

LakeN

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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

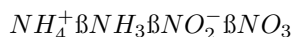
A steep temperature gradient in a body of water such as a lake, marked by a layer above and below which the water is at different temperatures. Because warmer water is less dense, the thermocline dictates the mixing depth of the lake, and therefore directly determines chemical properties of the lake's 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 build-up during lake stratification in the epilimnion
2. Ammonification build-up 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.

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.

read the data and load relevant libraries

```
##          Date          Depth          NH4          Nitrit
## 2012-06-03: 13   Min.    : 1.00   Min.    :0.0030   Min.    :0.00200
```

```

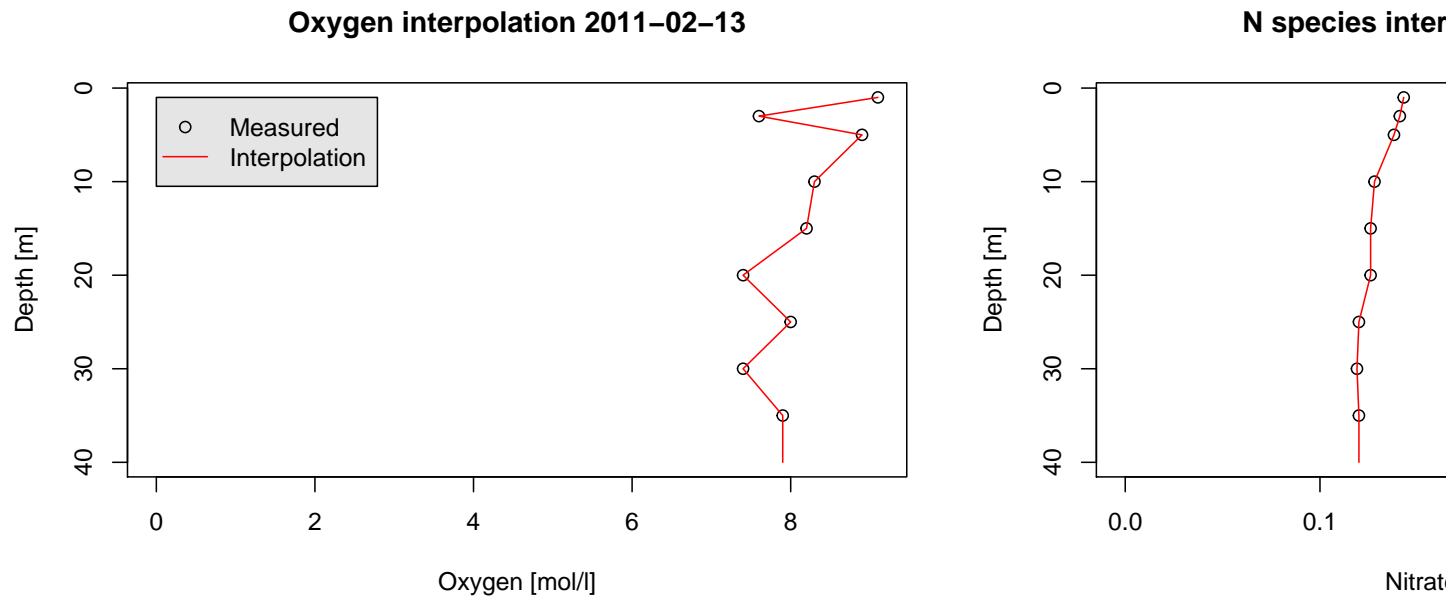
## 2012-06-24: 13 1st Qu.: 5.00 1st Qu.:0.0210 1st Qu.:0.00200
## 2012-07-08: 13 Median :16.00 Median :0.0850 Median :0.00300
## 2012-09-23: 13 Mean :16.91 Mean :0.2125 Mean :0.01409
## 2013-06-02: 13 3rd Qu.:25.00 3rd Qu.:0.2447 3rd Qu.:0.01400
## 2013-06-23: 13 Max. :40.00 Max. :2.5400 Max. :0.27300
## (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

```

Interpolate the Data 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

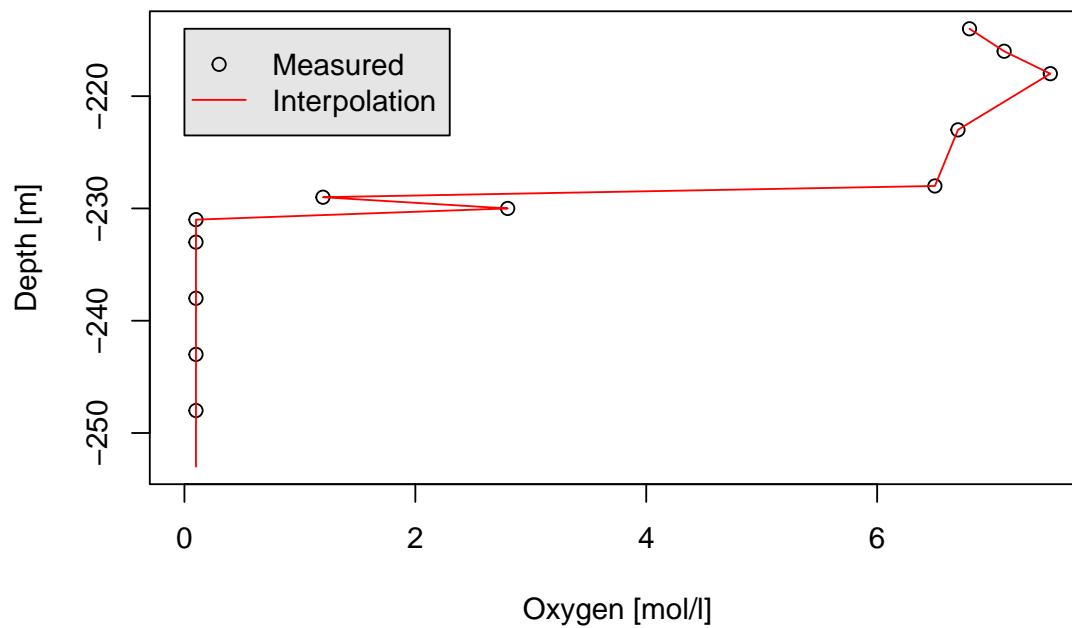


Depth and Level Corrections

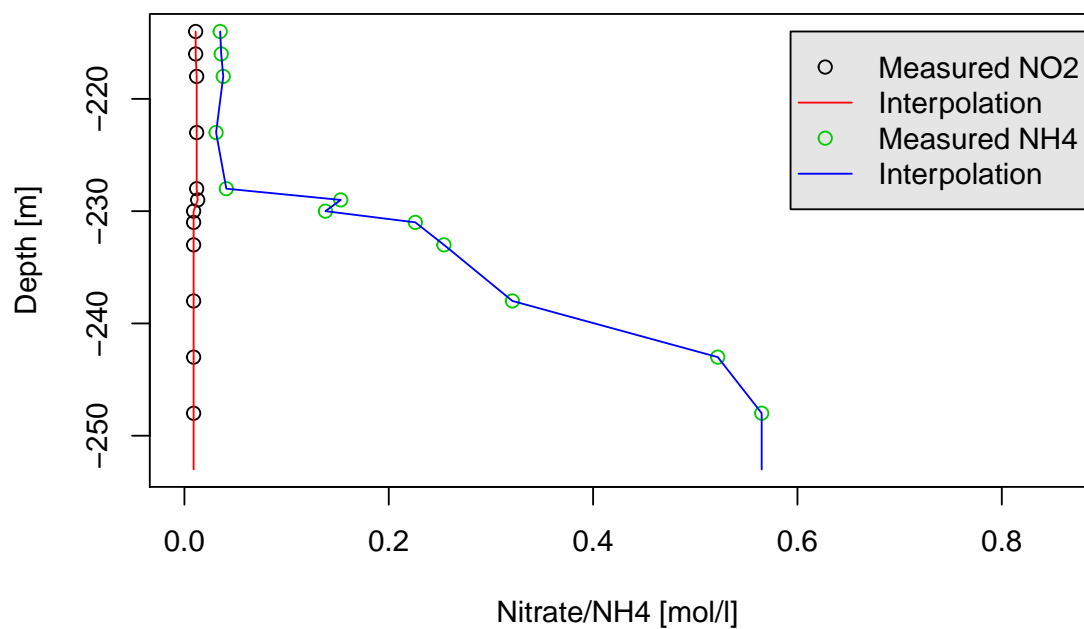
Calculate the appropriate depth for each measurement using available daily level measurements. Use function “realdepth” and use closest day if no level measurement of that day is available. This correction is essential for later calculation of depth to volume and concentration quantification of N species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

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

Oxygen interpolation 2010-06-27

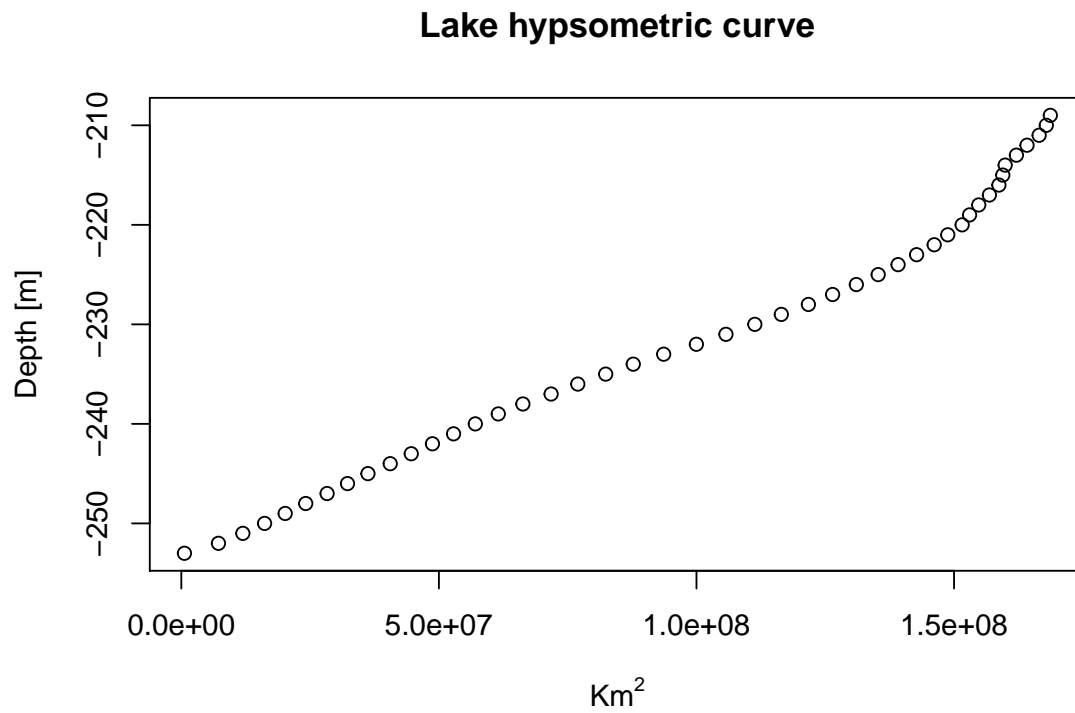


N species interpolation 2010-06-27



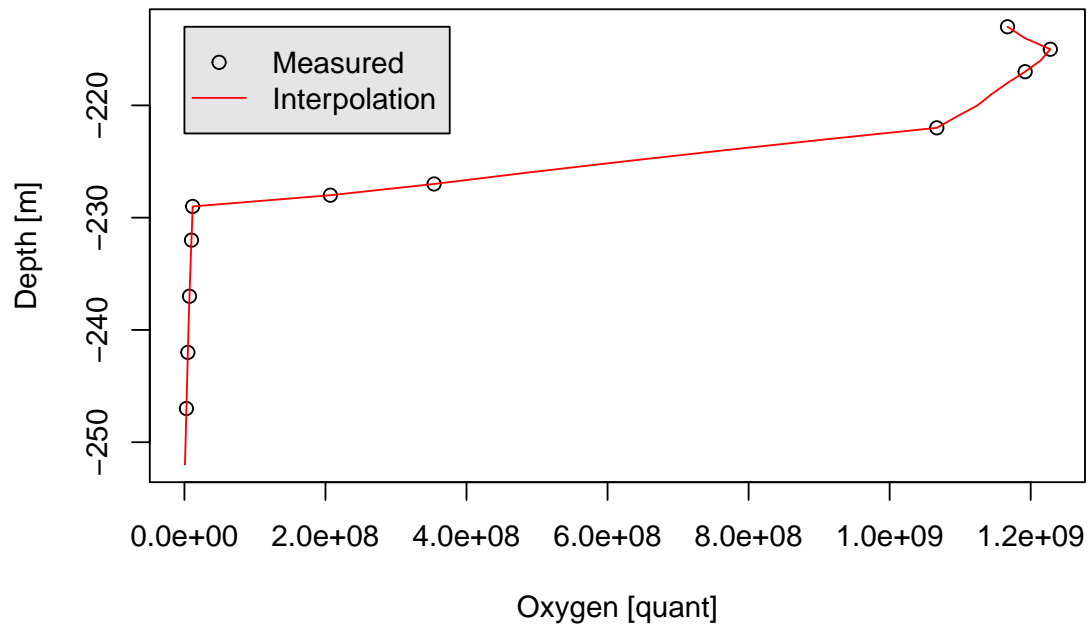
Quantify the data using lake hypsometric curve

The use of concentrations has limitations because it may enhance or demise a processes that is inherently “mass-based”. Quantify the amount of measured species using the hypsometric curve of the lake using function “conctoquant”. Multiply each depth value with its corresponding hypsometric value to

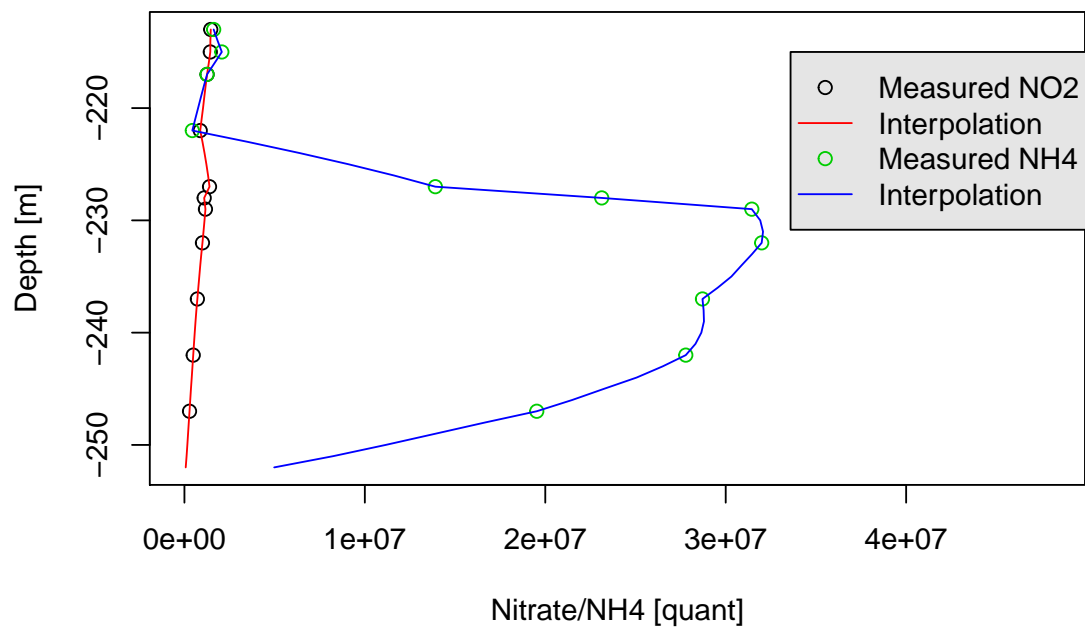


demonstrate the results according to the new depth scale of randomly selected data

