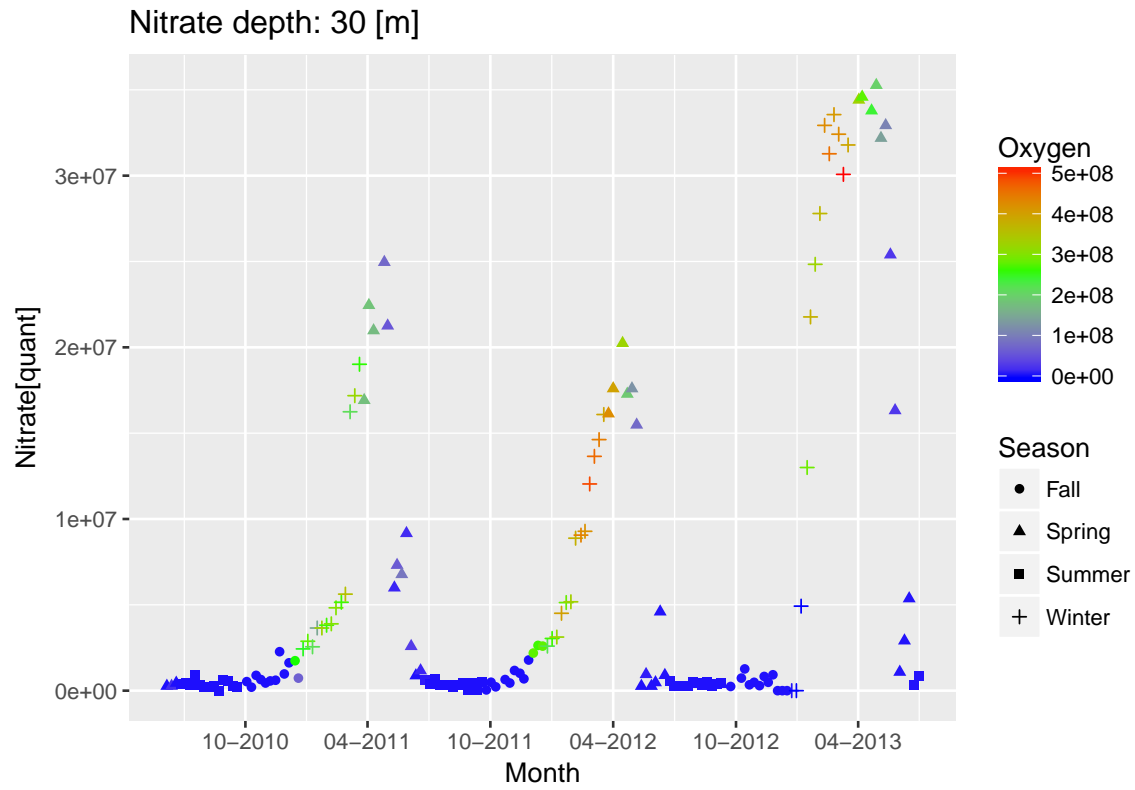




Model fitting estimation

Nitrification and denitrification are two opposing processes that take place in the presence or absence of oxygen. They therefore develop in the upper (nitrification) and lower (denitrification) parts of the lake during episodes of a stratified water column. The model therefore relies on the assumption that their development depends on the presence of oxygen and the time available for their accumulation. Lake mixing, which takes place during winter, disrupts their buildup, and uniformly distributes them across the lake, and mixing propagates towards the lake bottom. These two processes (stratification and mixing) can be examined in detail in two representative depths of 10m (nitrification) and 30m (denitrification). In the following section each of the processes is assumed to follow a linear fit. This assumption is tested via model fitting estimation described in the following section

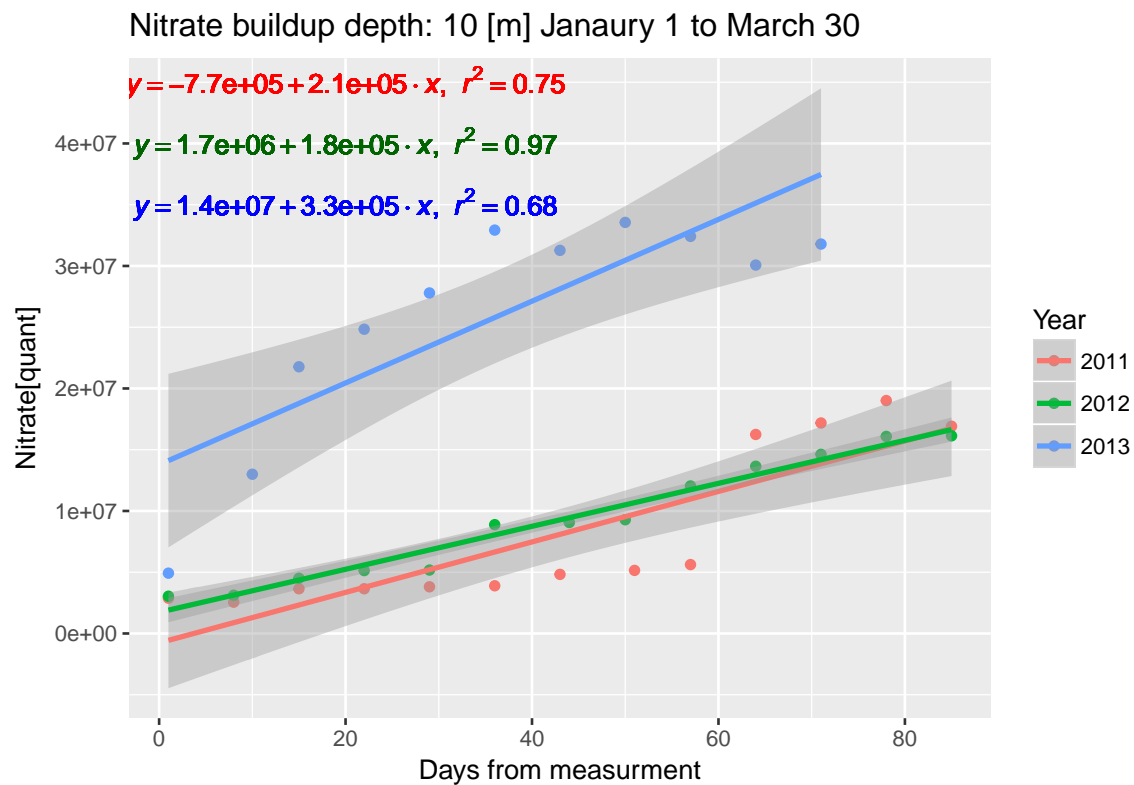




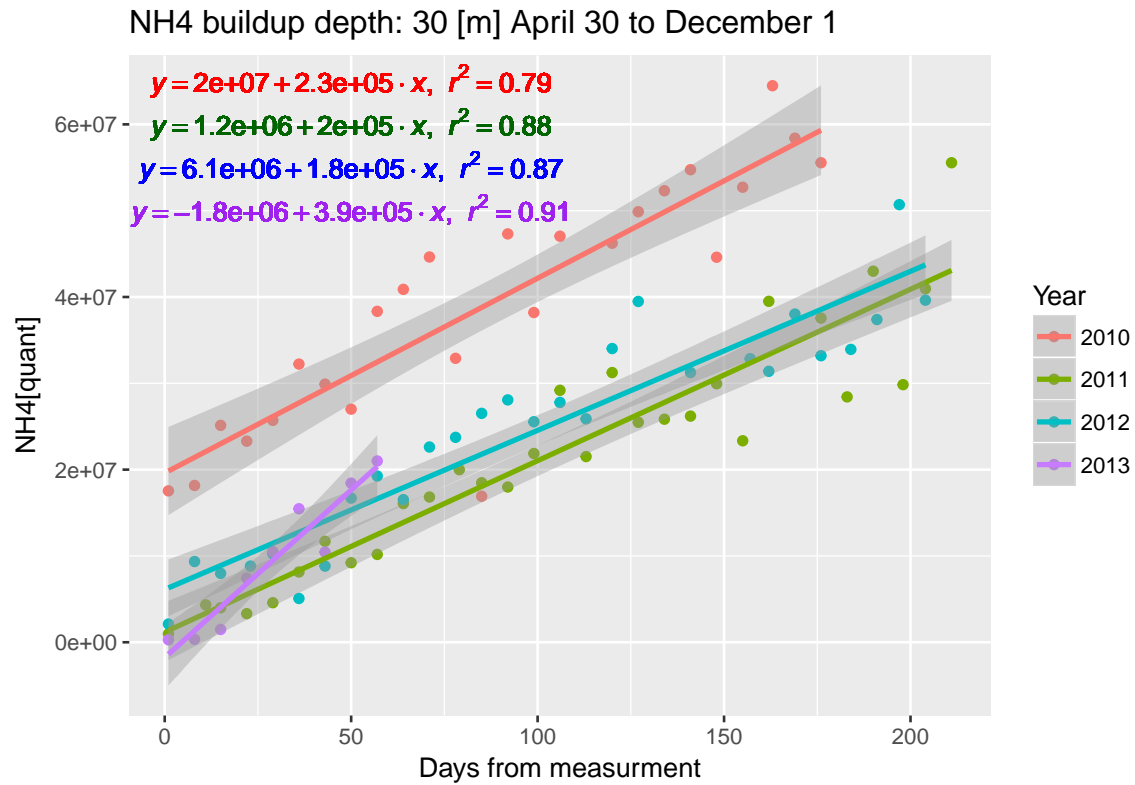
Process rate estimation

It can be observed from the figures presented above that nitrification is dominant in the upper portions of the lake (depicted for 10m depth), primarily between January and April. From April through August nitrate is consumed by primary producers. Ammonium, develops during the stratified lake conditions in its hypolimnion (depicted for depth 30 m), and peaks at during December, right before the mixing of the lake when the deeper lake is oxygenated once more. The ammonium is readily consumed by the producers in the epilimnion after its mixing. In the following section the time-dependent development of each of the processes is estimated in order to decide whether a linear fit is suited to simulate each of the buildup and consumption processes.

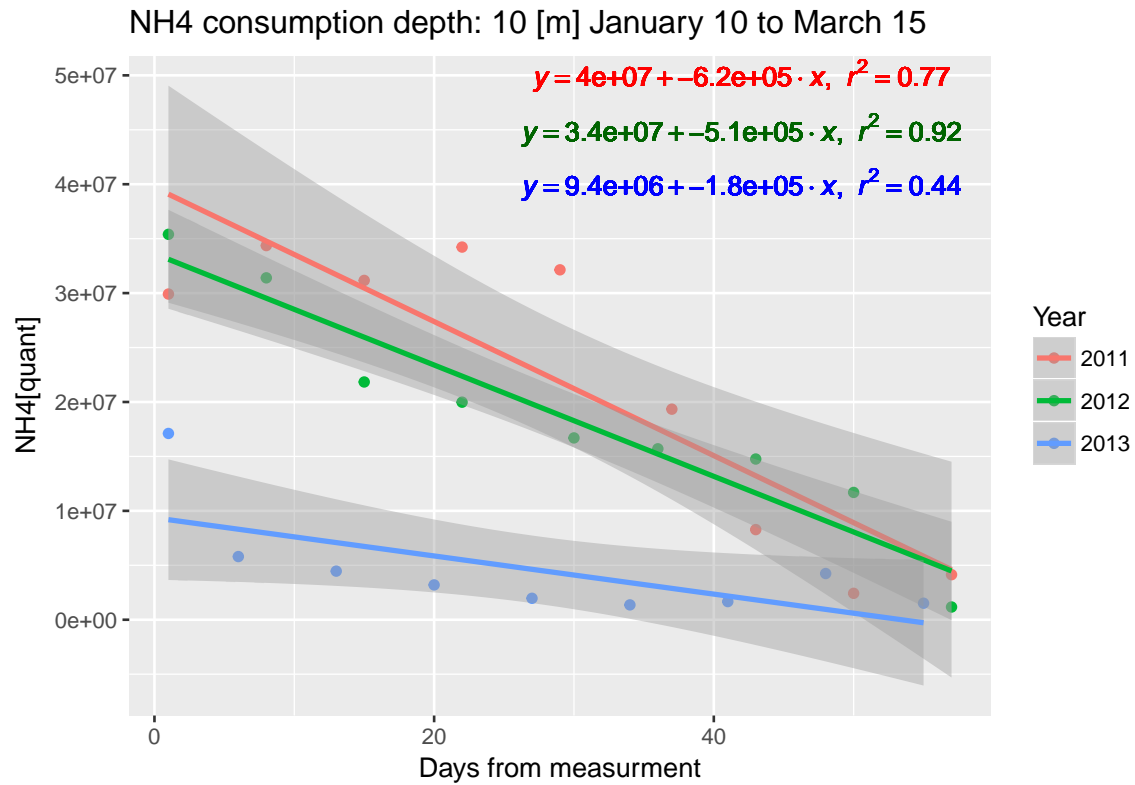
Simulate nitrate buildup between January 1st and March 30th in 10m depth in order to estimate processes rate