Oxygen interpolation 2012-08-19



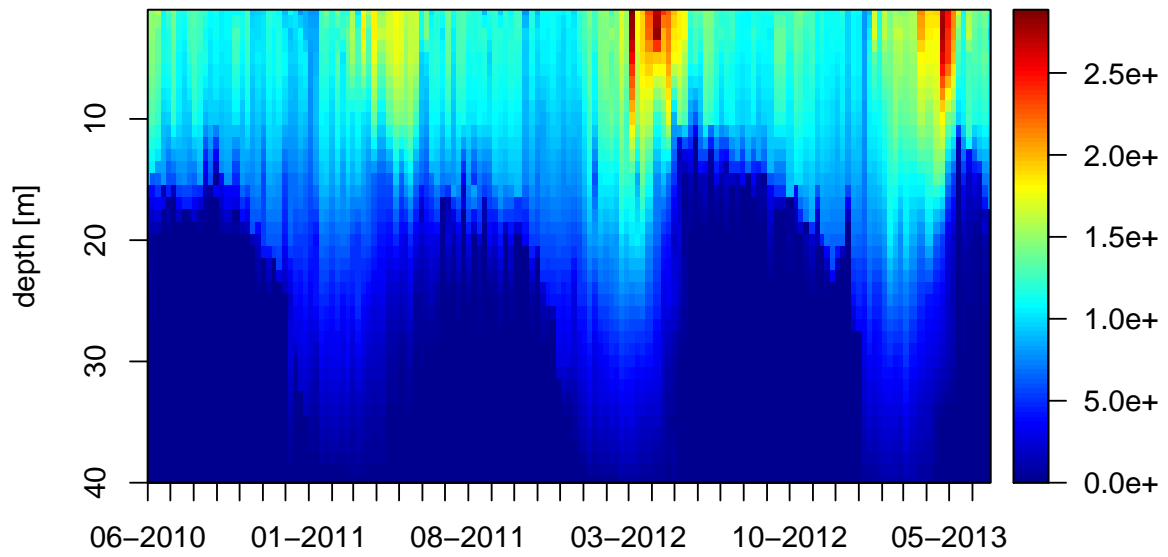
N species interpolation 2012-08-19



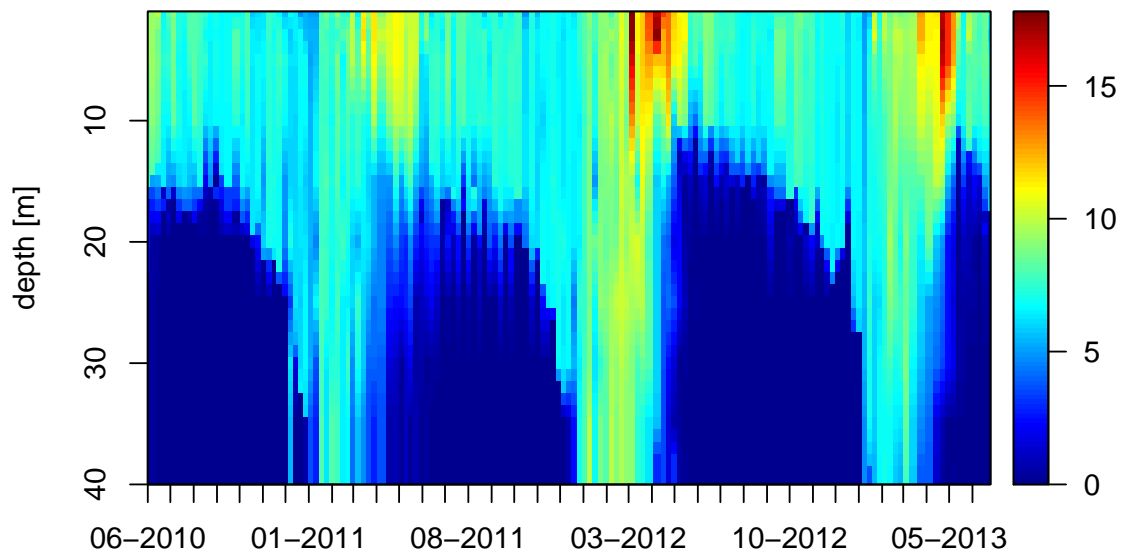
Time series plots

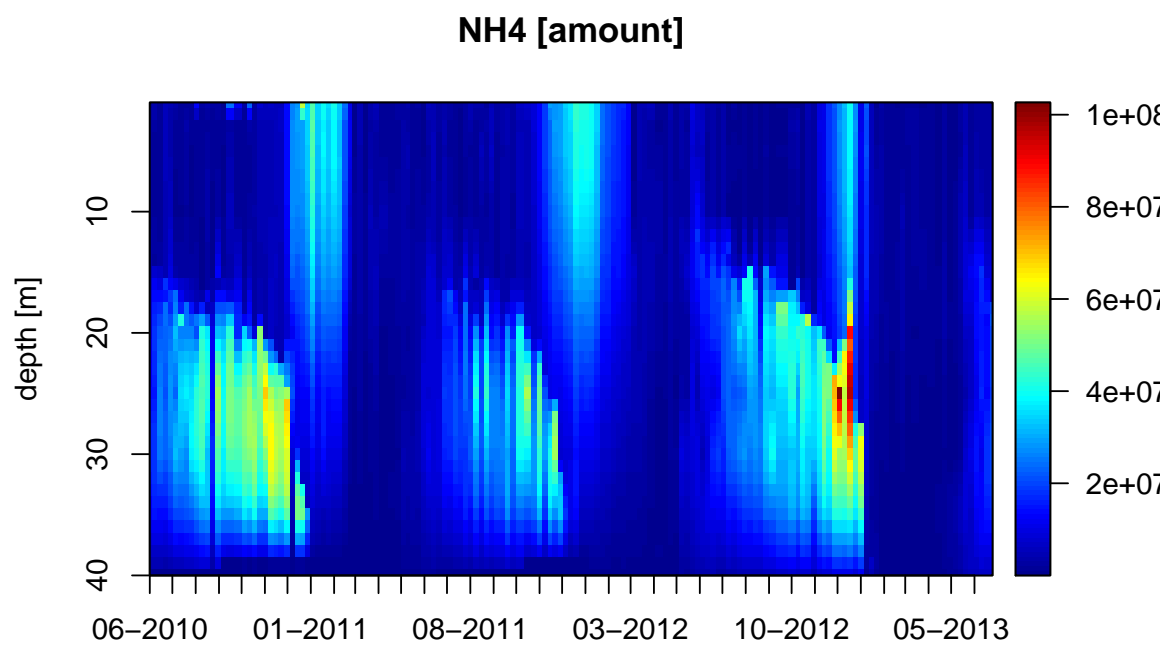
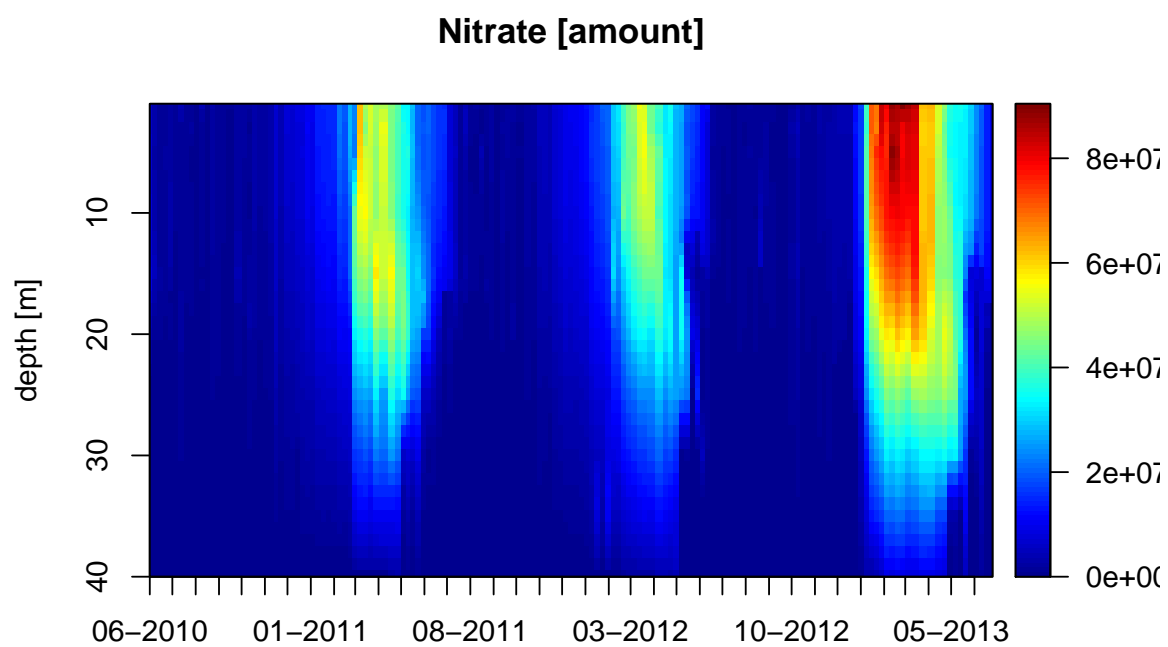
The following plots provide some visual estimation of the data to visualize time-depth processes for further considerations for the modelling of the processes

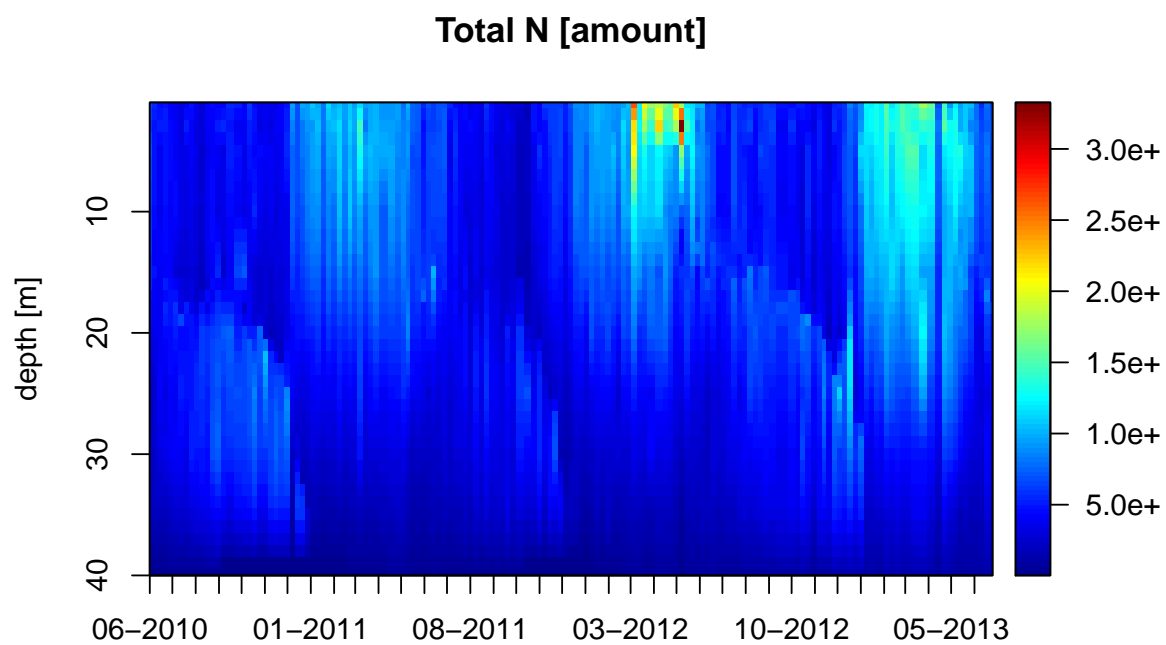
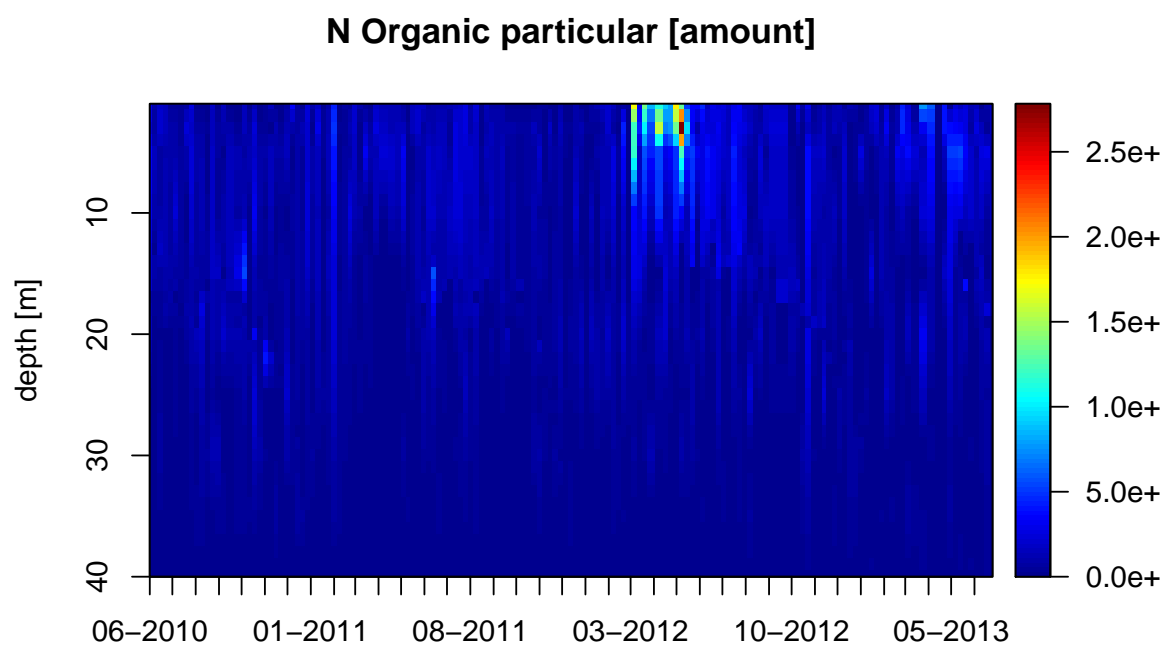
Oxygen [amount]



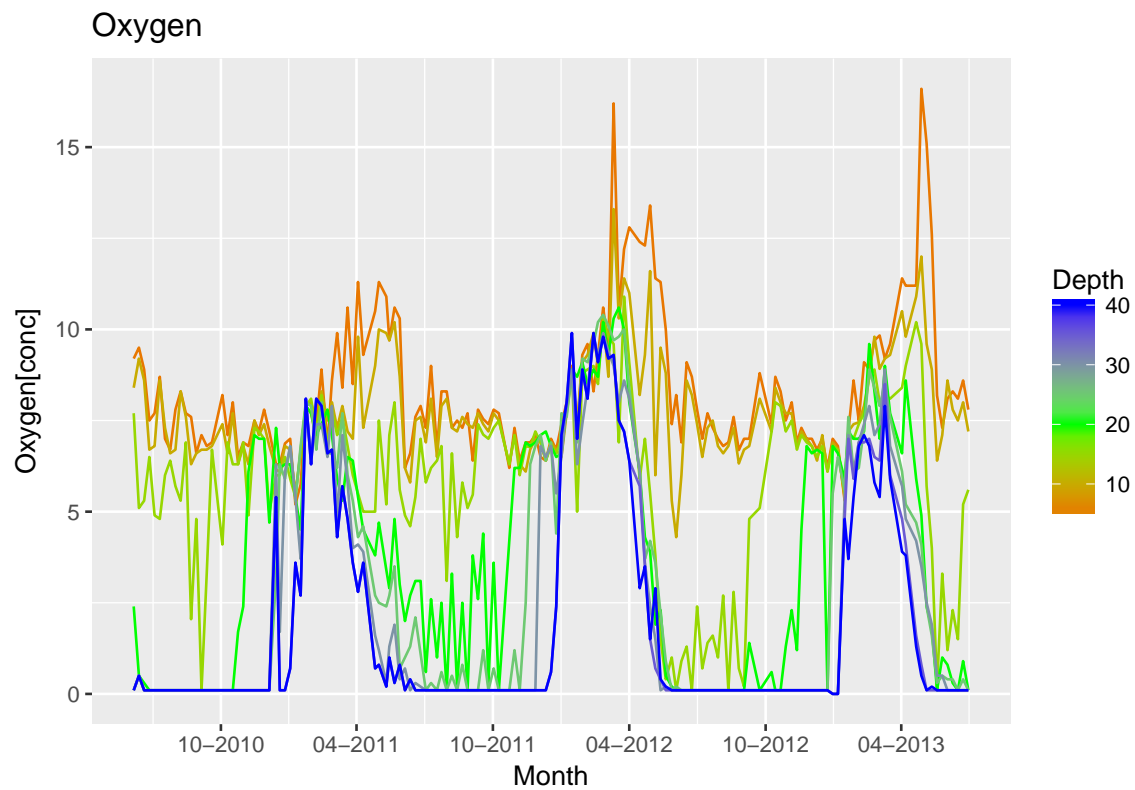
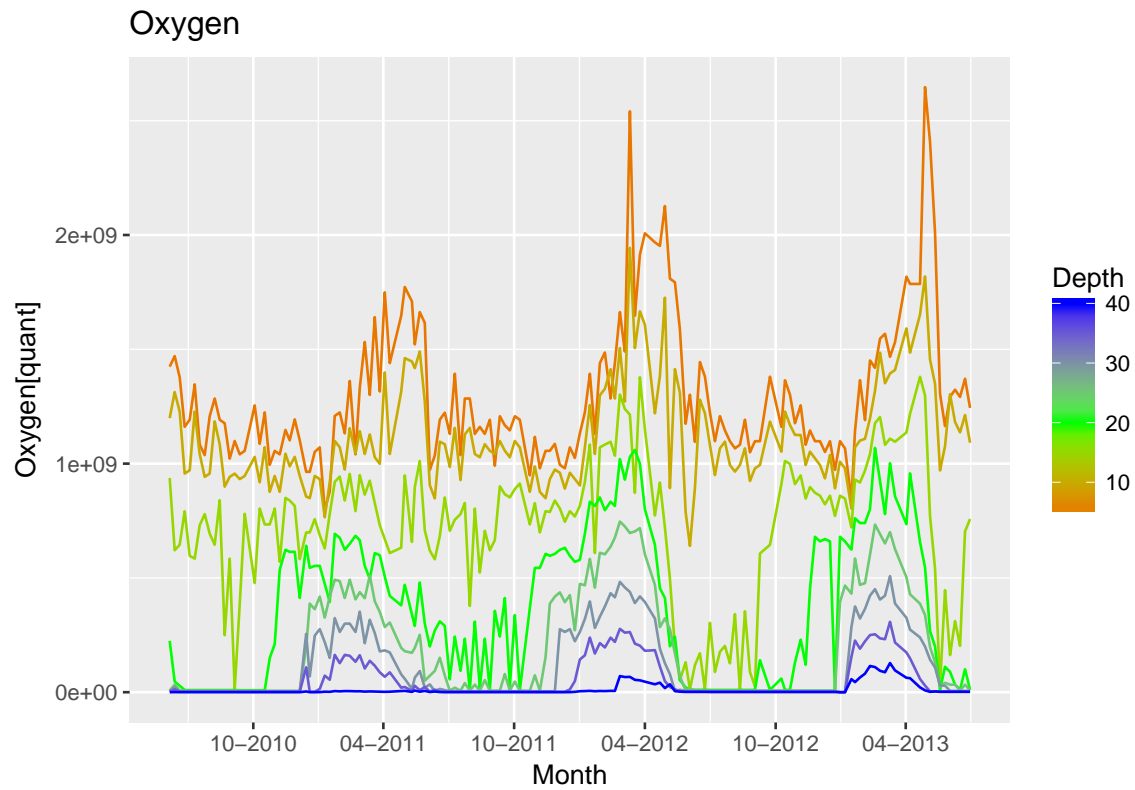
Oxygen [concentration]

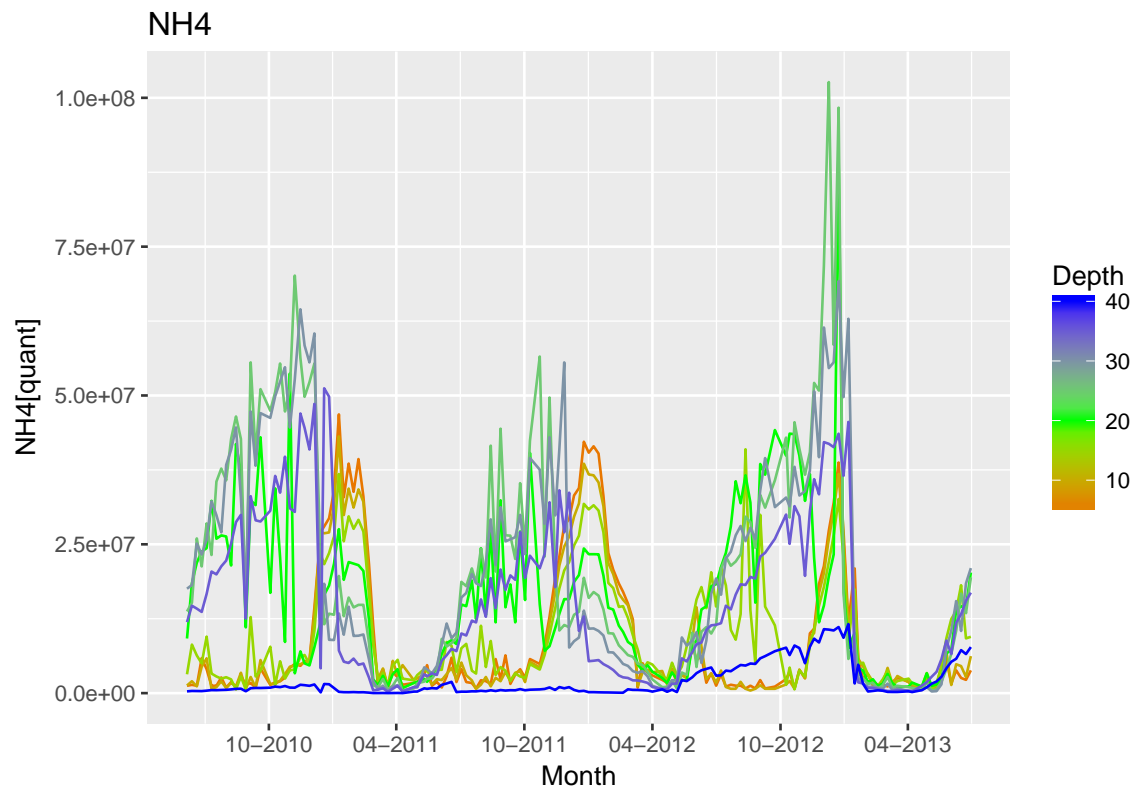
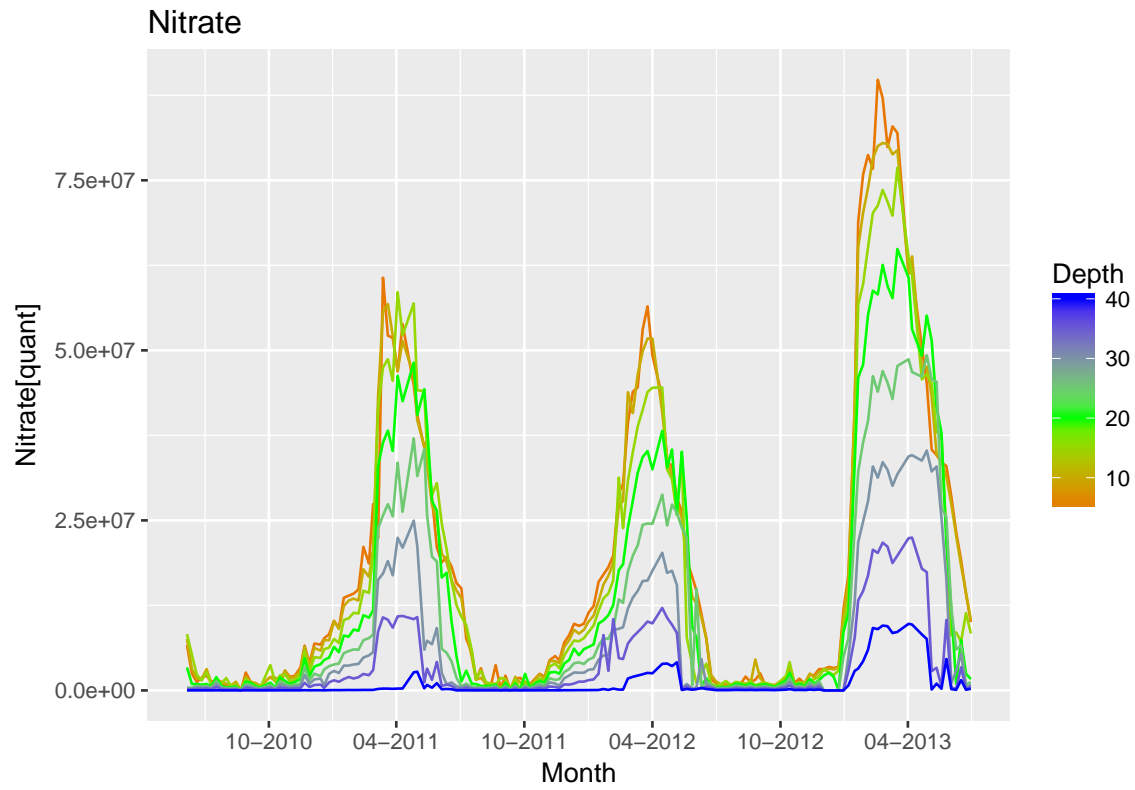