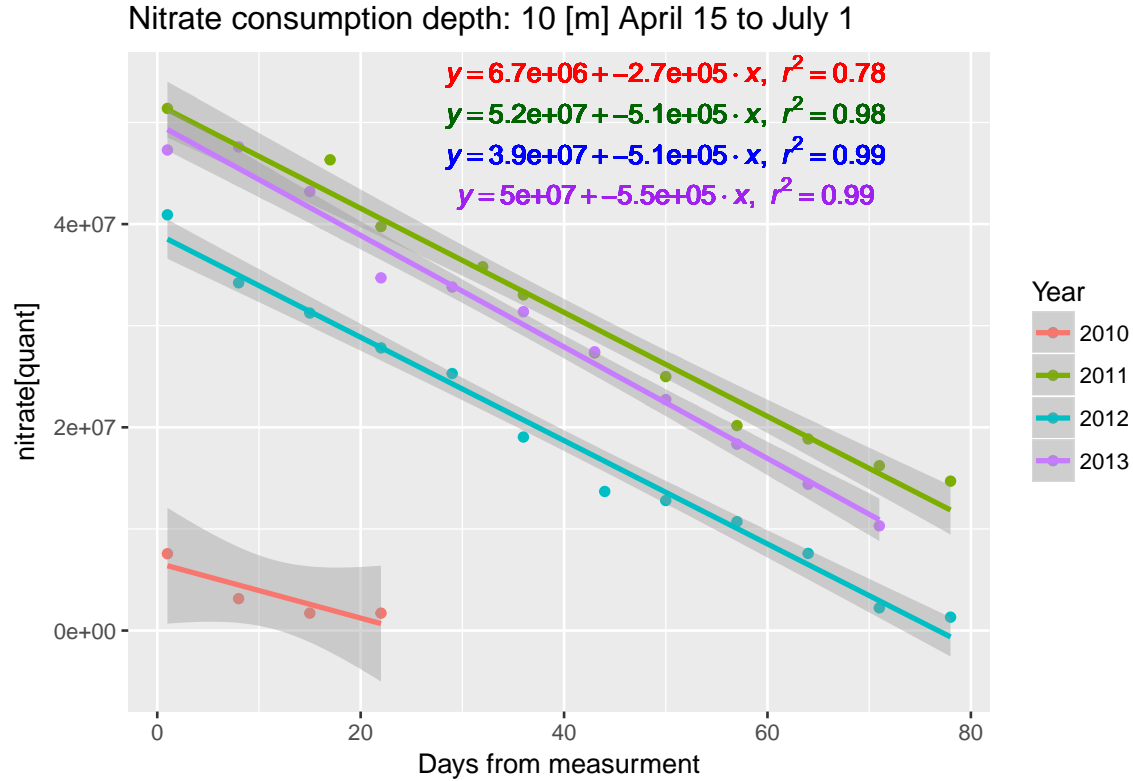
Simulate NH4 buildup between April 30th and December 1st in 30m depth in order to estimate reaction rate



Simulate NH₄ consumption between January 10th and March 15th in 10m depth in order to estimate reaction rate



Simulate nitrate consumption between April 10th and July 1st in 10m depth in order to estimate reaction rate



Coefficients assesment for all depths

After consideration of the dominant processes that control nitrate and ammonium content in the lake, the following section provides an assesment of the processes and their fit to a linear model separately for each depth. The R^2 value can be used to asses the best fit of the model for each depth. It can be observed that the quality of the fit varries greatly amongst different years. This elucidates the effect of other processes that are not considered in this project. These include varying nitrate additions from the lake's sorrounding, but also relates to the hydrological differences, since every year the lake receives different amounts of water, and therefore the amount of water that leaves it through the southern dam also varies. Furthermore, variations in lake level also introduce some compexities since they affect the range of the hypsometric curve that is used for the calculations. These inherent complexities are not fully solved within the scope of this project.

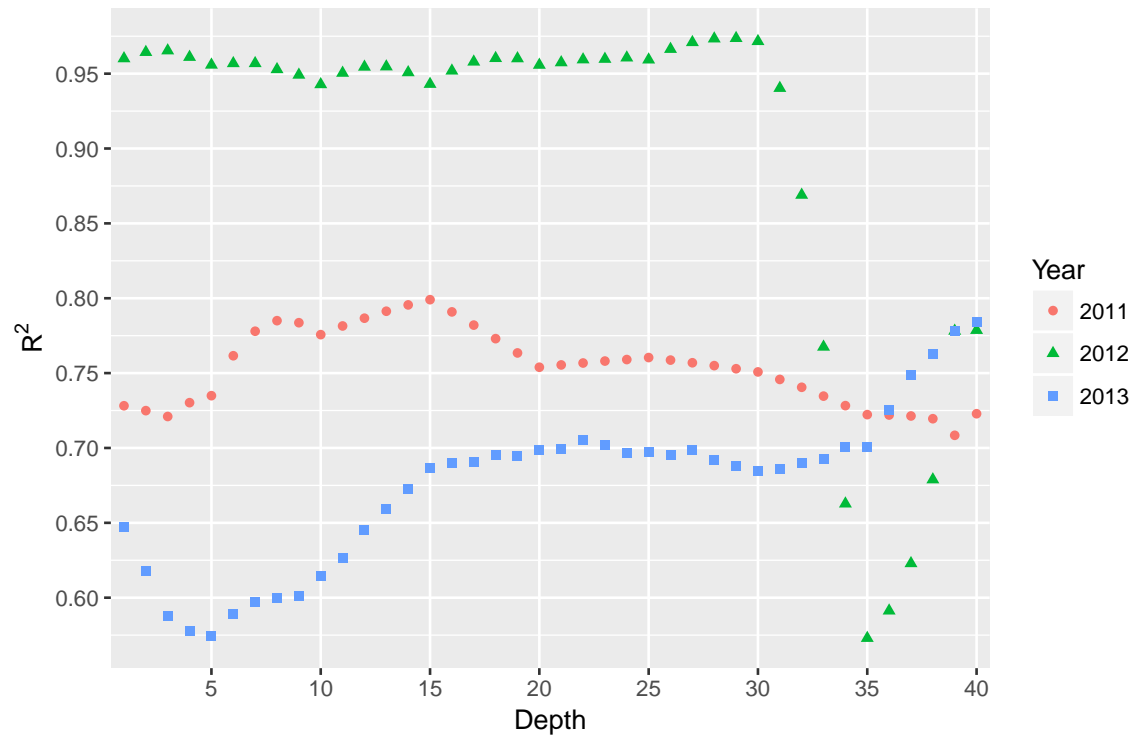
It can be observed, for example, that ammonium buildup does fit the linear model in most depths as nicely as nitrate. Intraannual changes are significatn, and once more illustrate the complexity of the system and its divergence from linearity. Unsurprisingly, the model has the best fit for depths of 20 to 35m, where oxygenation solely depends on annual stratification and mixing.

Nitrate buildup during stratification between January 1st and March 30th

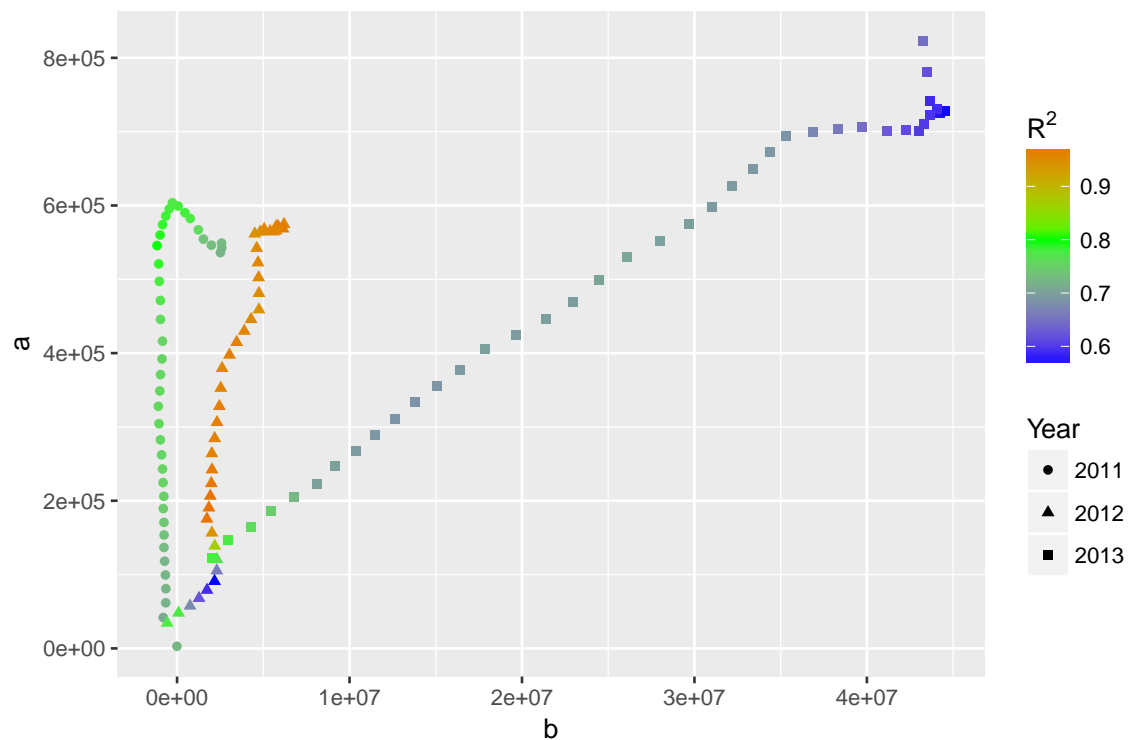
| ## | Depth | a | b | r2 |
|----|----------------|-----------------|------------------|-----------------|
| ## | Min. : 1.00 | Min. : 2837 | Min. : -1163352 | Min. : 0.5730 |
| ## | 1st Qu.: 10.75 | 1st Qu.: 223195 | 1st Qu.: -315929 | 1st Qu.: 0.6953 |
| ## | Median : 20.50 | Median : 437797 | Median : 2589163 | Median : 0.7545 |

| | | | | | | | | |
|----|---------|--------|---------|---------|---------|-----------|---------|---------|
| ## | Mean | :20.50 | Mean | :409771 | Mean | : 9884307 | Mean | :0.7765 |
| ## | 3rd Qu. | :30.25 | 3rd Qu. | :569284 | 3rd Qu. | :12924573 | 3rd Qu. | :0.9409 |
| ## | Max. | :40.00 | Max. | :822536 | Max. | :44544584 | Max. | :0.9737 |

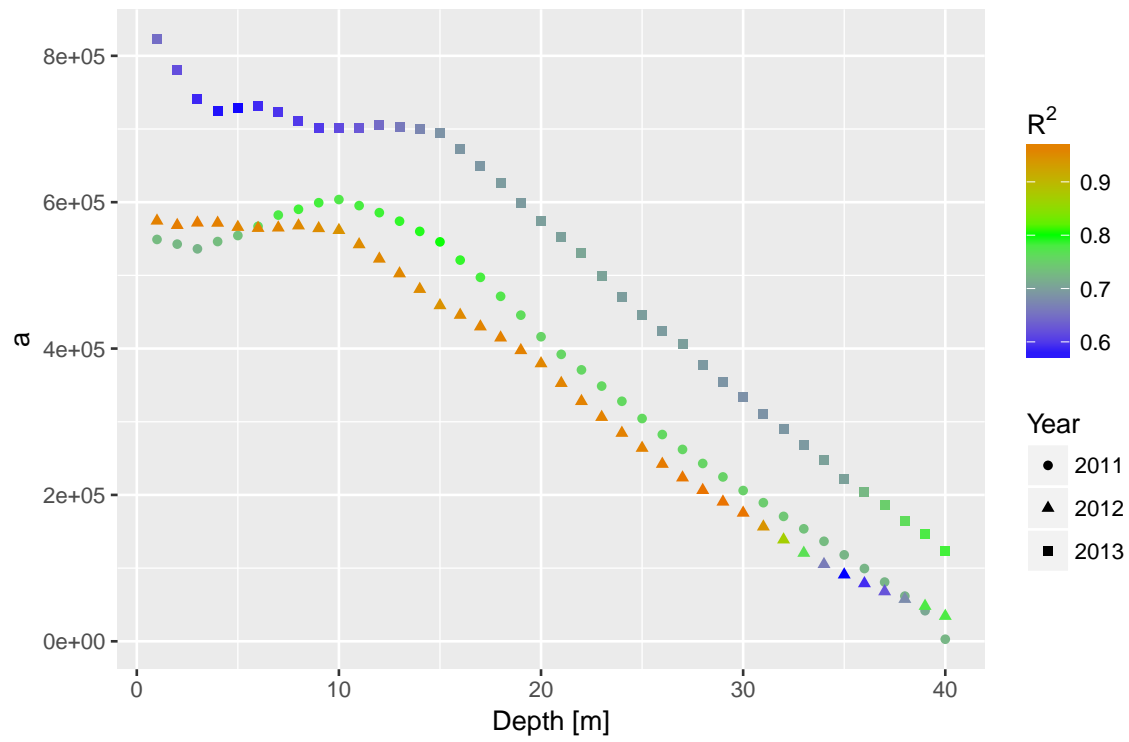
Nitrate buildup Linear Modeling: Janaury 1 to March 30



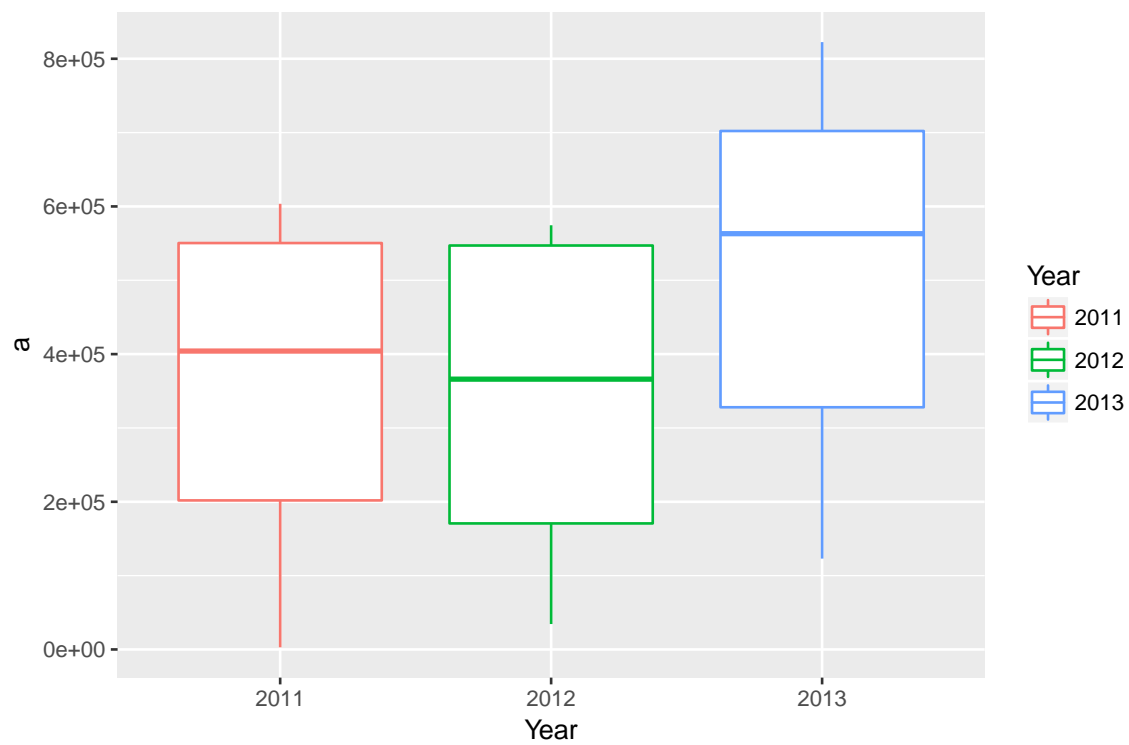
Nitrate buildup Linear Modeling: Janaury 1 to March 30



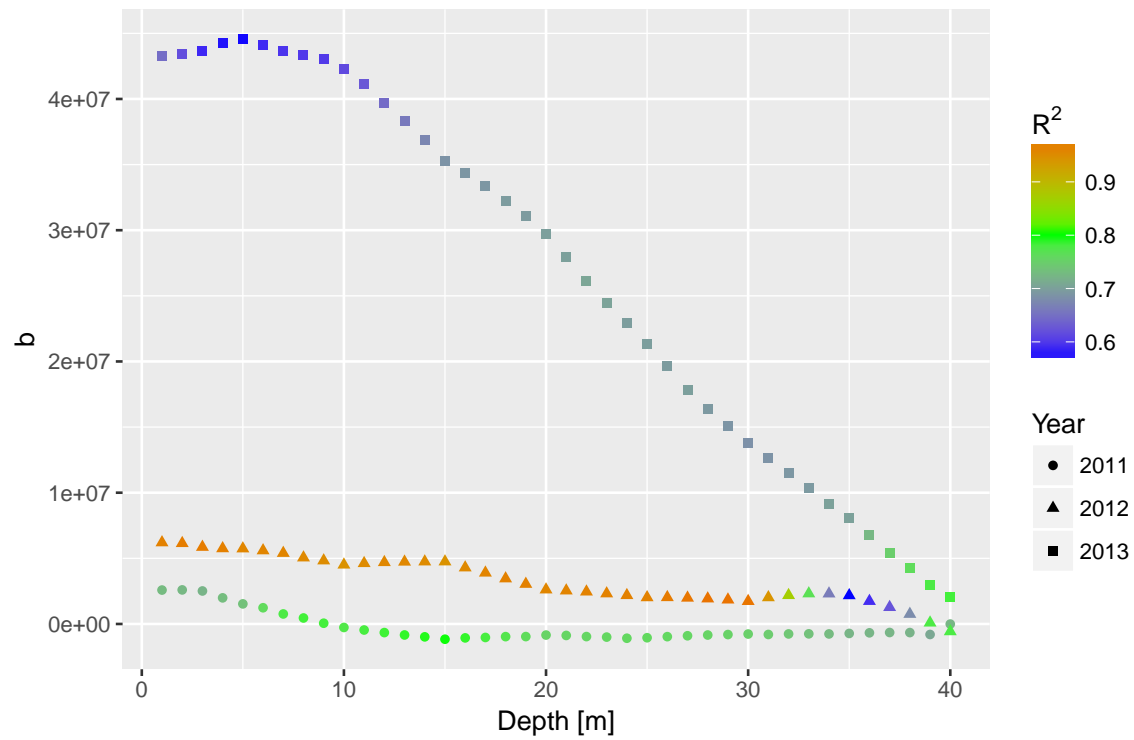
Nitrate buildup Linear Modeling: Janaury 1 to March 30



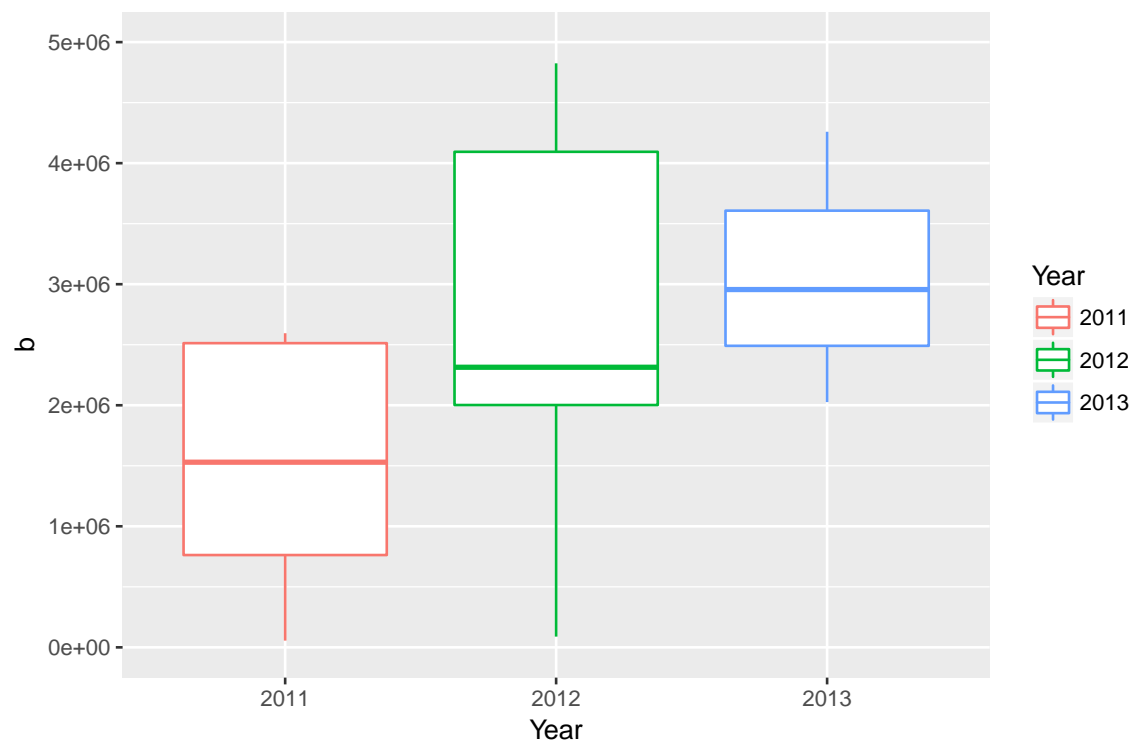
a parameter for Nitrate buildup: Janaury 1 to March 30



Nitrate buildup Linear Modeling: Janaury 1 to March 30



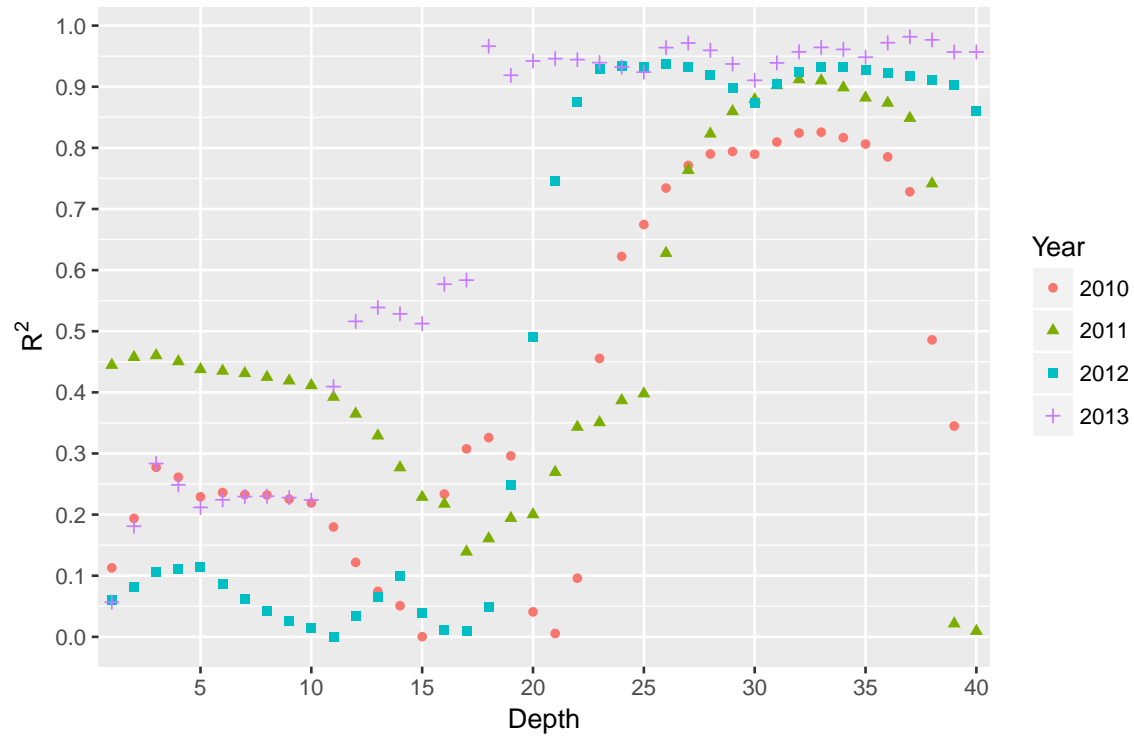
b parameter for Nitrate buildup: Janaury 1 to March 30