Time-depth cross sections

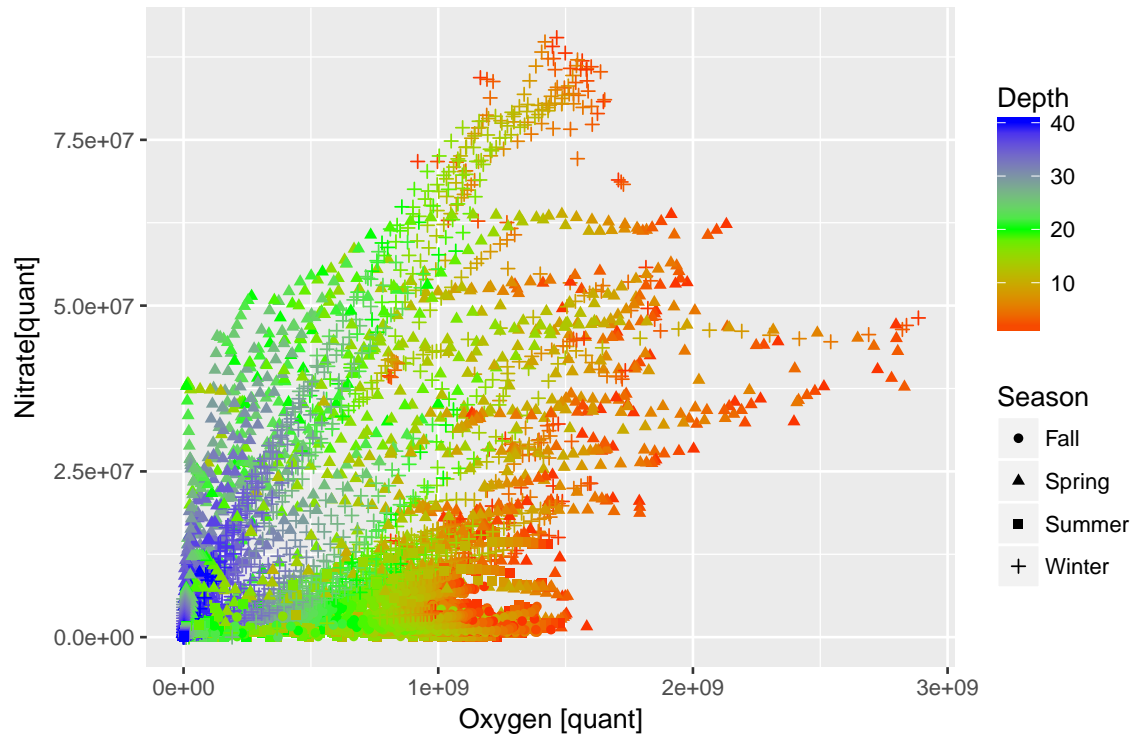




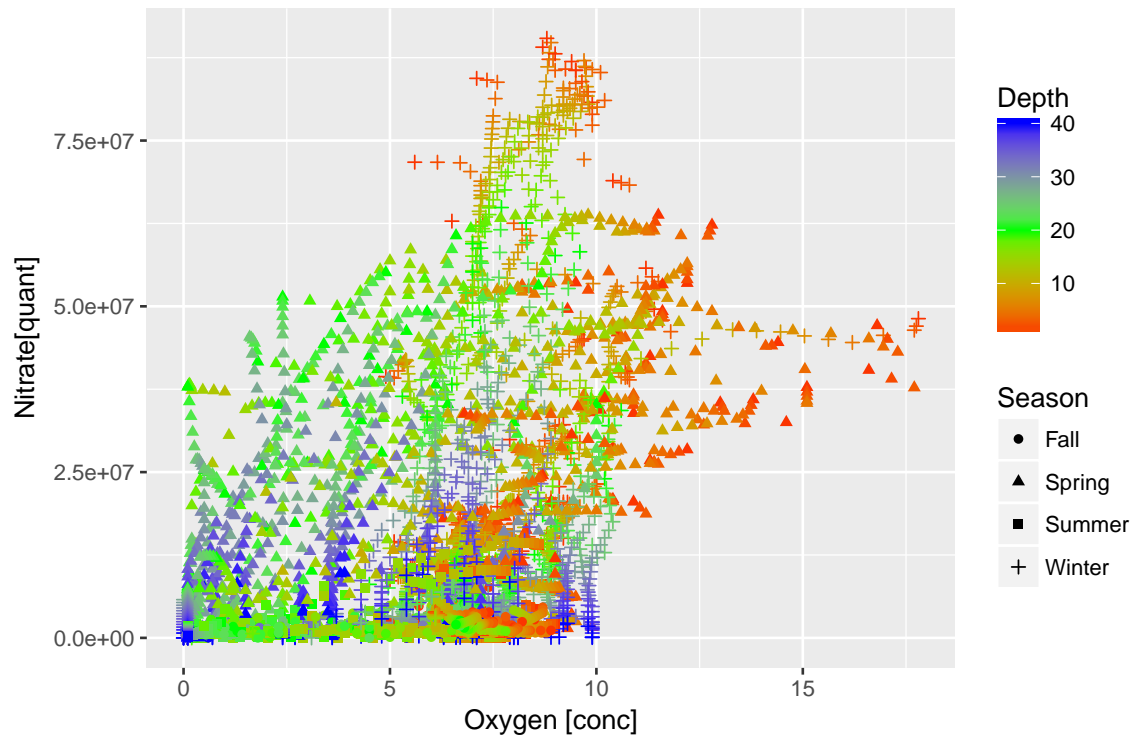
Correlation plots

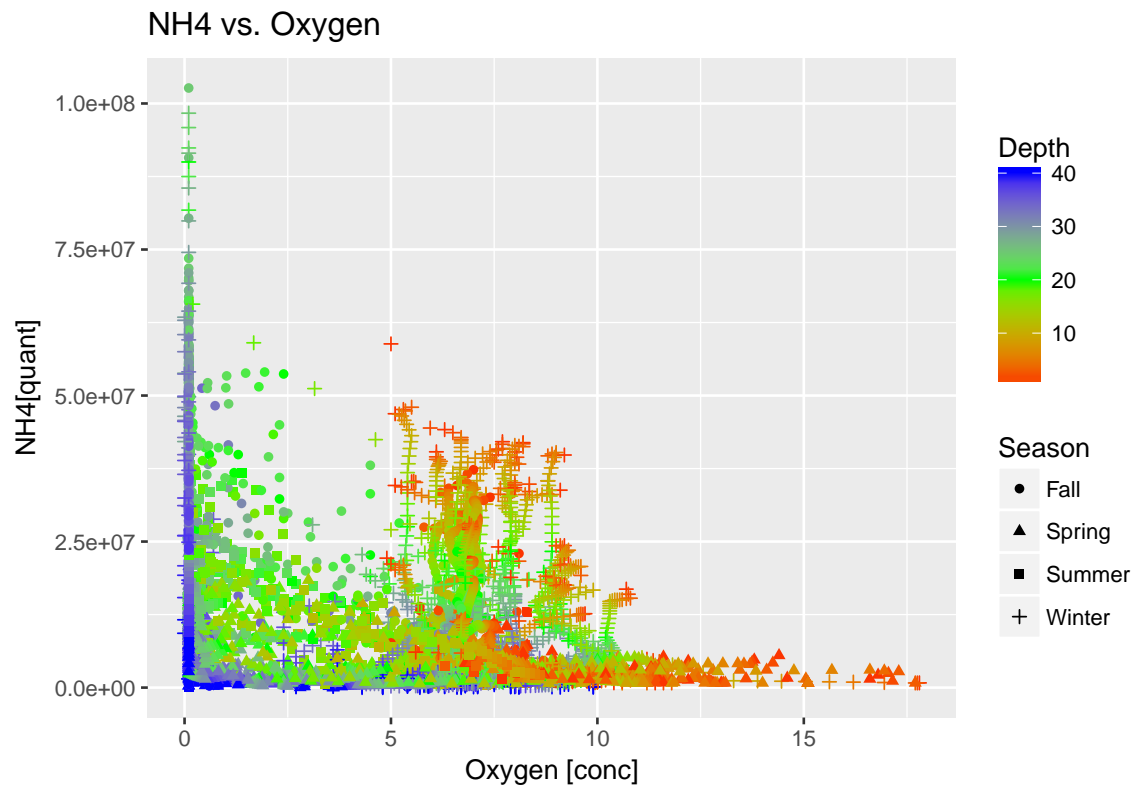
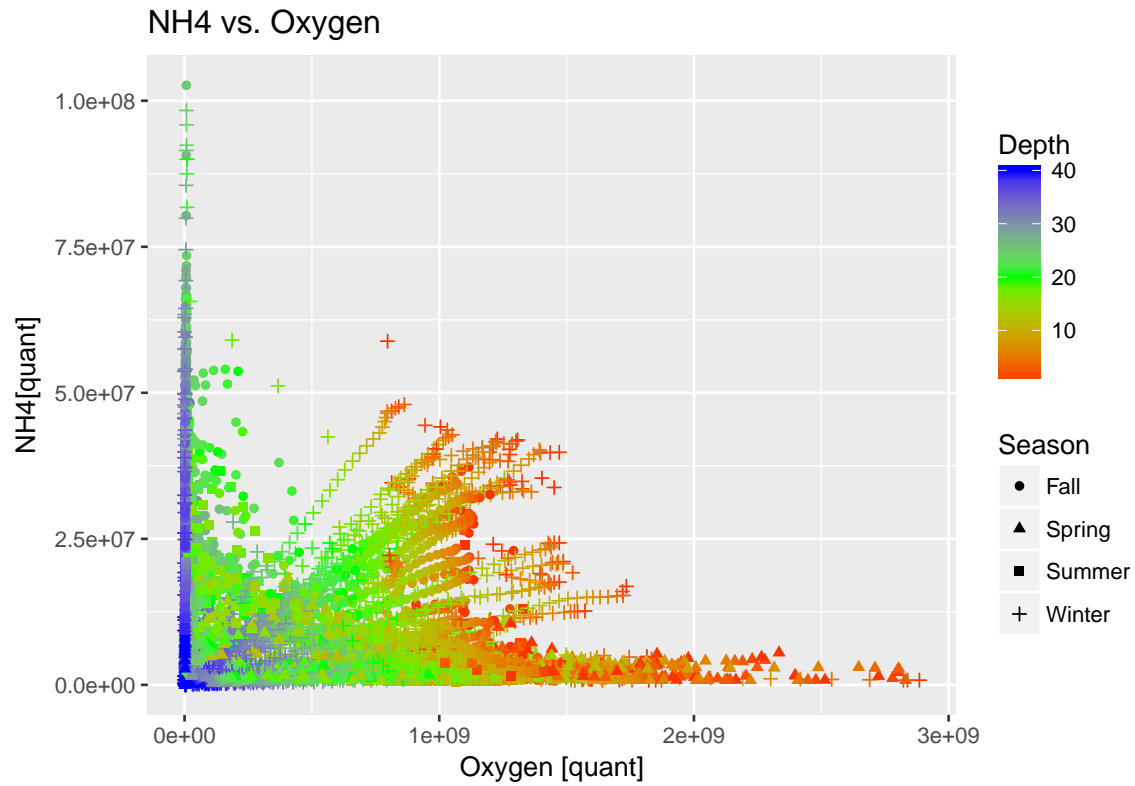
The following plots provide some visual estimation of data correlation

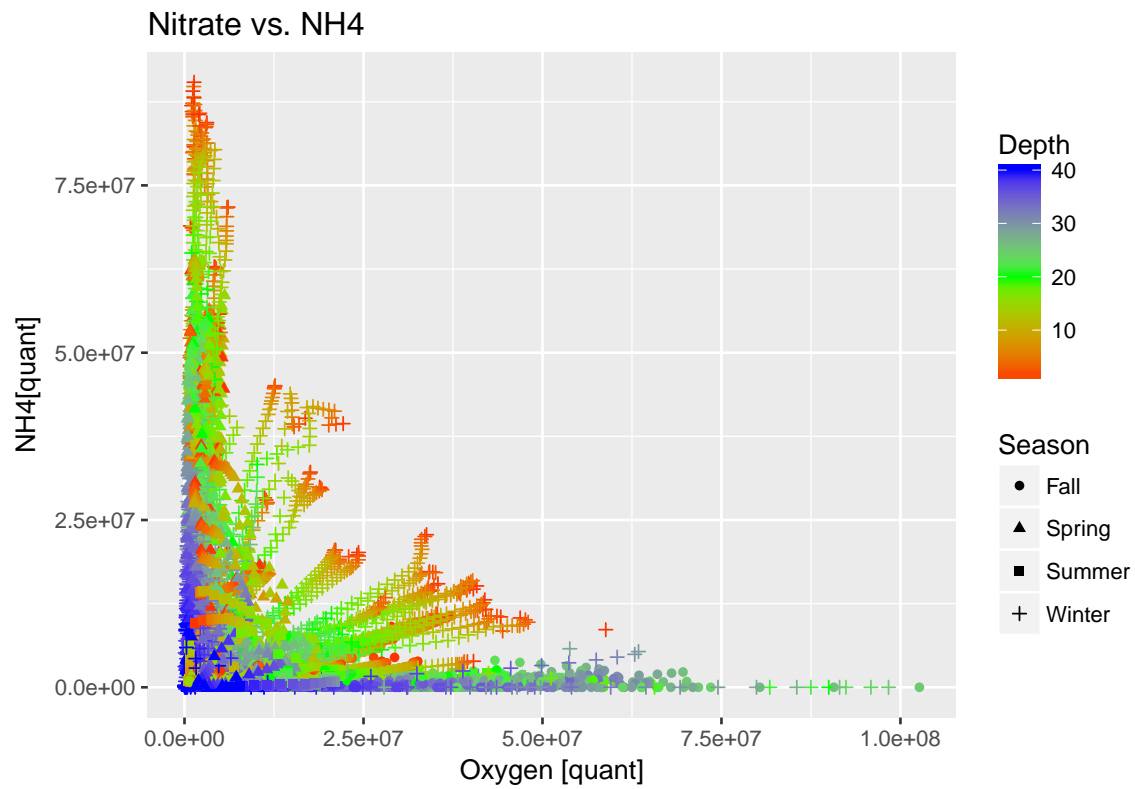
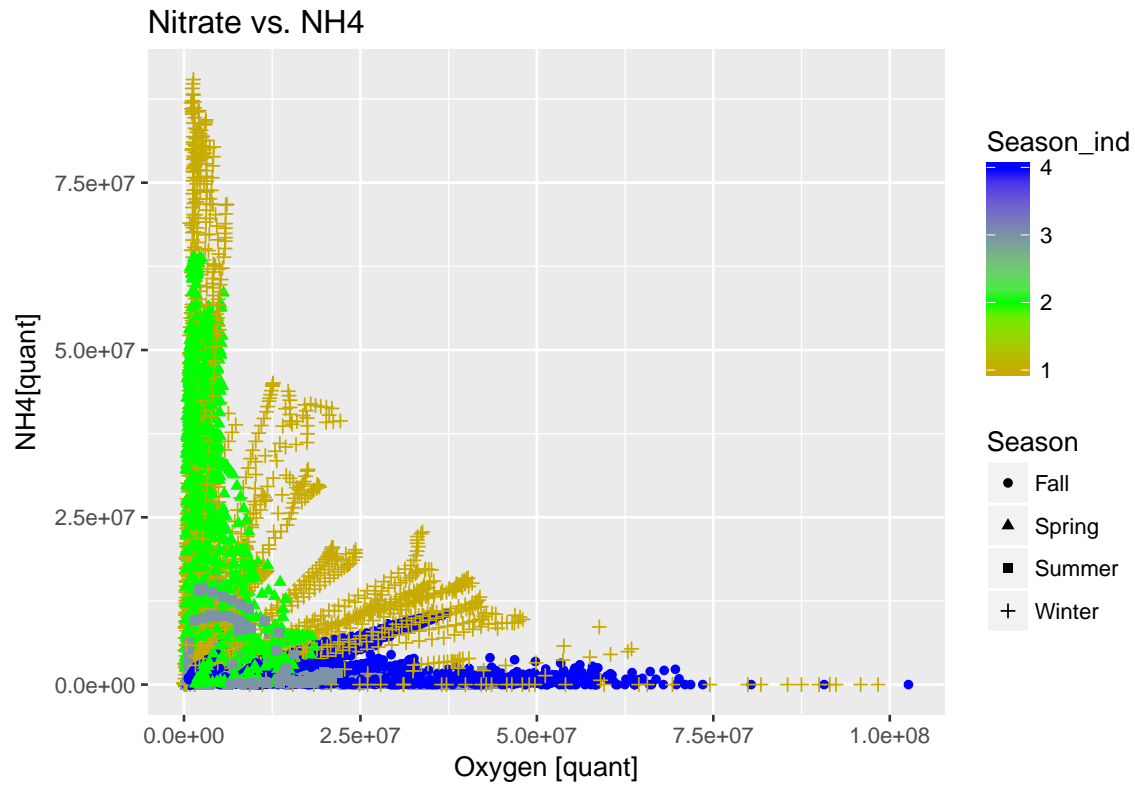
Nitrate vs. Oxygen



Nitrate vs. Oxygen

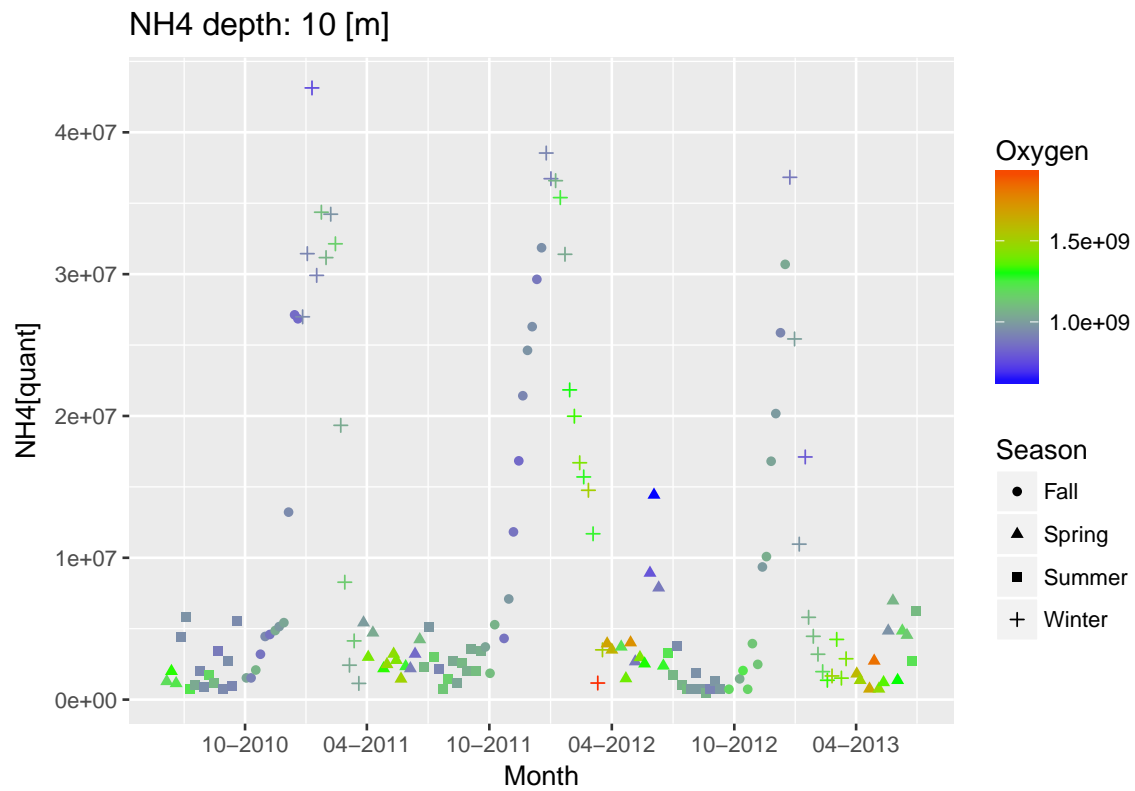
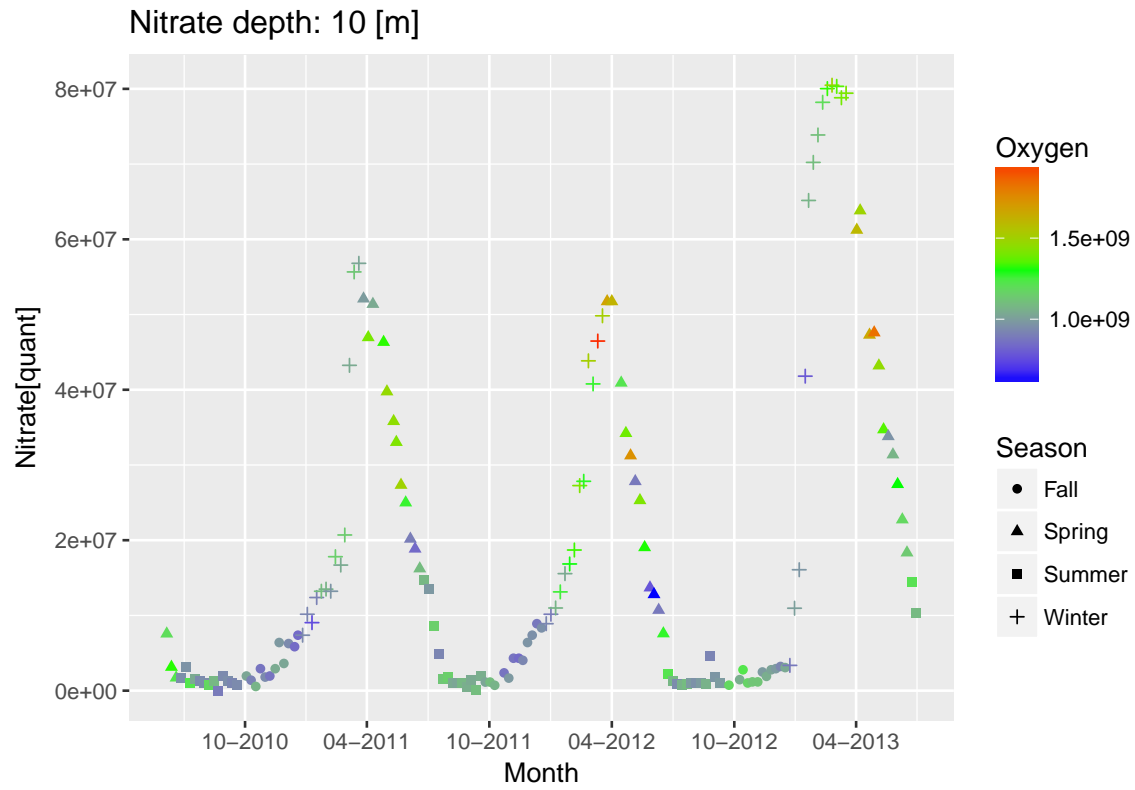