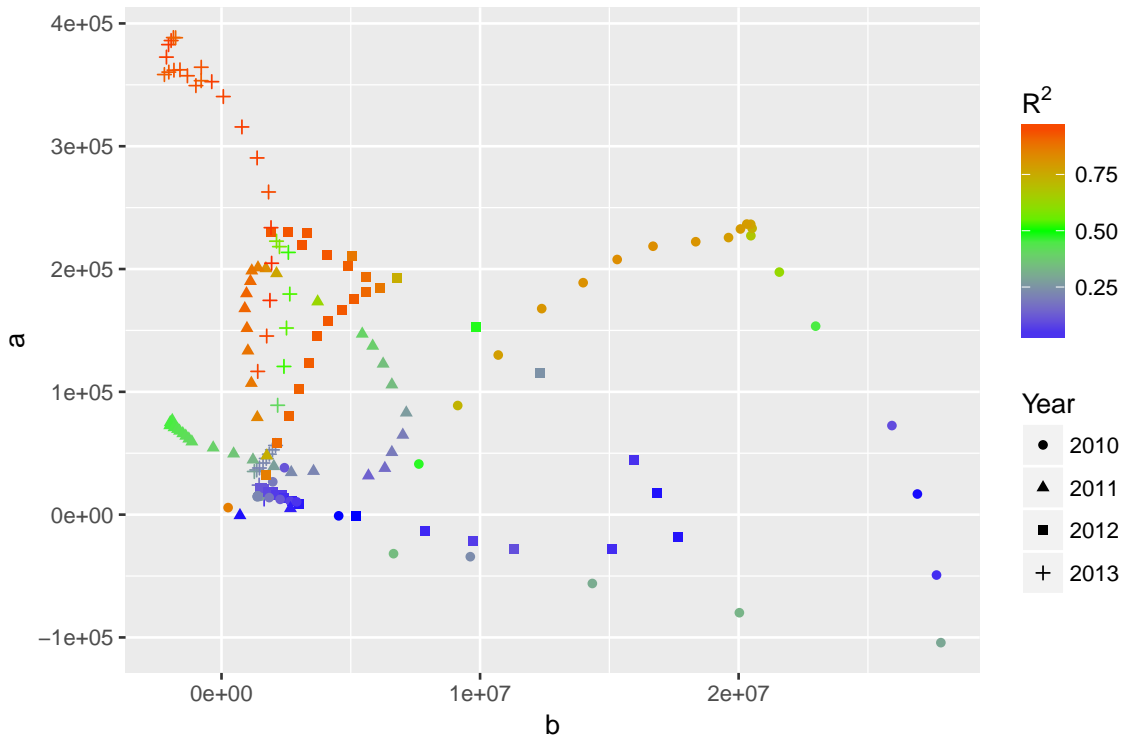
Ammonium buildup during stratification between April 30th and December 12th

| ## | Depth | a | b | r2 |
|----|----------------|-----------------|------------------|--------------------|
| ## | Min. : 1.00 | Min. : -104262 | Min. : -2209182 | Min. : 0.0003153 |
| ## | 1st Qu.: 10.75 | 1st Qu.: 21419 | 1st Qu.: 1373549 | 1st Qu.: 0.2240937 |
| ## | Median : 20.50 | Median : 81791 | Median : 2140742 | Median : 0.4588809 |
| ## | Mean : 20.50 | Mean : 120362 | Mean : 4868893 | Mean : 0.5247795 |
| ## | 3rd Qu.: 30.25 | 3rd Qu.: 200613 | 3rd Qu.: 6149996 | 3rd Qu.: 0.9020609 |
| ## | Max. : 40.00 | Max. : 388468 | Max. : 27822019 | Max. : 0.9818000 |

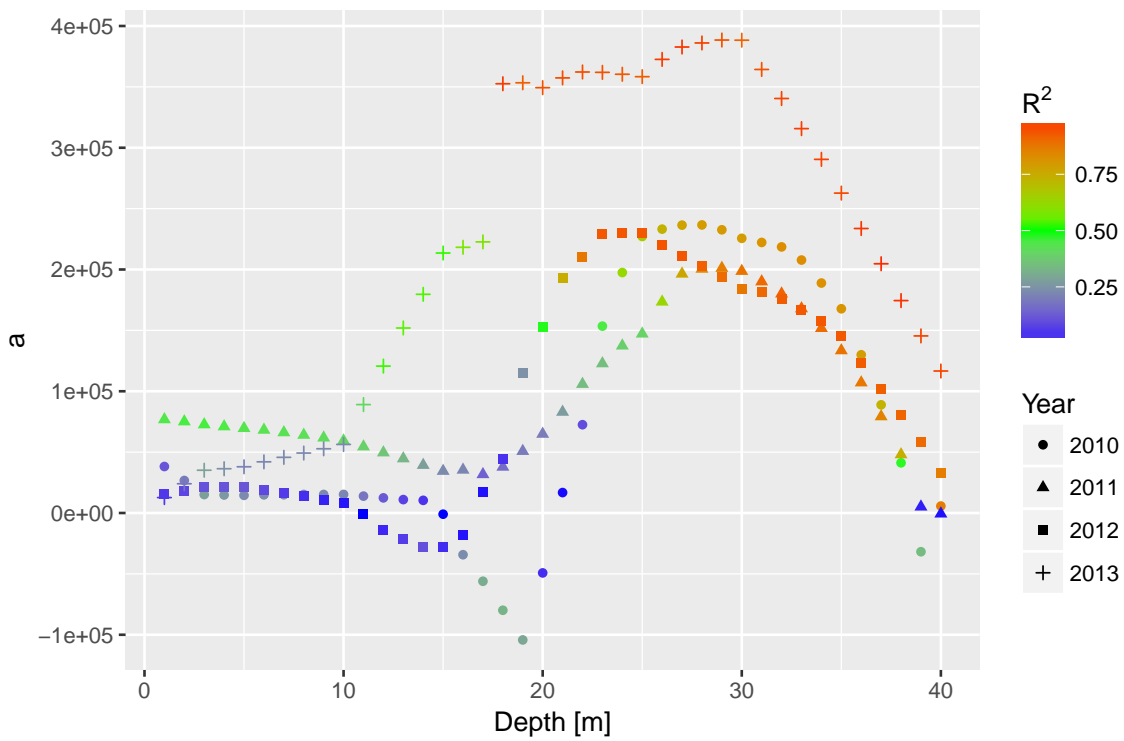
NH4 buildup Linear Modeling: April 30 to December 1



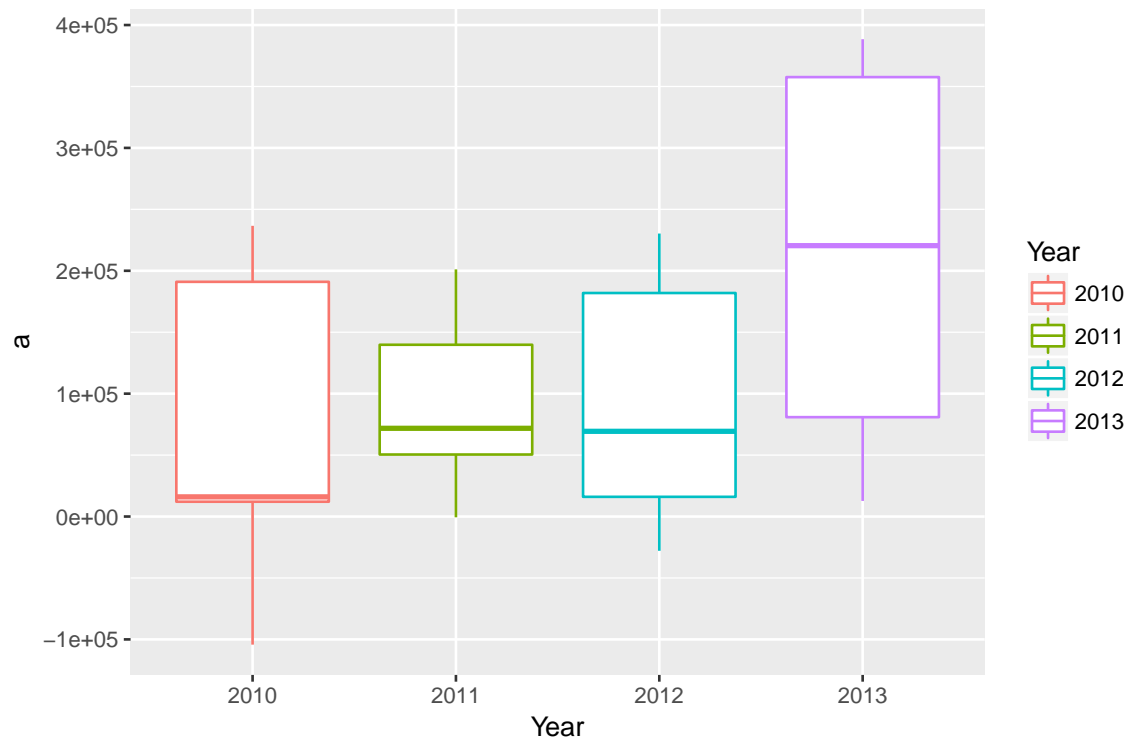
NH4 buildup Linear Modeling: April 30 to December 1



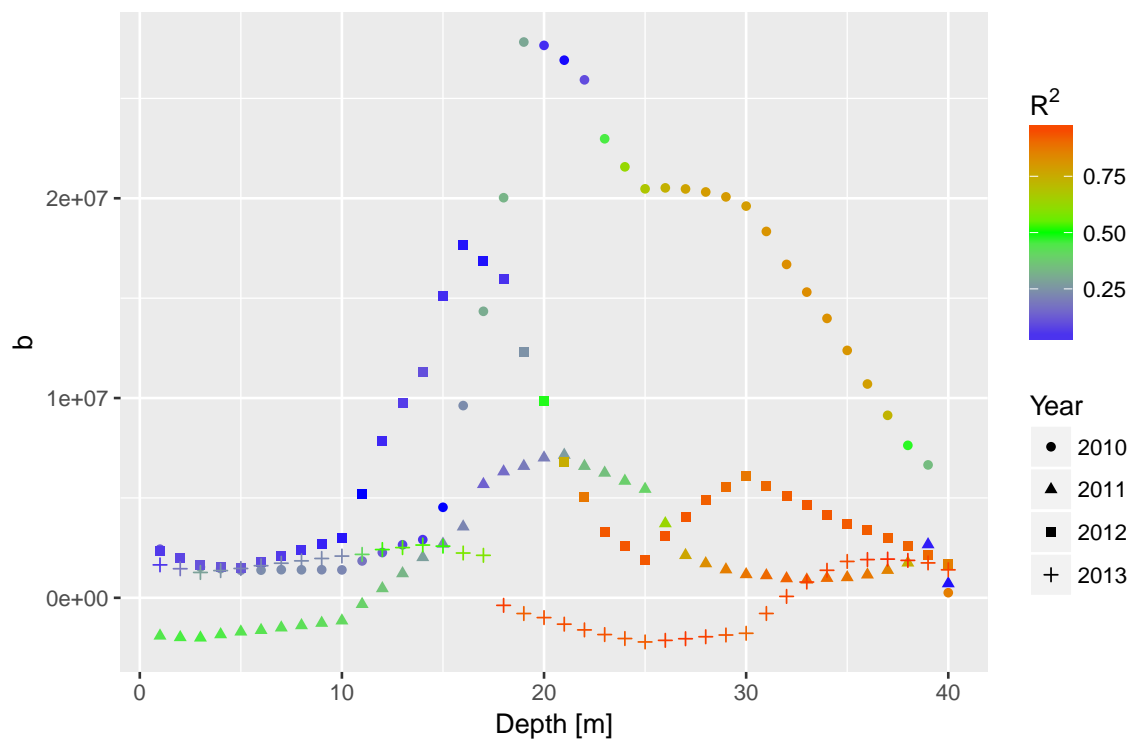
NH4 buildup Linear Modeling: April 30 to December 1