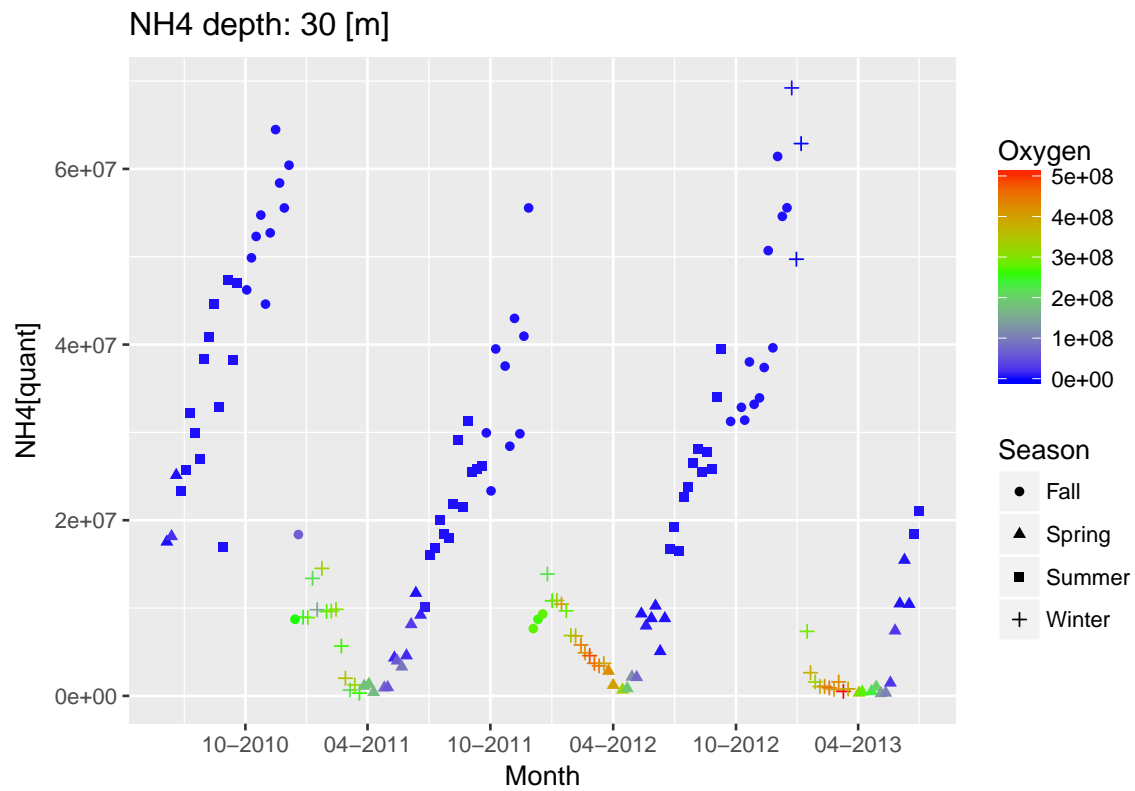
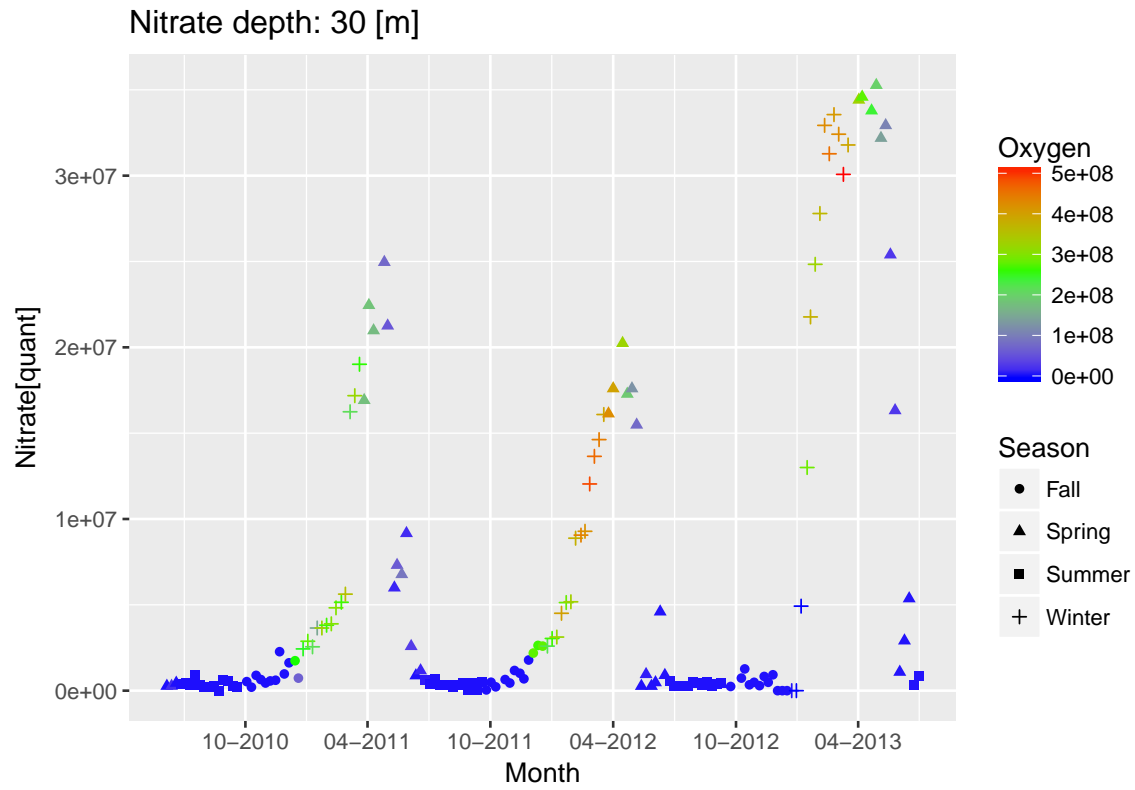




Model fitting estimation

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 build-up, 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).

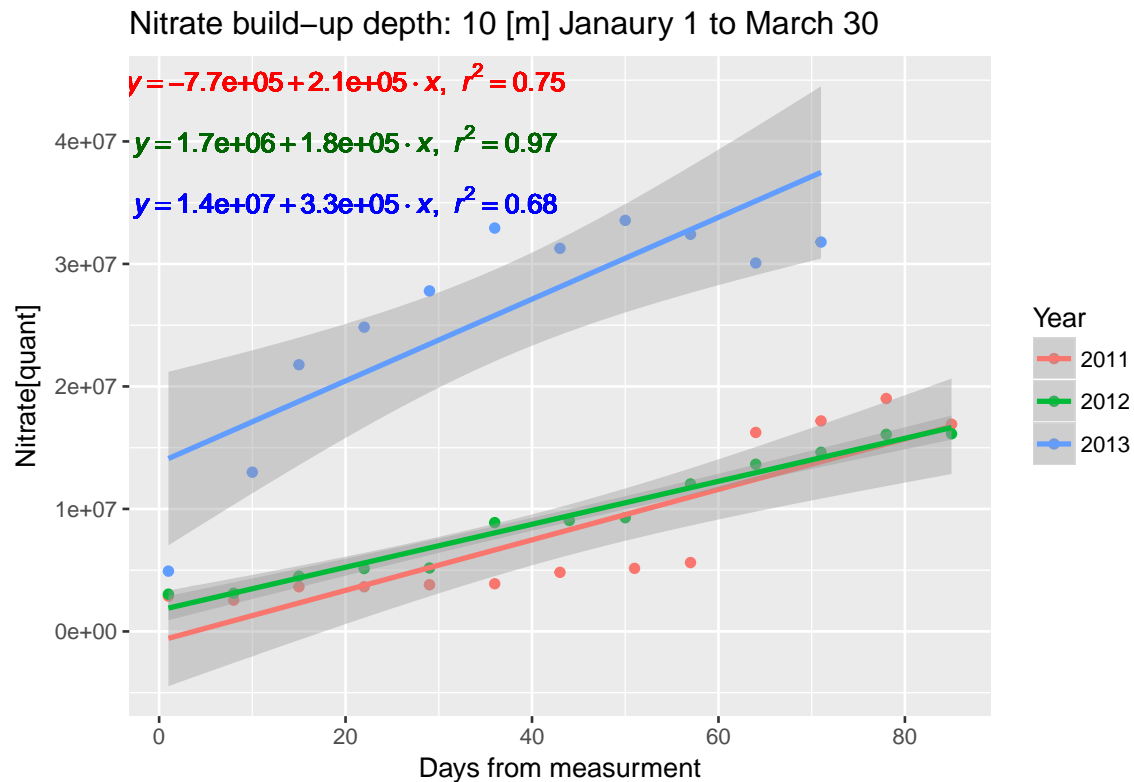




Process rate estimation

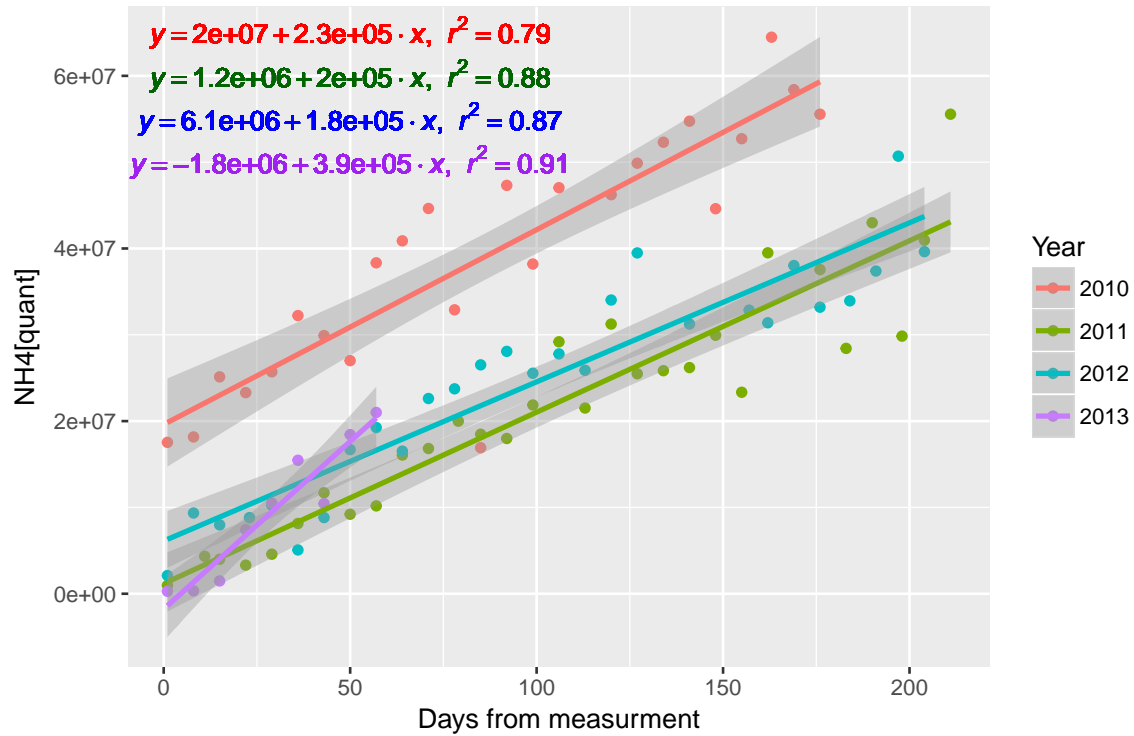
It can be observed from the figures presented above that nitrification is dominant in the upper portions of the lake (depicted for 10m depth), primarily between January and April, when the mixing of the lake decreases its content through a down-ward propagating mixing of the oxygenated epilimnion with the lower, oxygen-depleted hypolimnion. Ammonium, on the other hand, develops during the stratified lake conditions in its hypolimnion (depicted for depth 30 m), and peaks at the beginning of May, right before the mixing of the lake reaches the deeper parts of the lake, denitrification is halted, and the deeper lake is oxygenated once more.

Simulate Nitrate build-up between November 1st and April 30st in 10m depth in order to estimate processes rate



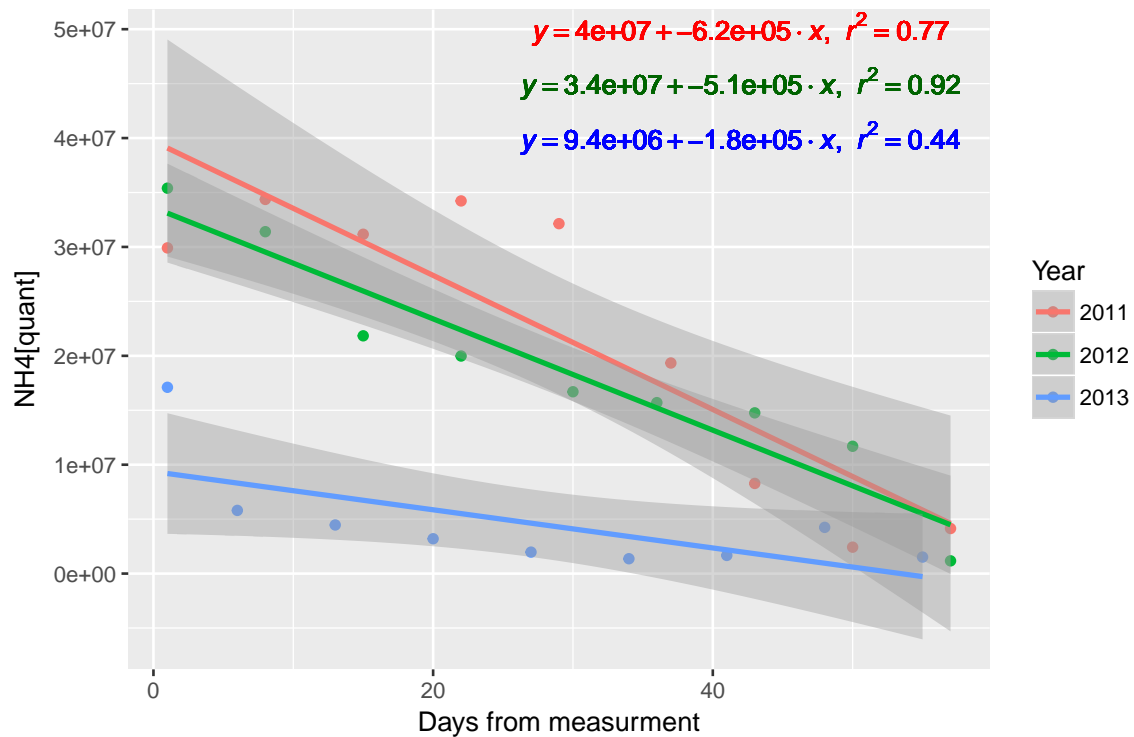
simulate NH4 build-up between April 30st and December 1st in 30m depth in order to estimate reaction rate

NH4 build-up depth: 30 [m] April 30 to December 1



simulate NH4 consumption between January 10th and March 15th in 30m depth in order to estimate reaction rate