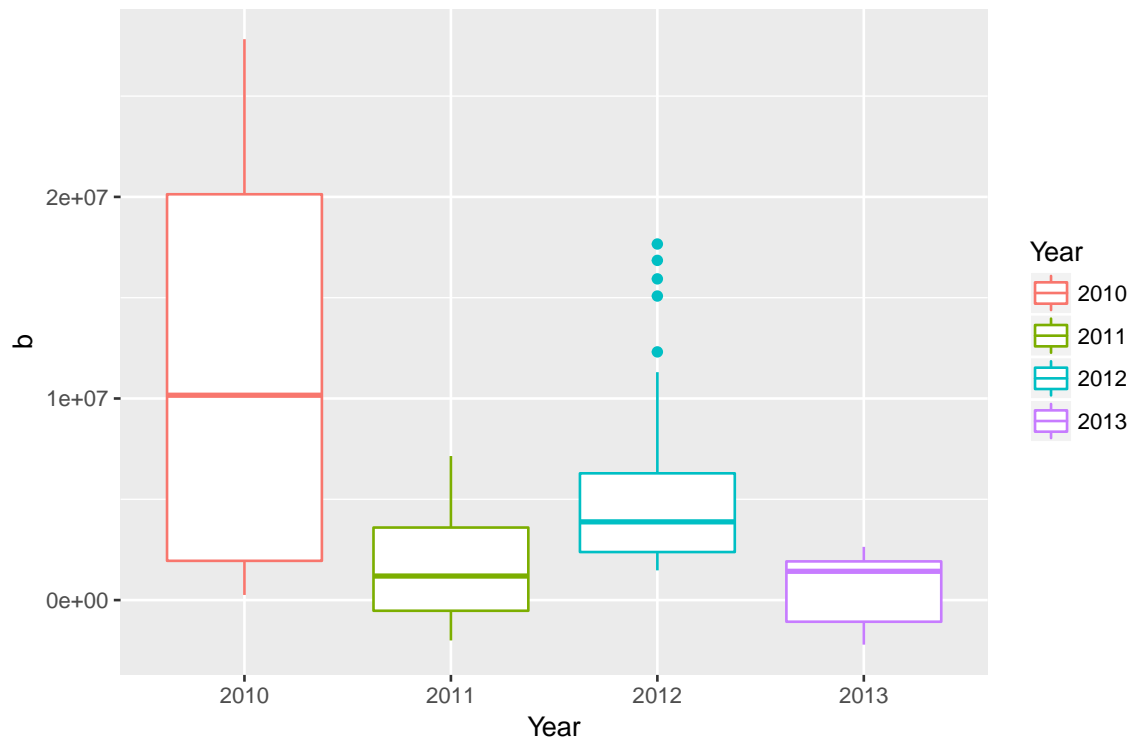
a parameter for NH4 buildup: April 30 to December 1



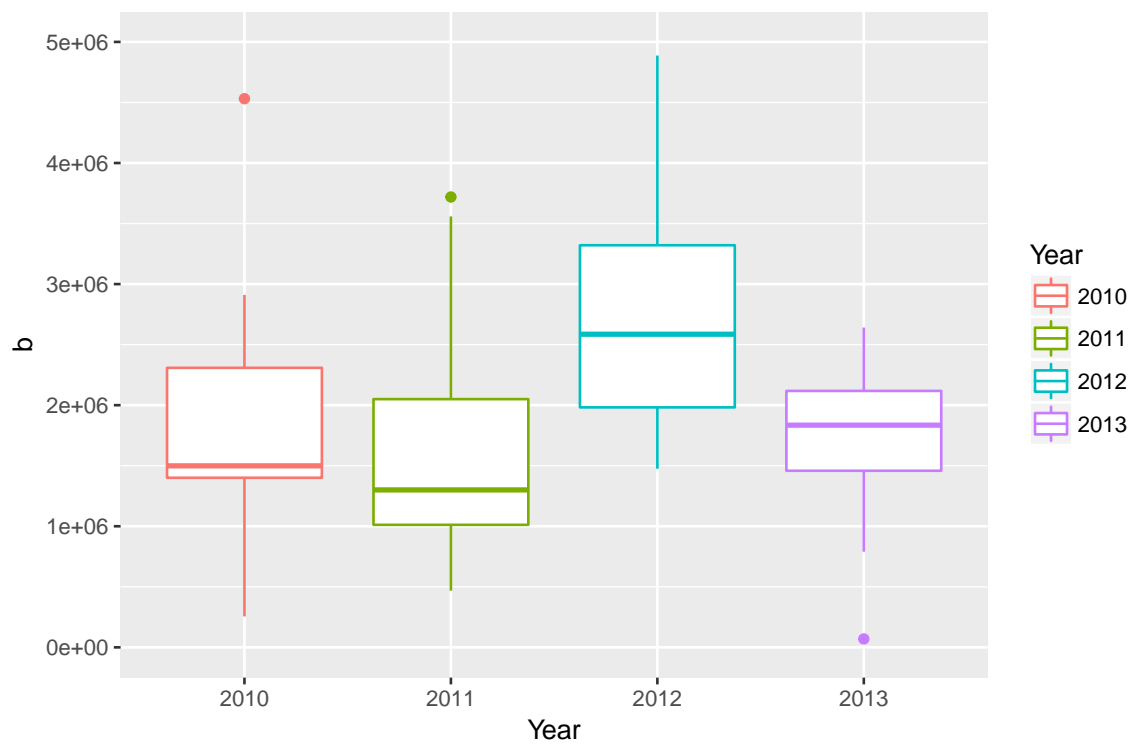
NH4 buildup Linear Modeling: April 30 to December 1



b parameter for NH4 buildup: April 30 to December 1

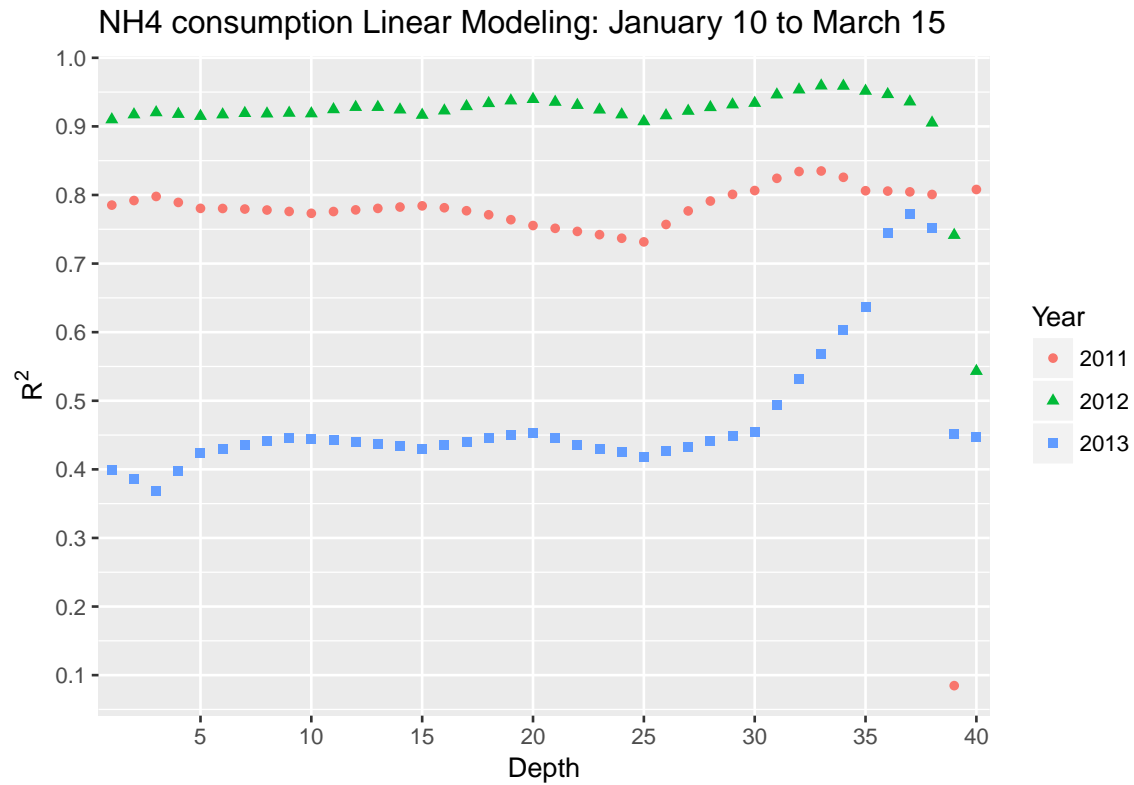


b parameter for NH4 buildup: April 30 to December 1

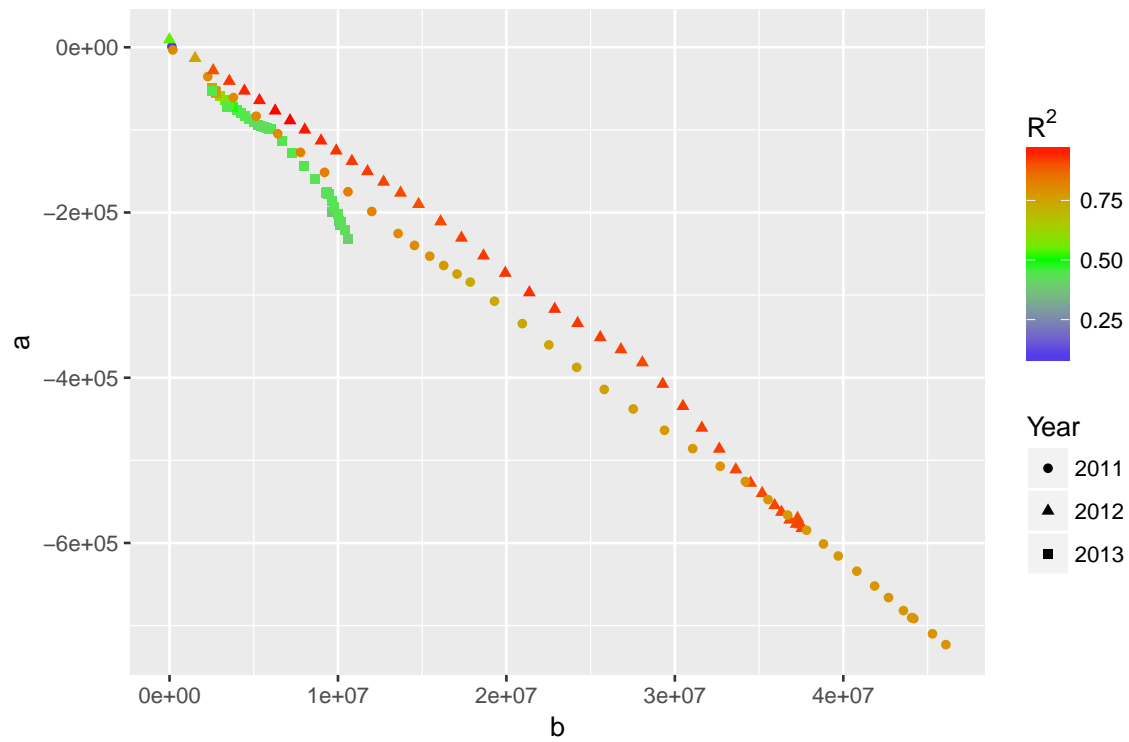


Ammonium consumption after mixing between January 15th to March 15th

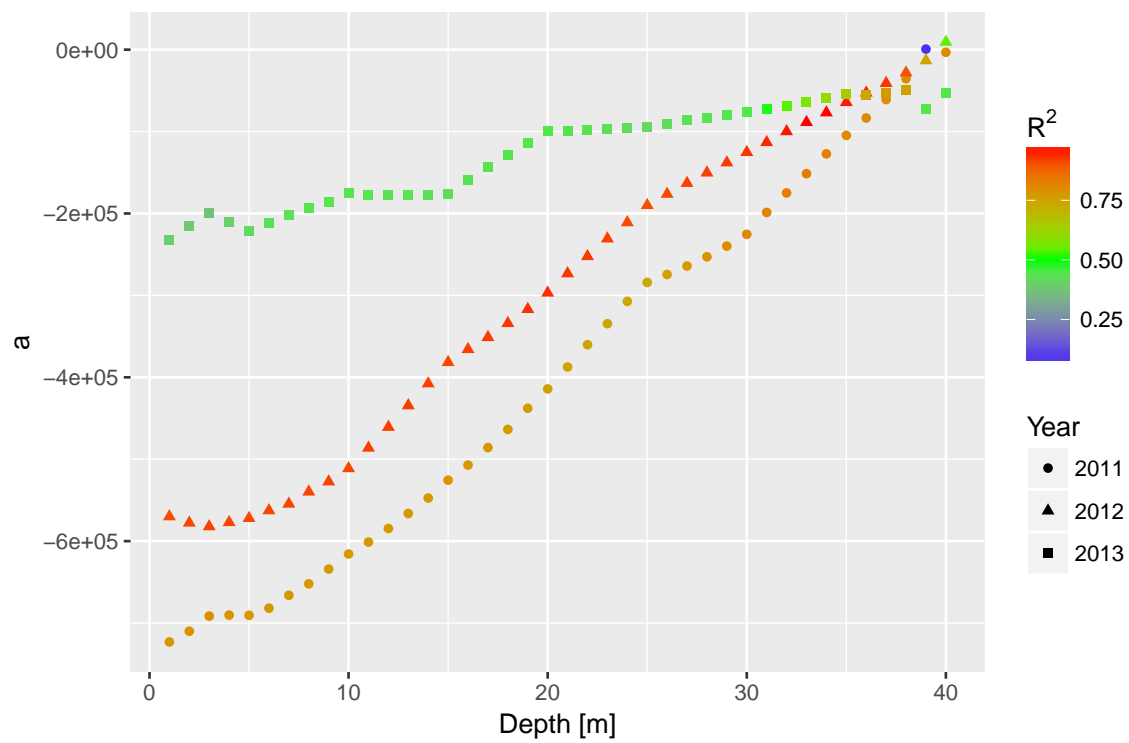
| ## | Depth | a | b | r2 |
|----|----------------|------------------|-------------------|------------------|
| ## | Min. : 1.00 | Min. : -723066 | Min. : -9510 | Min. : 0.08467 |
| ## | 1st Qu.: 10.75 | 1st Qu.: -443545 | 1st Qu.: 5888522 | 1st Qu.: 0.45085 |
| ## | Median : 20.50 | Median : -200589 | Median : 10710844 | Median : 0.77990 |
| ## | Mean : 20.50 | Mean : -272712 | Mean : 17447156 | Mean : 0.71780 |
| ## | 3rd Qu.: 30.25 | 3rd Qu.: -96653 | 3rd Qu.: 29659587 | 3rd Qu.: 0.91716 |
| ## | Max. : 40.00 | Max. : 9290 | Max. : 46089838 | Max. : 0.95925 |

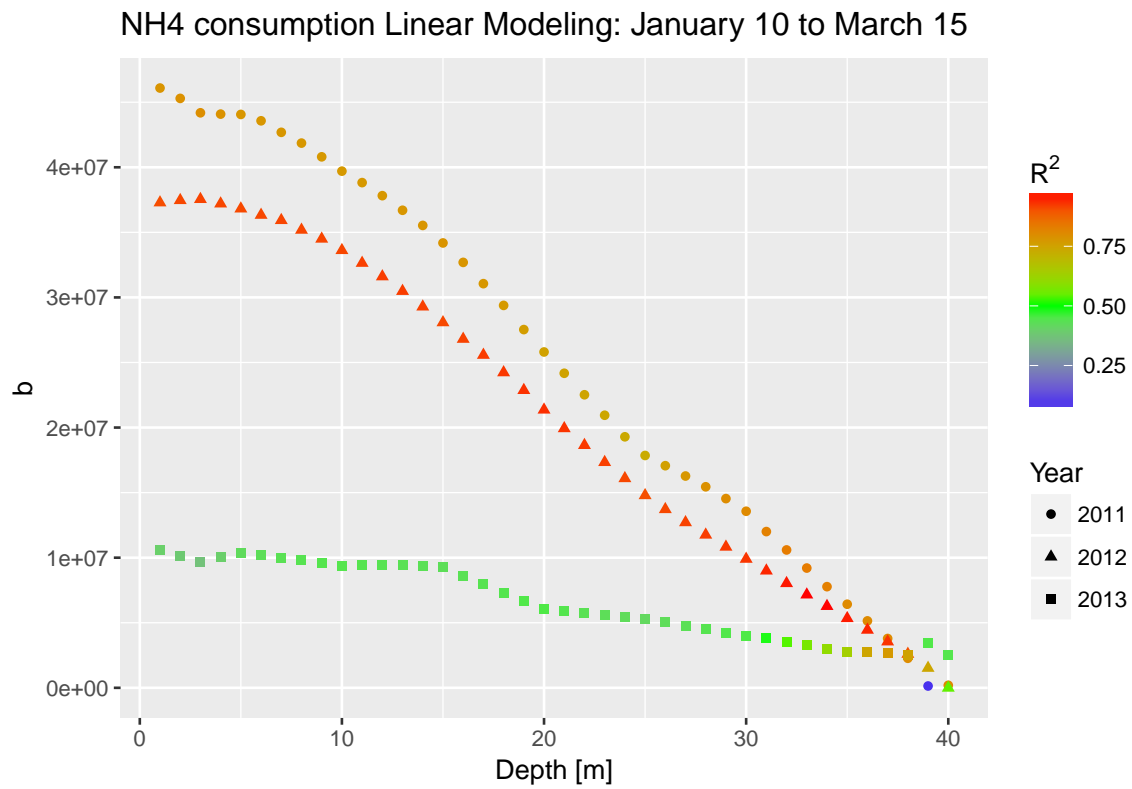
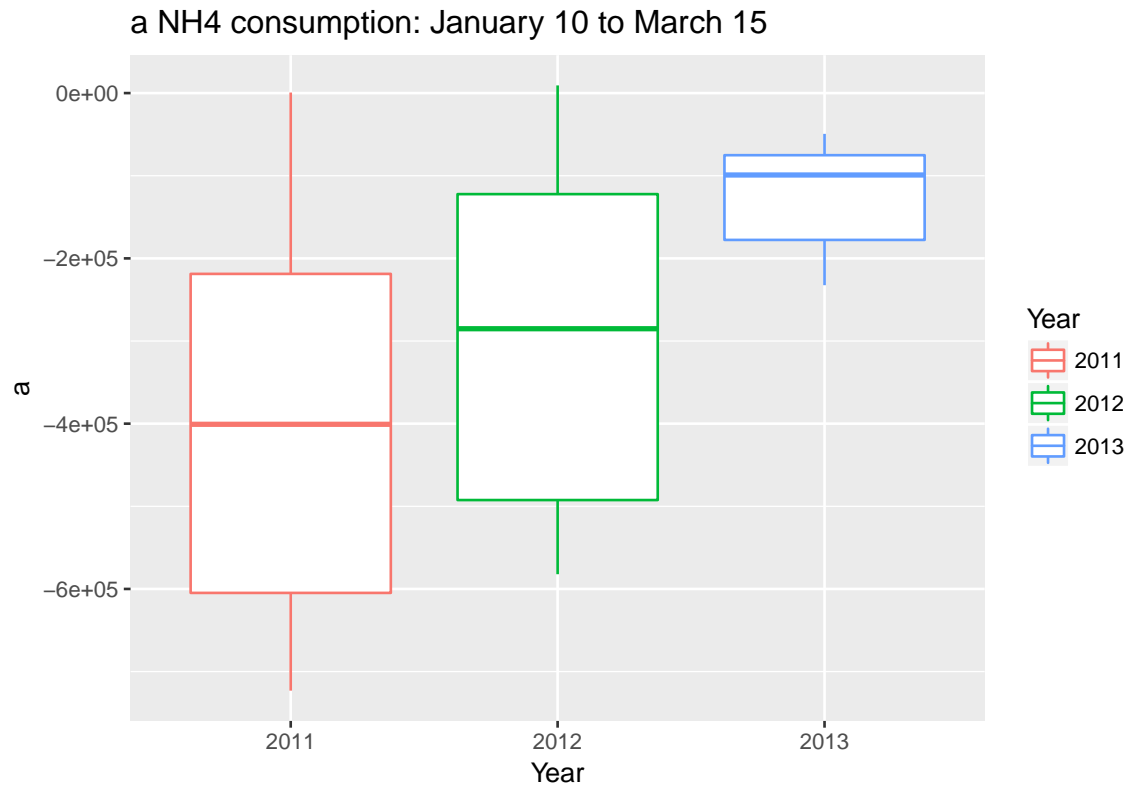


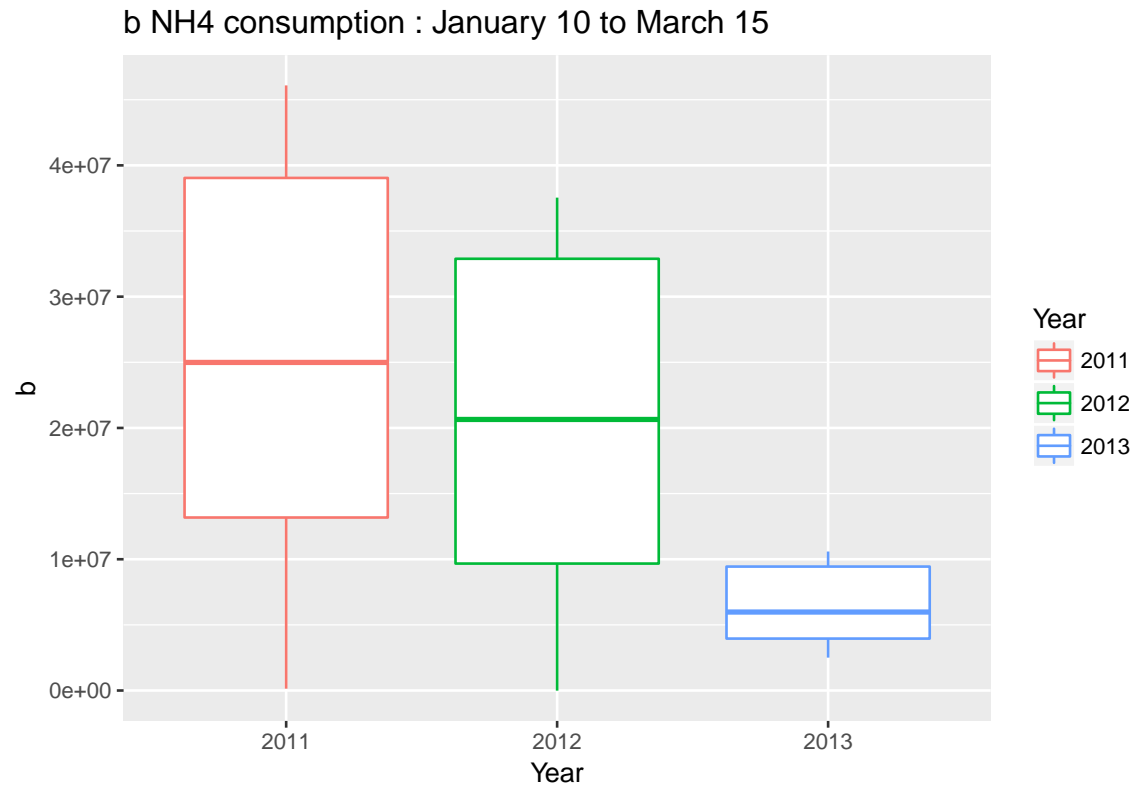
NH4 consumption Linear Modeling: January 10 to March 15