NH4 consumption depth: 10 [m] January 10 to March 15



Coefficients assesment for all depths

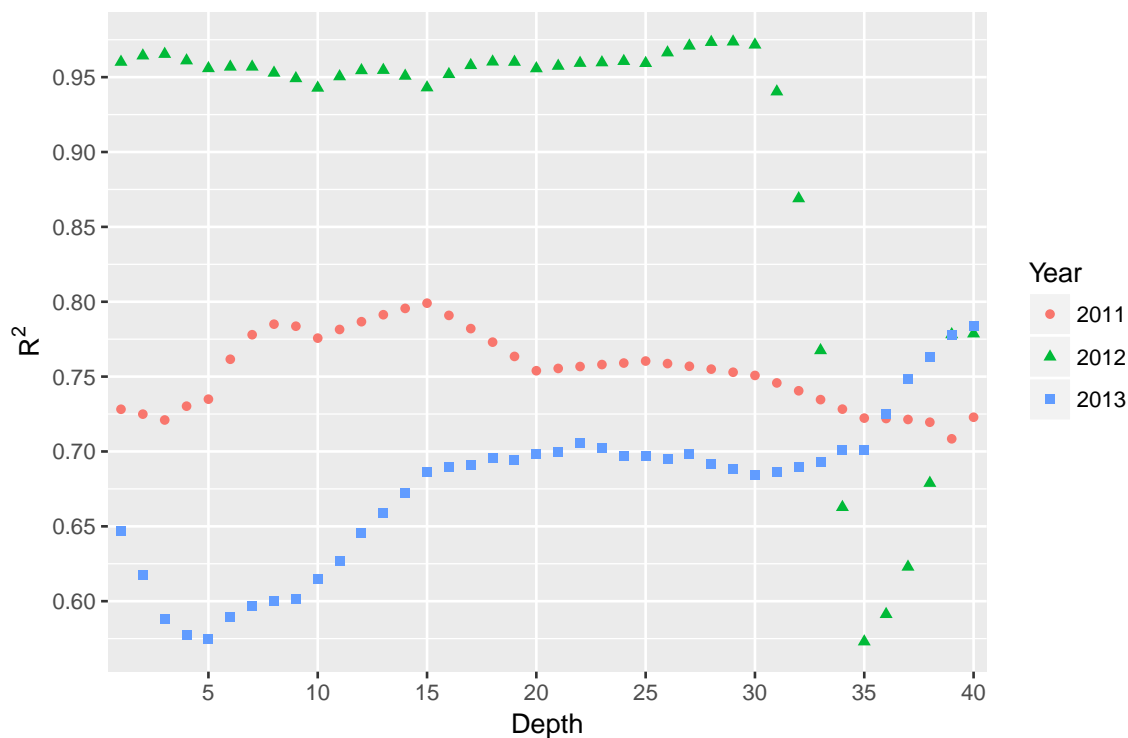
After consideration of the dominant processes that control nitrate and ammonium content in the lake, the following section provides an assesment of the processes and their fit to a linear model in each depth. The R^2 value can be used to asses the best fit of the model for each depth. It can be observed that nitrate buildup fits a linear model in most depths, although some intraannual changes illustrate the complexity of the system and its divergence from linearity. The coefficients of the model also show a wide range, and illustrate that the best R^2 values were found for the year 2012 (triangles) and values of ca. $a = 5 * 10^6$ and $b = 4 * 10^5$ that describe nitrate build up between Novemebr 1st and April 31st using the following equation:

$$NO_3 = 5 * 10^6 * t + 4 * 10^5$$

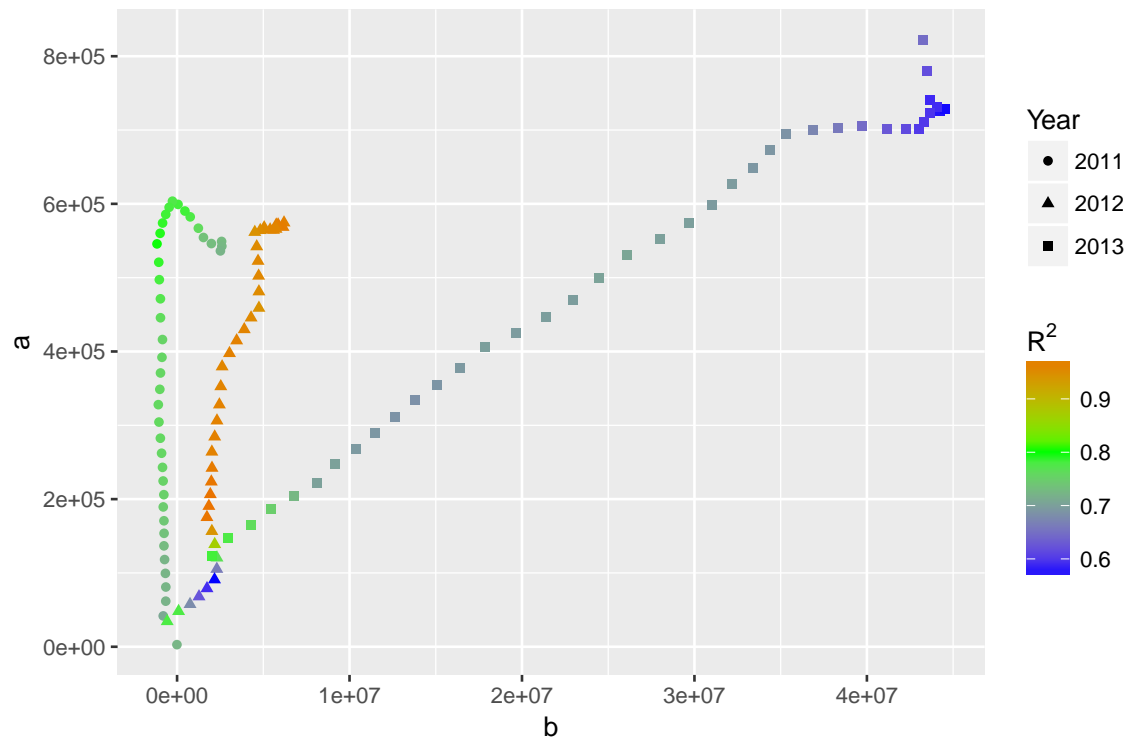
, where t is provided in days.

##	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

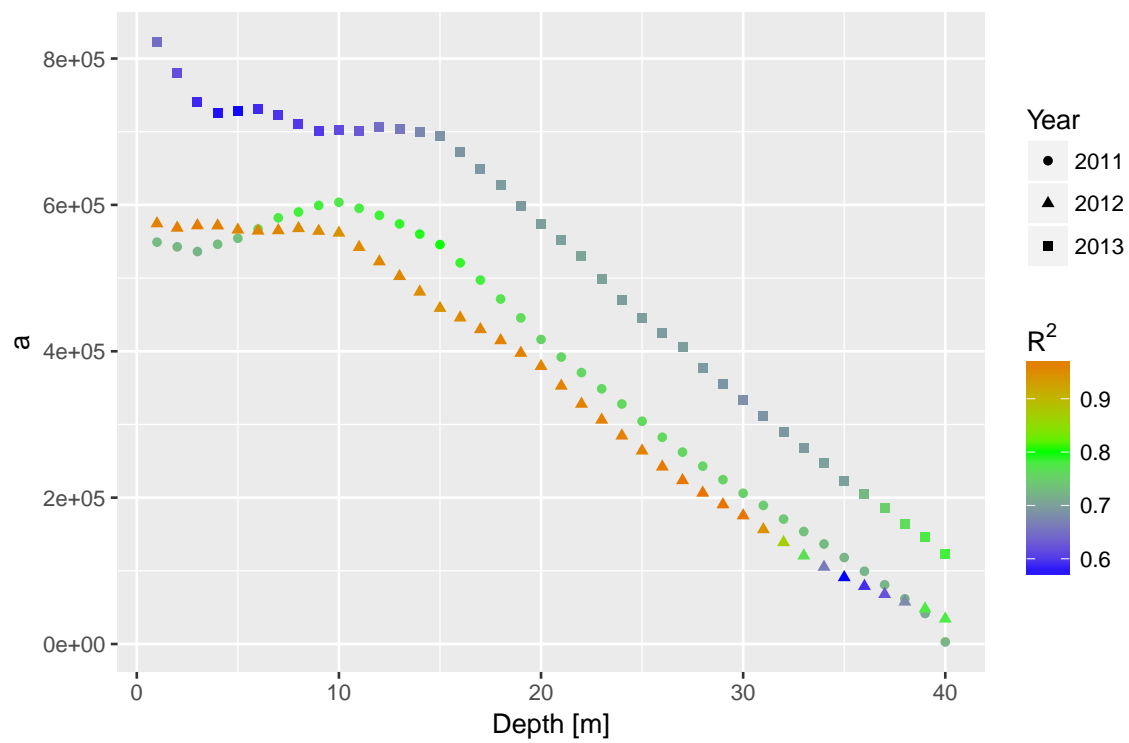
Nitrate build-up Linear Modeling: Janaury 1 to March 30



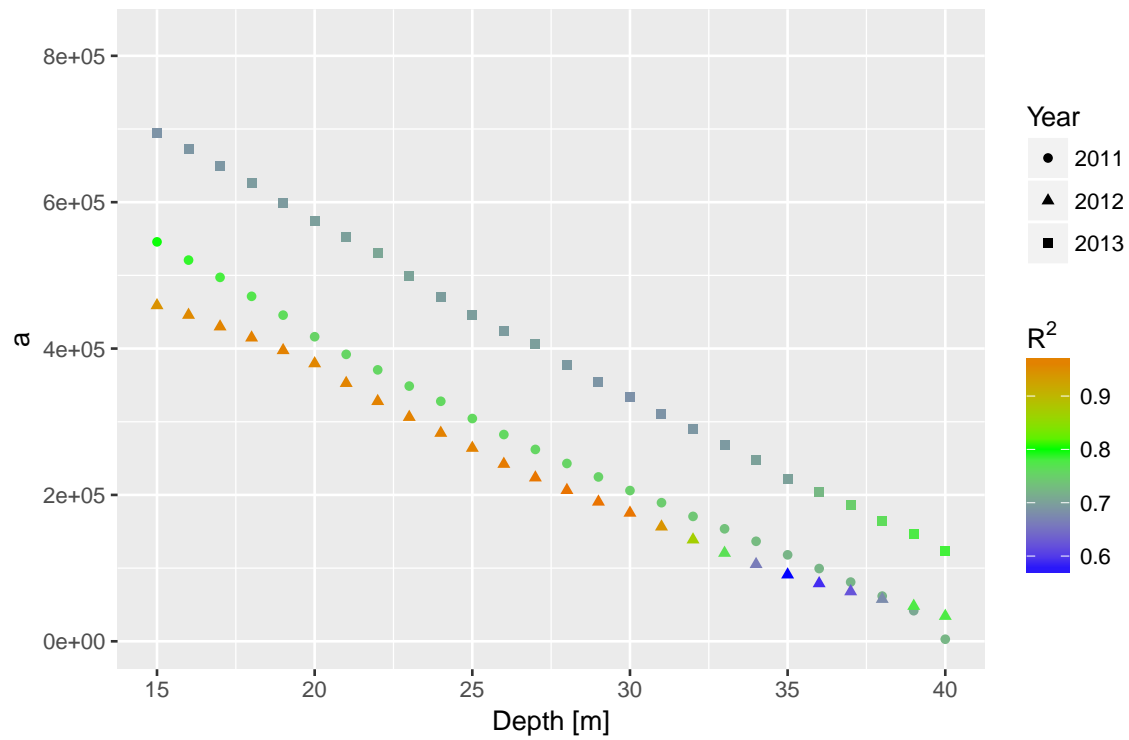
Nitrate build-up Linear Modeling: Janaury 1 to March 30



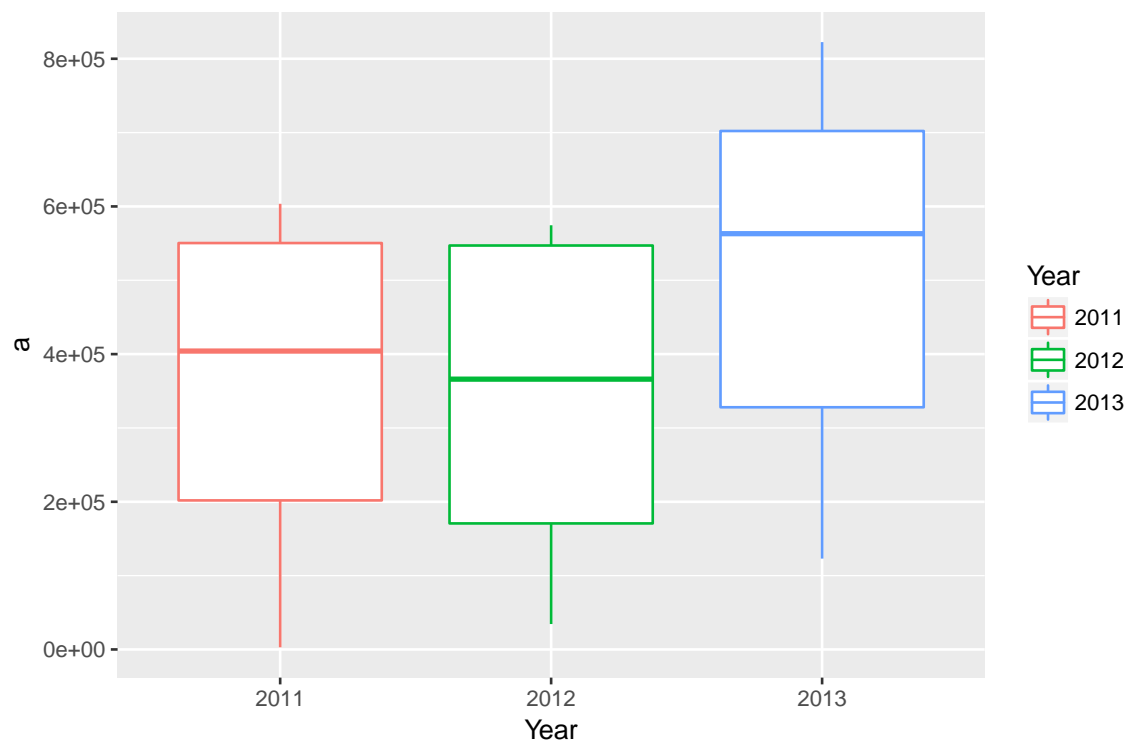
Nitrate build-up Linear Modeling: Janaury 1 to March 30



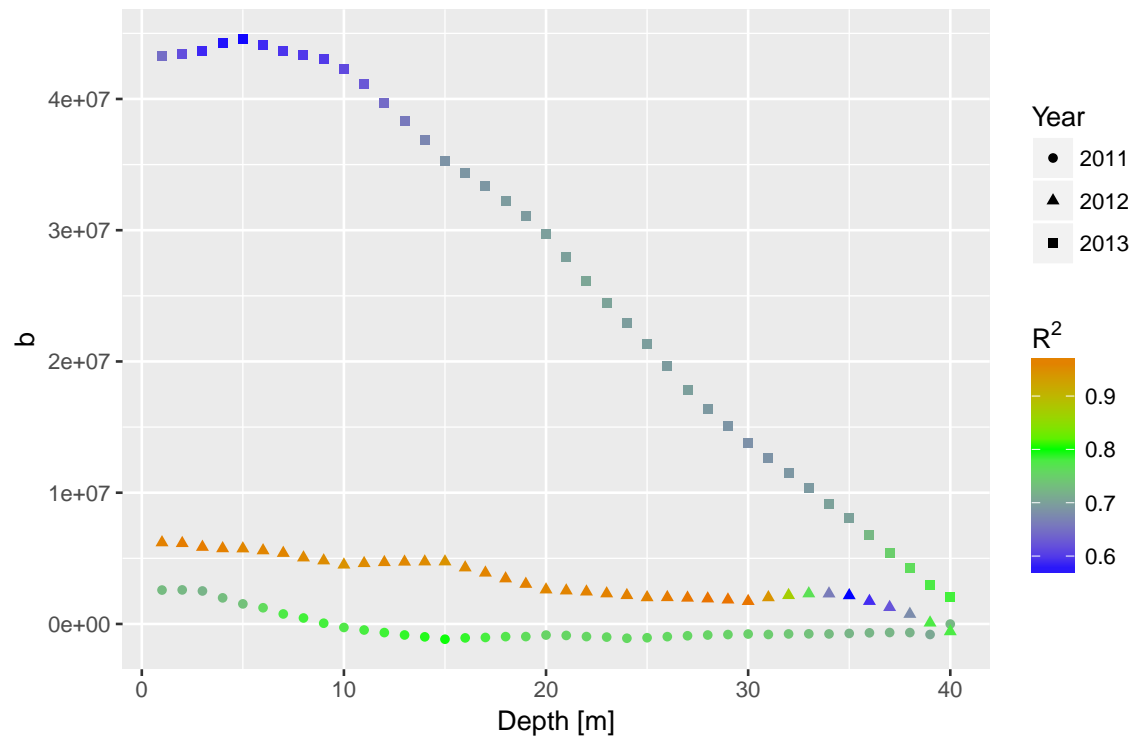
Nitrate build-up Linear Modeling: Janaury 1 to March 30



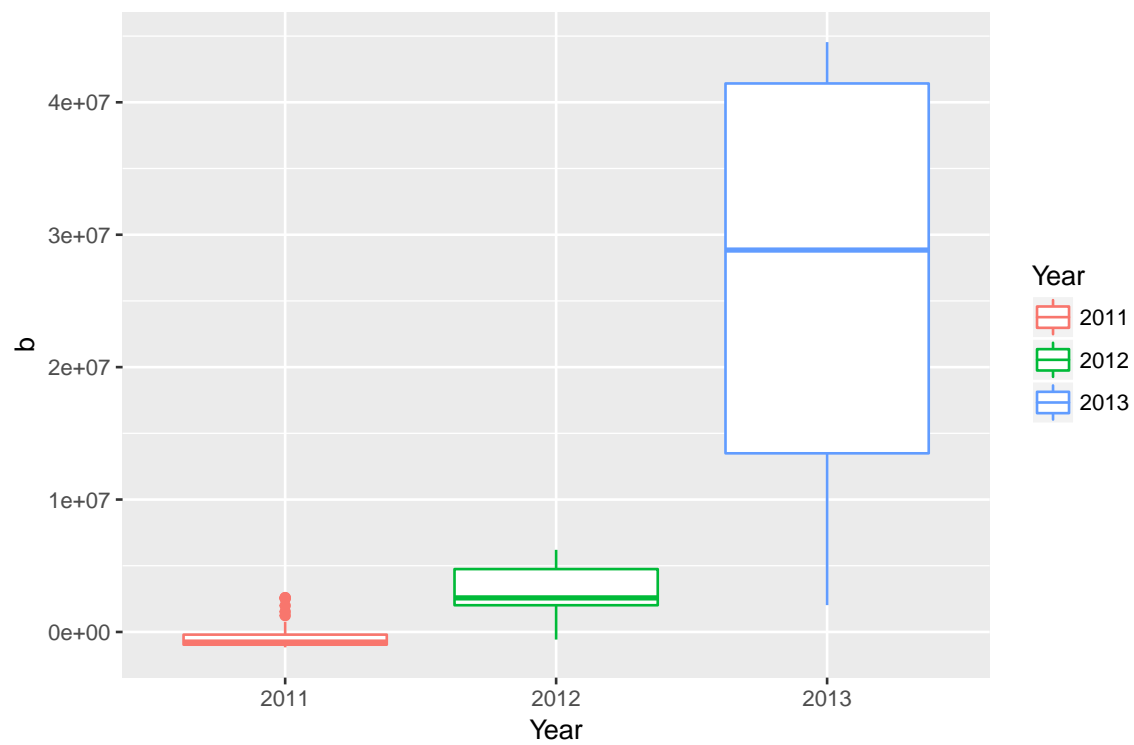
a parameter for Nitrate build-up: Janaury 1 to March 30