NH4 consumption Linear Modeling: January 10 to March 15



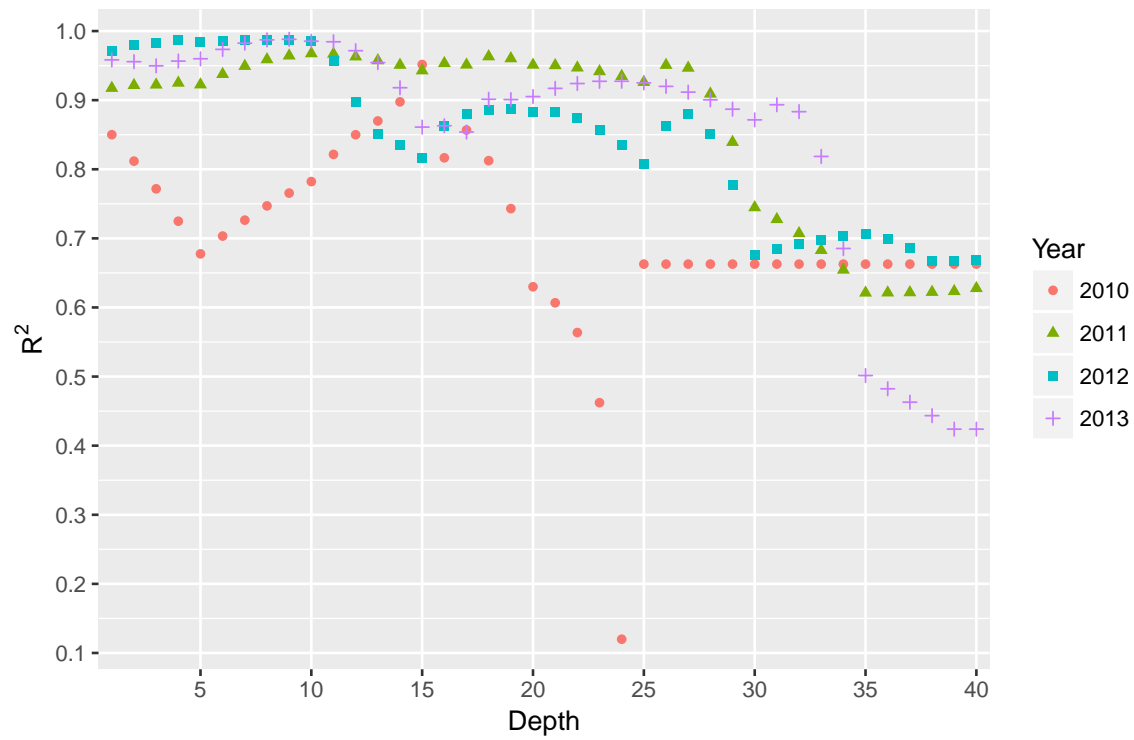




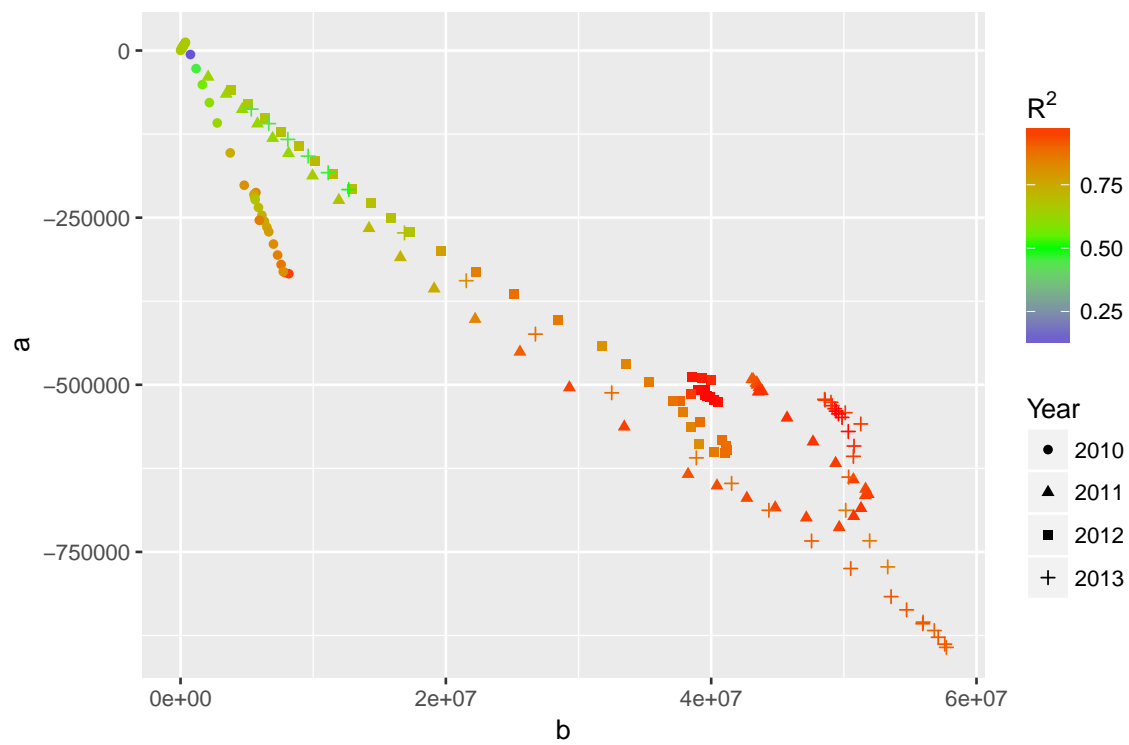
Nitrate consumption after mixing between January 10th to March 15th

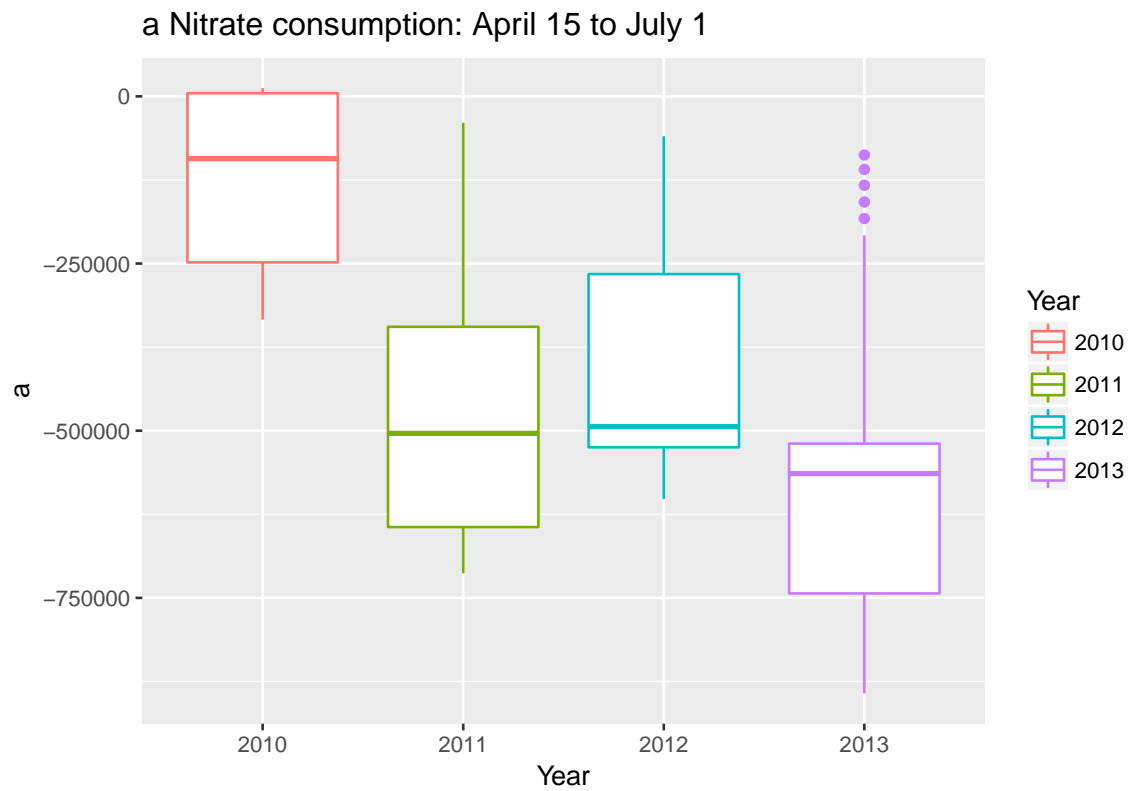
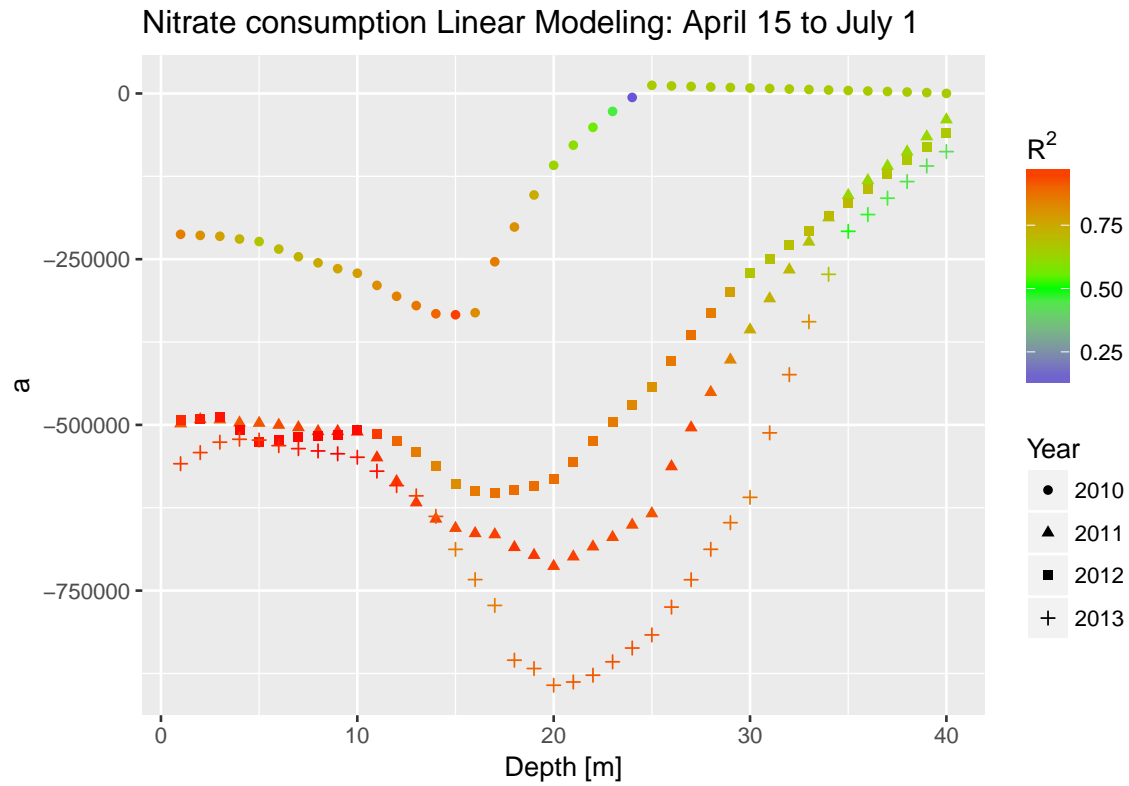
| ## | Depth | a | b | r2 |
|----|----------------|------------------|-------------------|-----------------|
| ## | Min. : 1.00 | Min. : -892768 | Min. : 3394 | Min. : 0.1199 |
| ## | 1st Qu.: 10.75 | 1st Qu.: -564564 | 1st Qu.: 6471333 | 1st Qu.: 0.6841 |
| ## | Median : 20.50 | Median : -489261 | Median : 32975722 | Median : 0.8628 |
| ## | Mean : 20.50 | Mean : -393441 | Mean : 27172061 | Mean : 0.8151 |
| ## | 3rd Qu.: 30.25 | 3rd Qu.: -186772 | 3rd Qu.: 43982135 | 3rd Qu.: 0.9475 |
| ## | Max. : 40.00 | Max. : 12313 | Max. : 57730907 | Max. : 0.9880 |