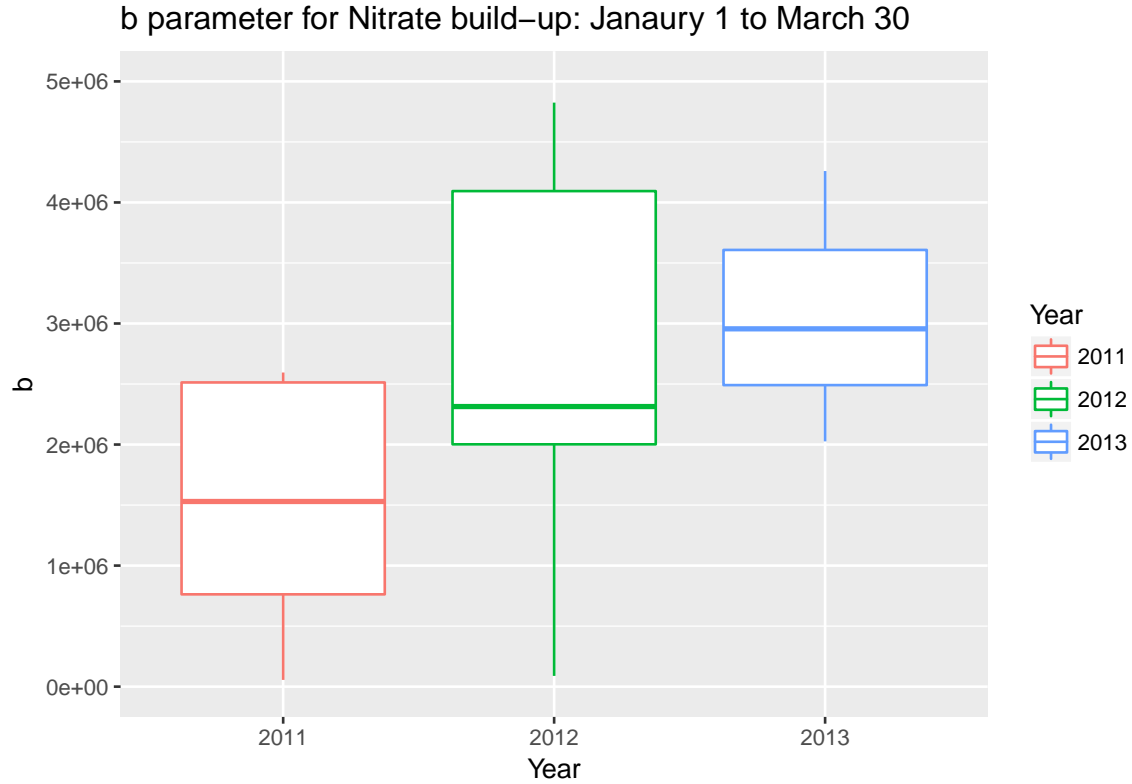


Nitrate build-up Linear Modeling: Janaury 1 to March 30



b parameter for Nitrate build-up: Janaury 1 to March 30





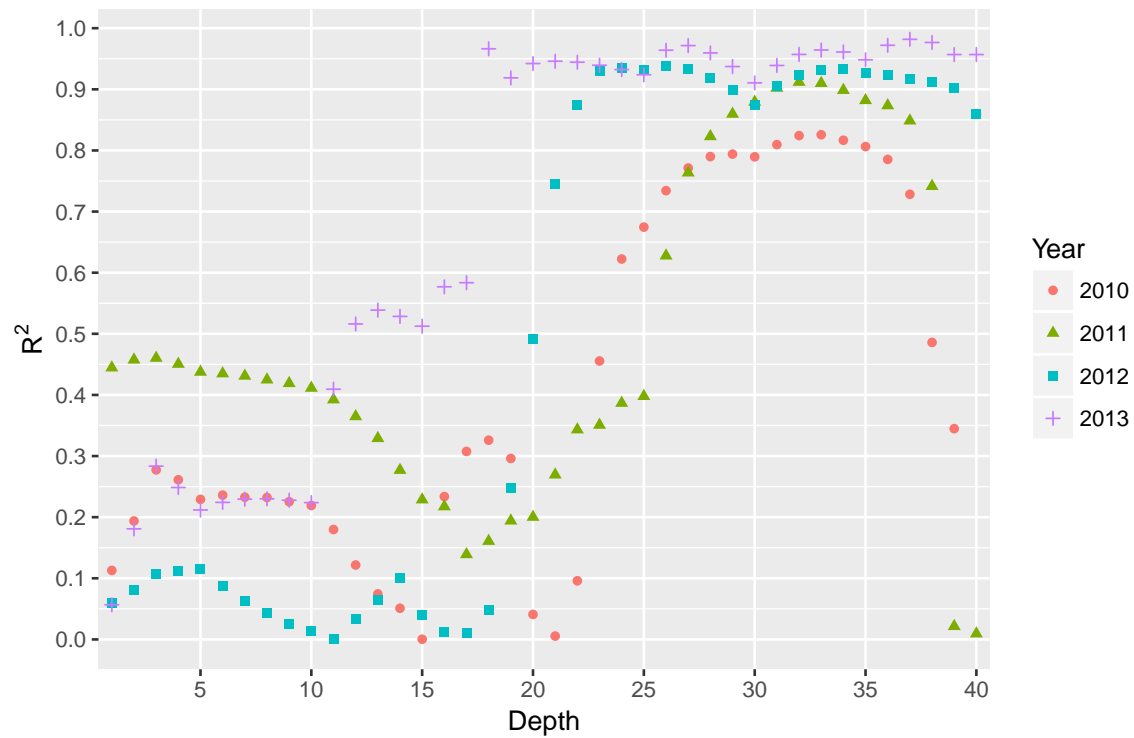
It can be observed that ammonium buildup does fit the linear model in most depths as nicely as nitrate. Intraannual changes are significant, and once more illustrate the complexity of the system and its divergence from linearity. The coefficients of the model show a slightly smaller range, and illustrate that the best R^2 values of ca. $a = 5 * 10^6$ and $b = 5 * 10^5$ that describe ammonium build up between April 30th and December 1st using the following equation:

$$NH_4 = 5 * 10^6 t + 5 * 10^5$$

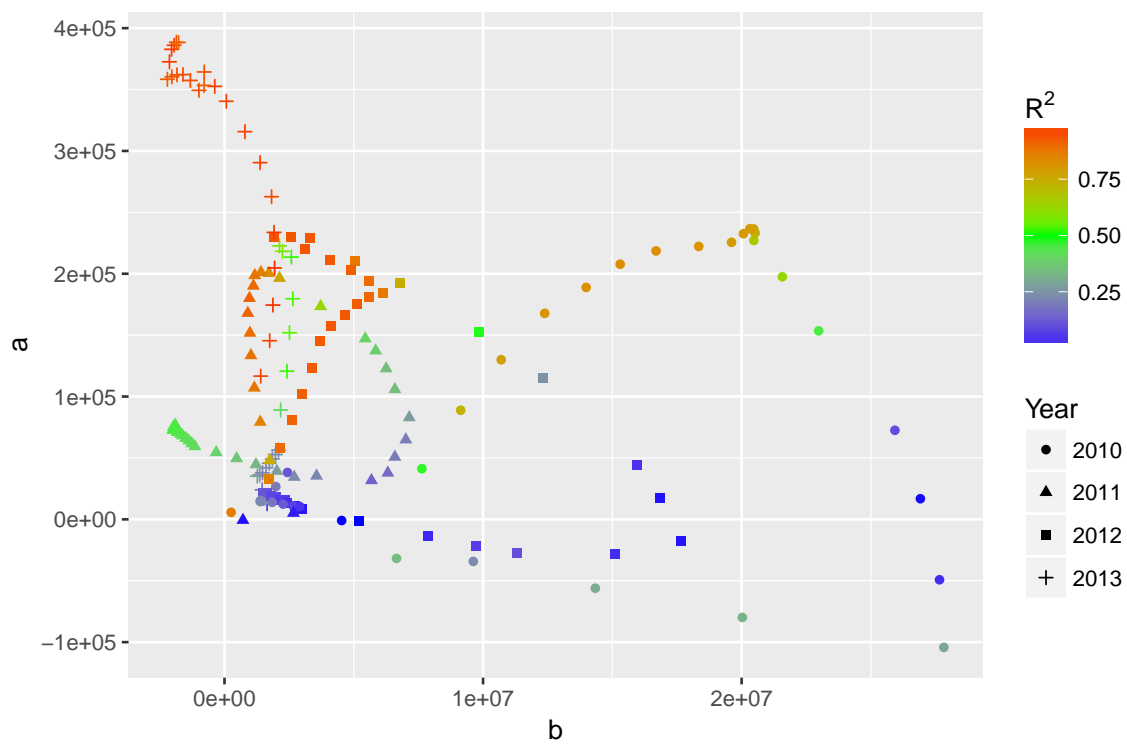
, where t is provided in days. Unsurprisingly, the model has the best fit for depths of 20 to 35m, where oxygenation is solely depends on annual stratification and monomictic mixing.

##	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

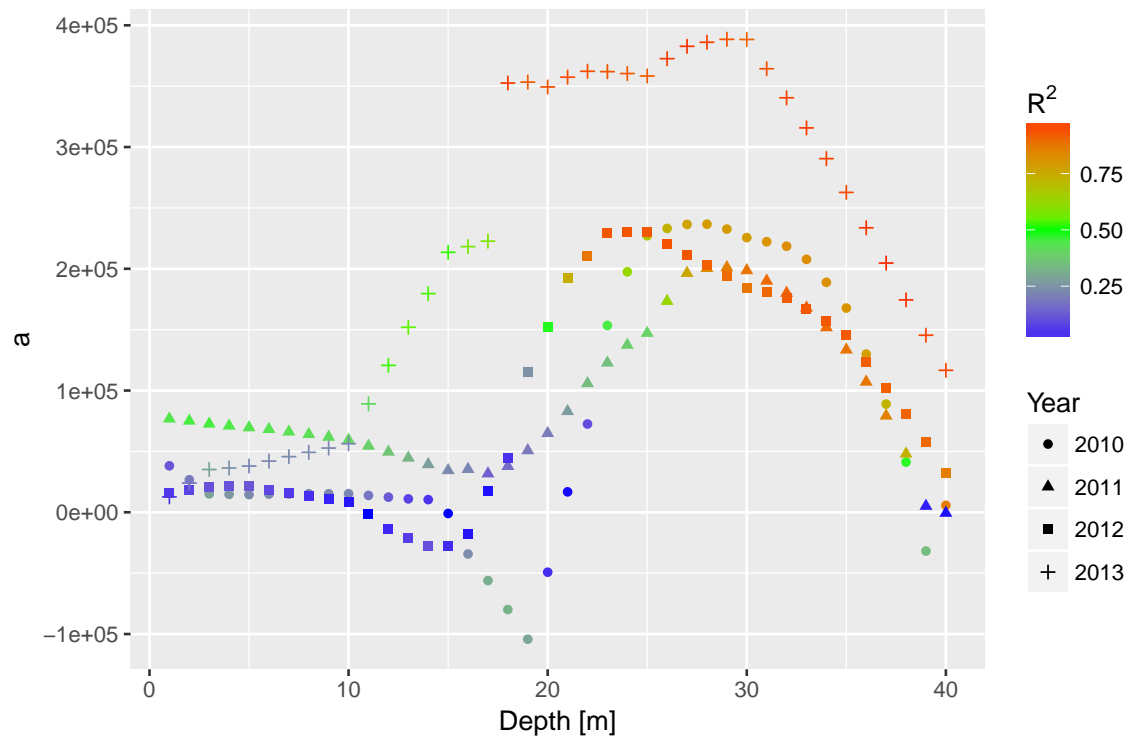
NH4 build-up Linear Modeling: April 30 to December 1



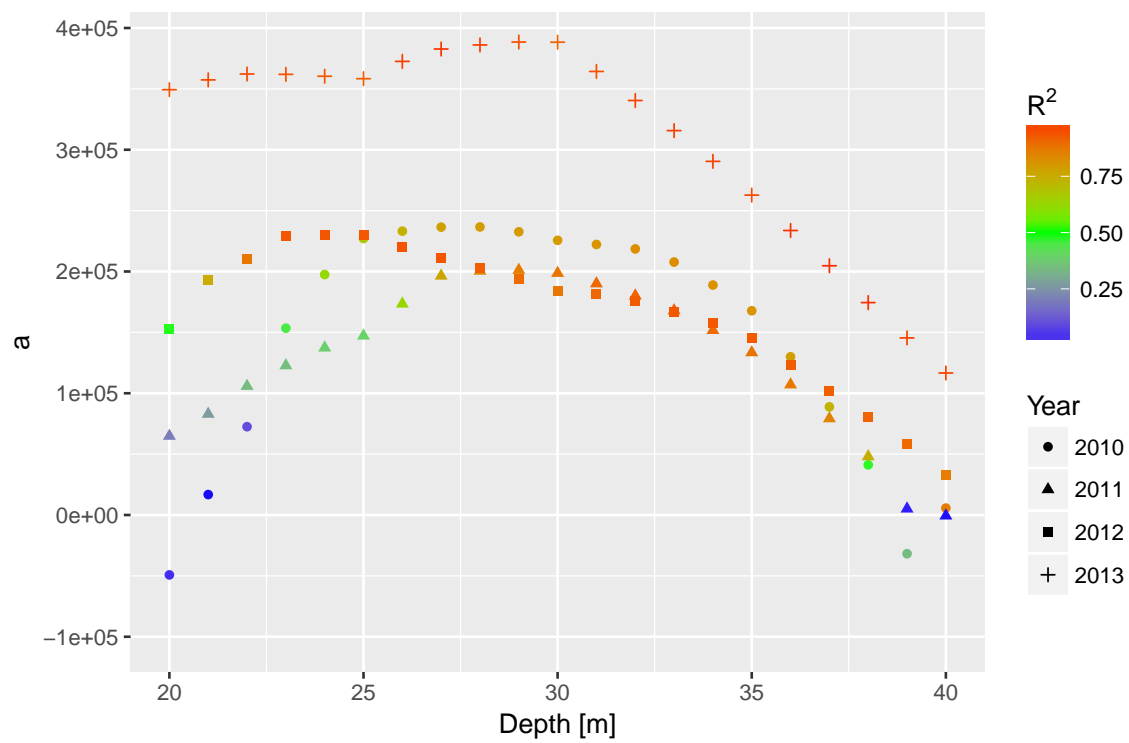
NH4 build-up Linear Modeling: April 30 to December 1