Nitrate consumption Linear Modeling: April 15 to July 1

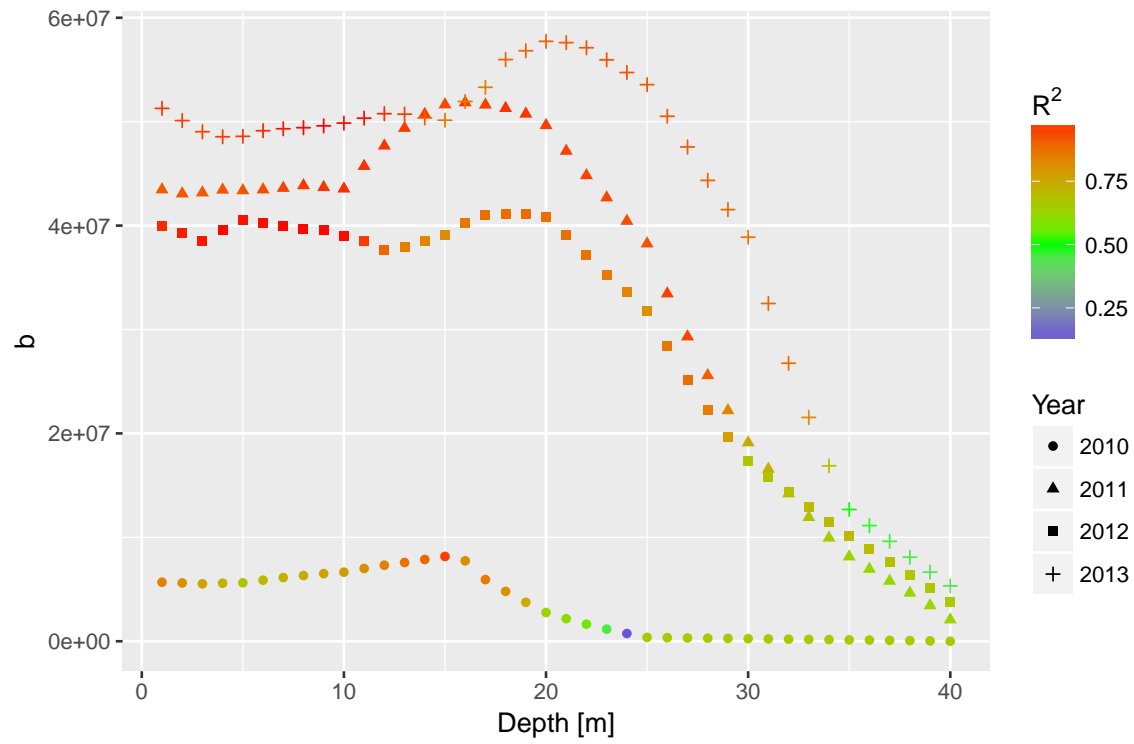


Nitrate consumption Linear Modeling: April 15 to July 1

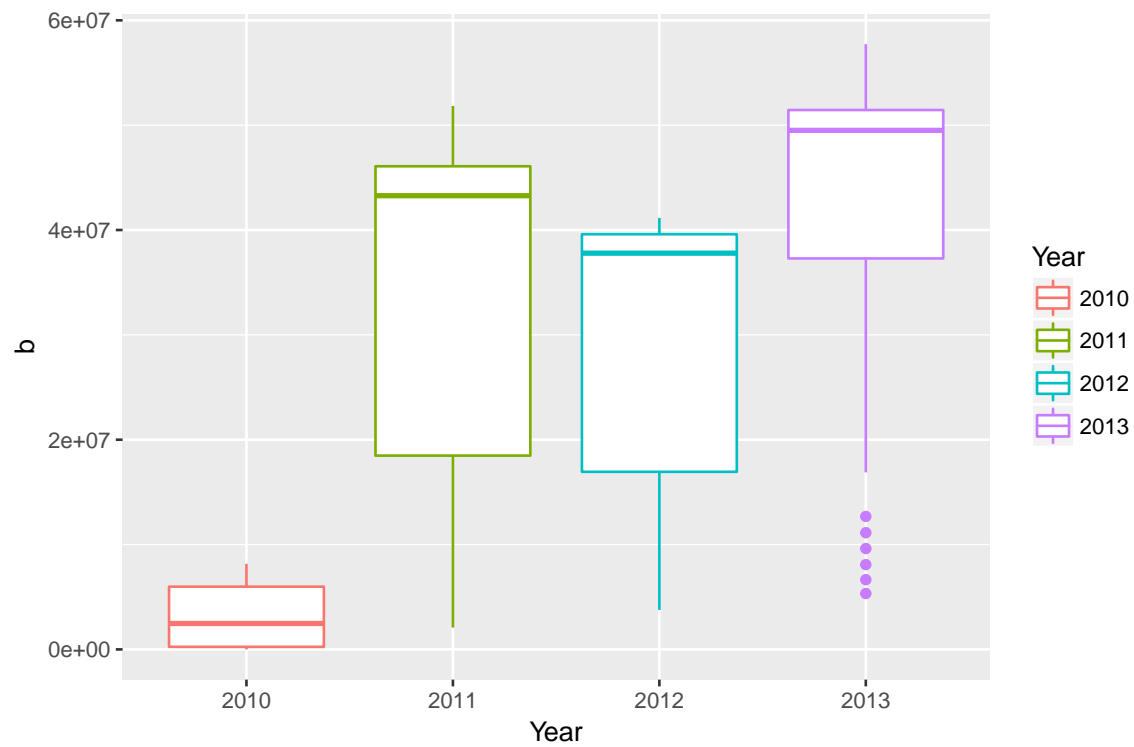




Nitrate consumption Linear Modeling: April 15 to July 1

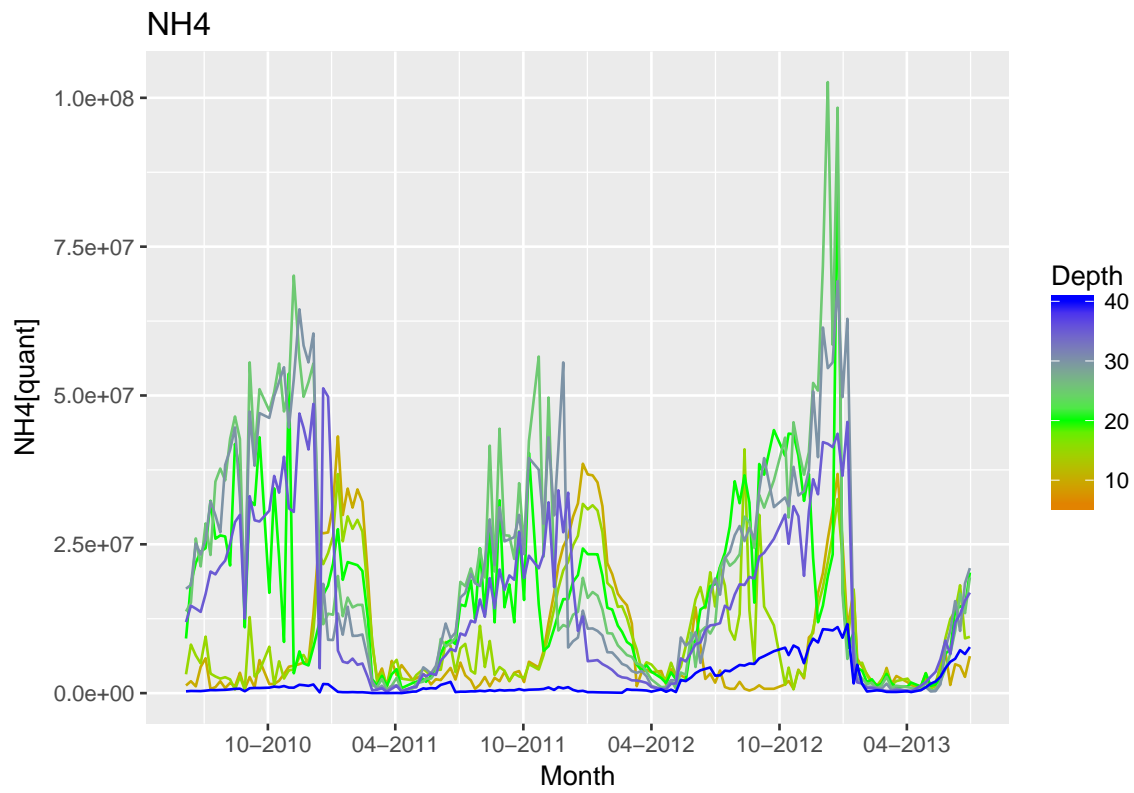
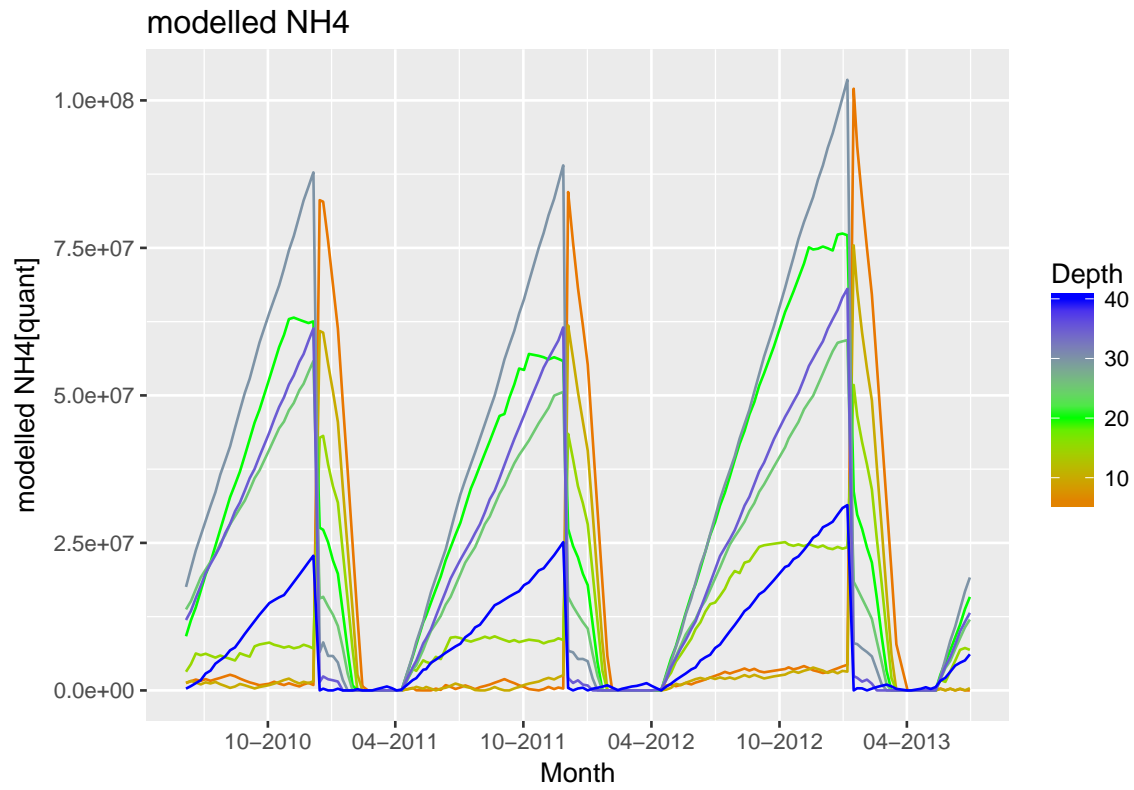


b Nitrate consumption : April 15 to July 1

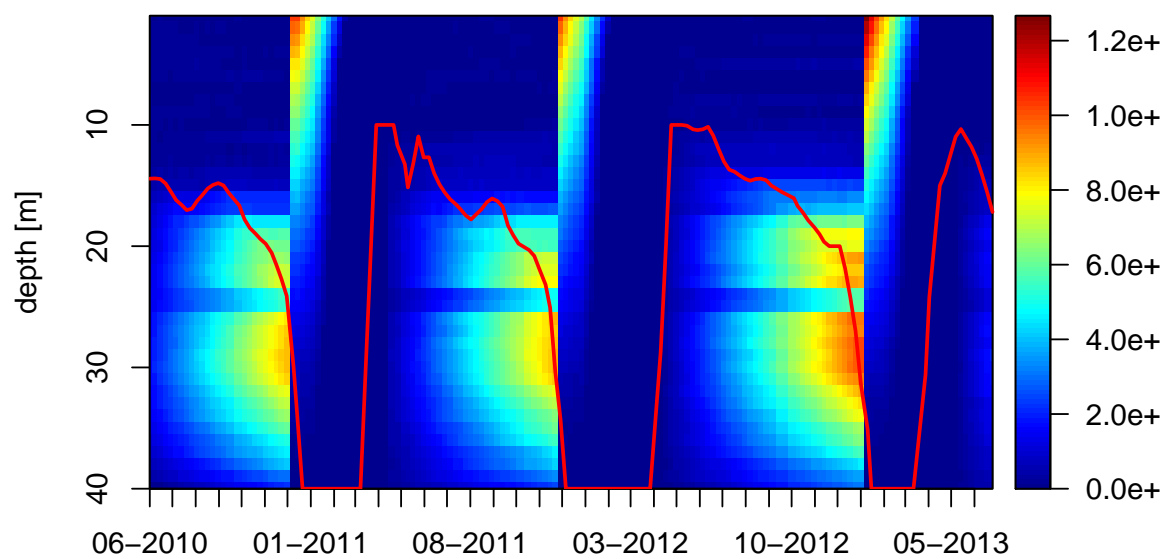


Lake Modelling

In the following section the previously estimated parameters are used to simulate annual NH_4^+ development in the lake. The parameters that are used for this model include the linear fit parameters that were calculated in the previous section, as well as several parameters that define the intensity of the lake mixing, and the durations of the delay in the consumption of NH_4^+ , and the consumption itself.



modelled NH4 [amount]



NH4 [amount]