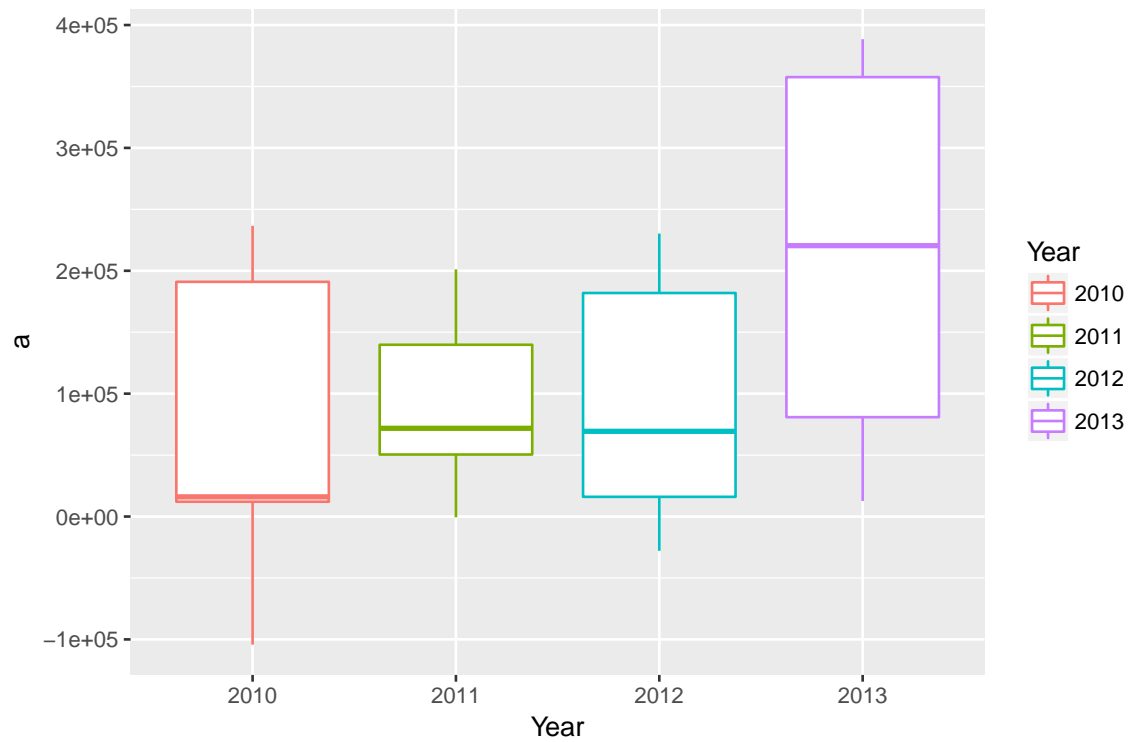
NH4 build-up Linear Modeling: April 30 to December 1



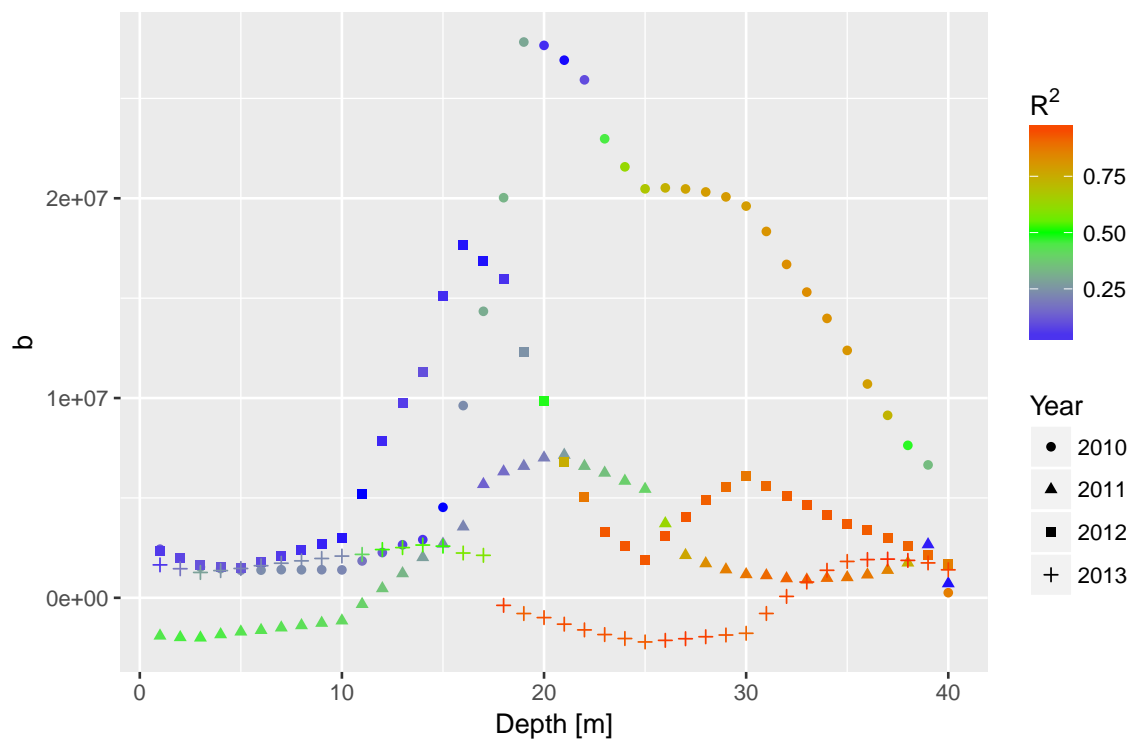
NH4 build-up Linear Modeling: April 30 to December 1



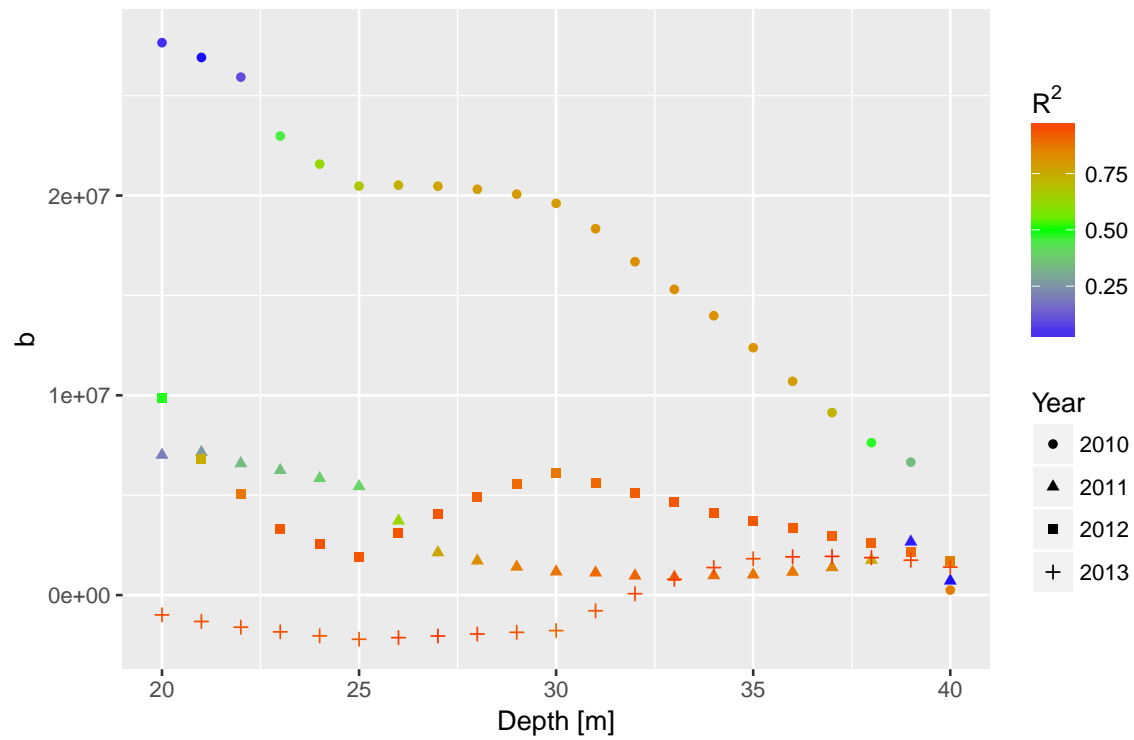
a parameter for NH4 build-up: April 30 to December 1



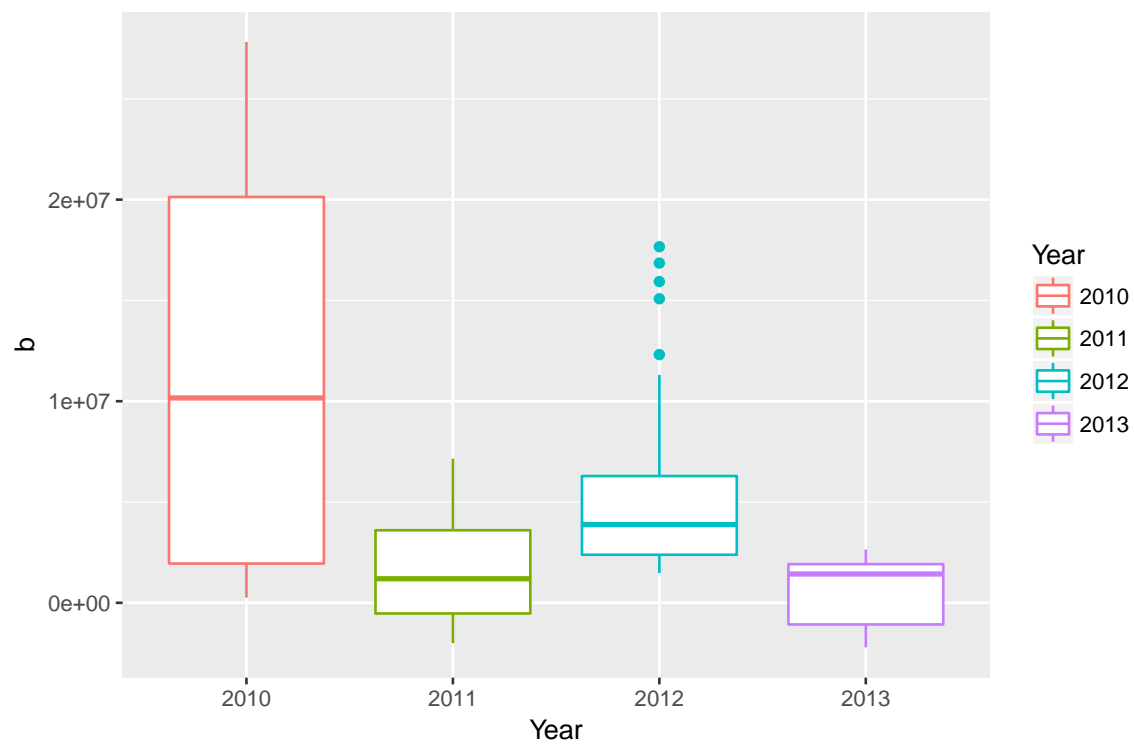
NH4 build-up Linear Modeling: April 30 to December 1

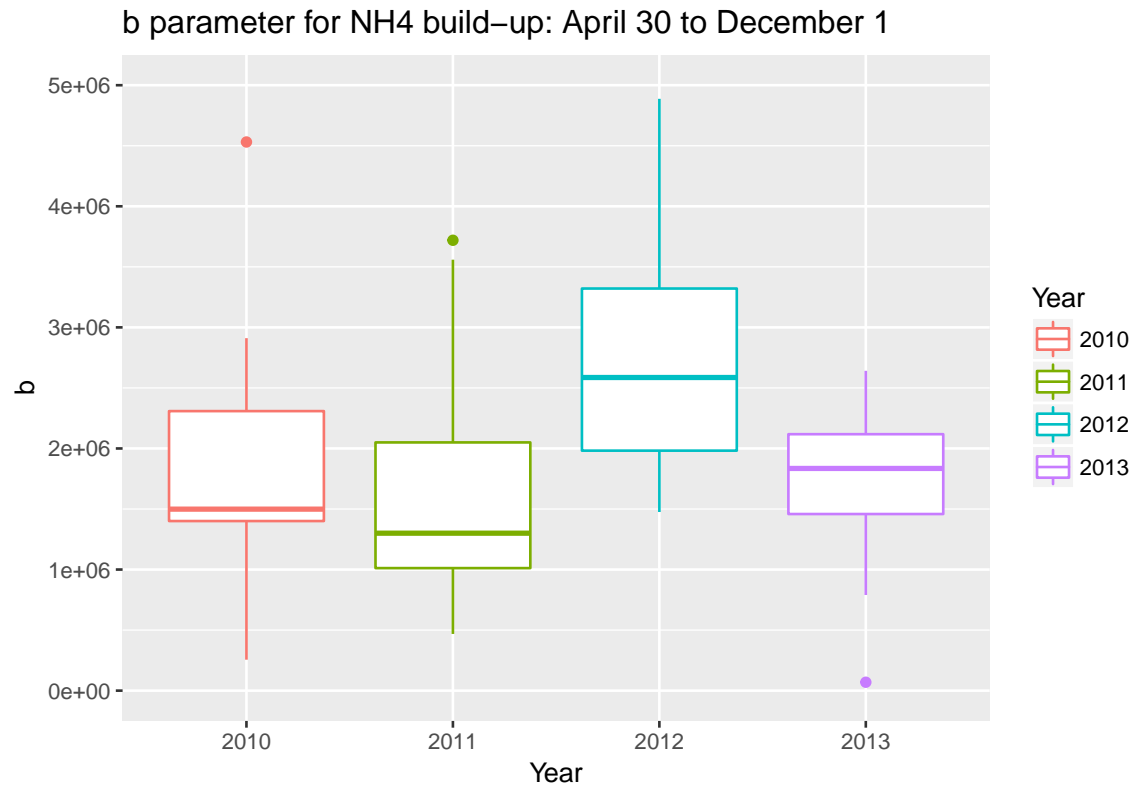


NH4 build-up Linear Modeling: April 30 to December 1



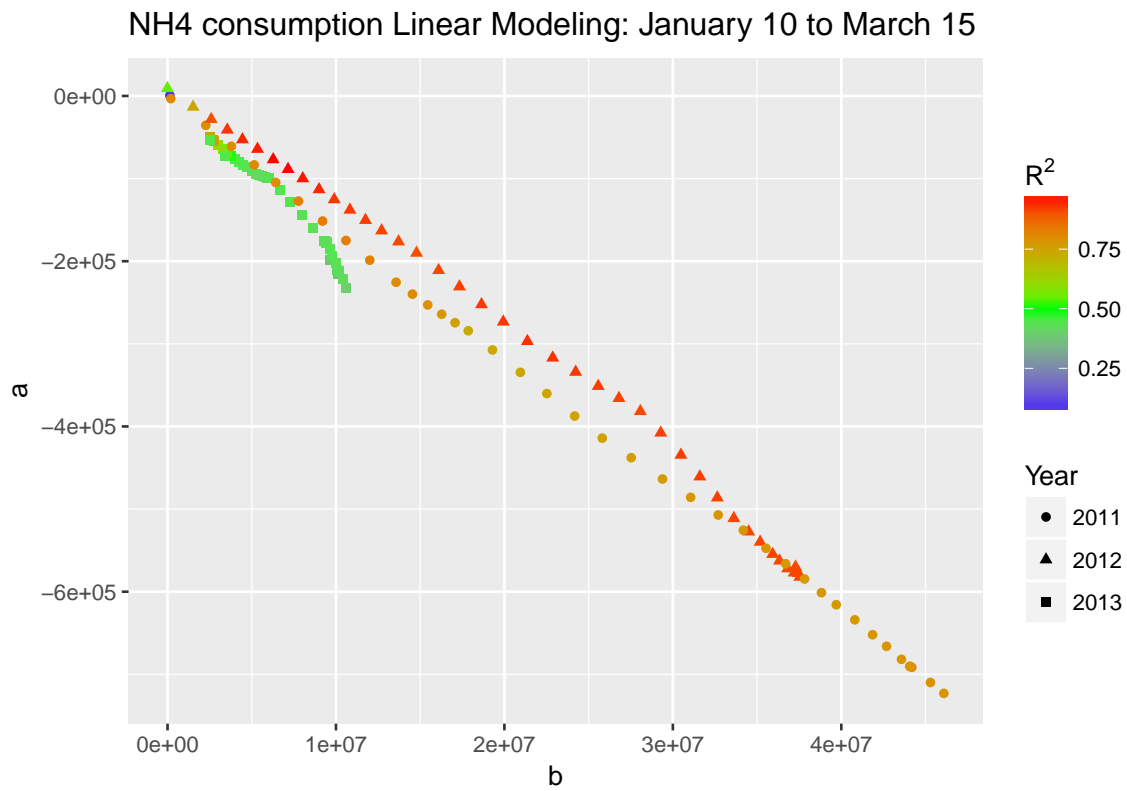
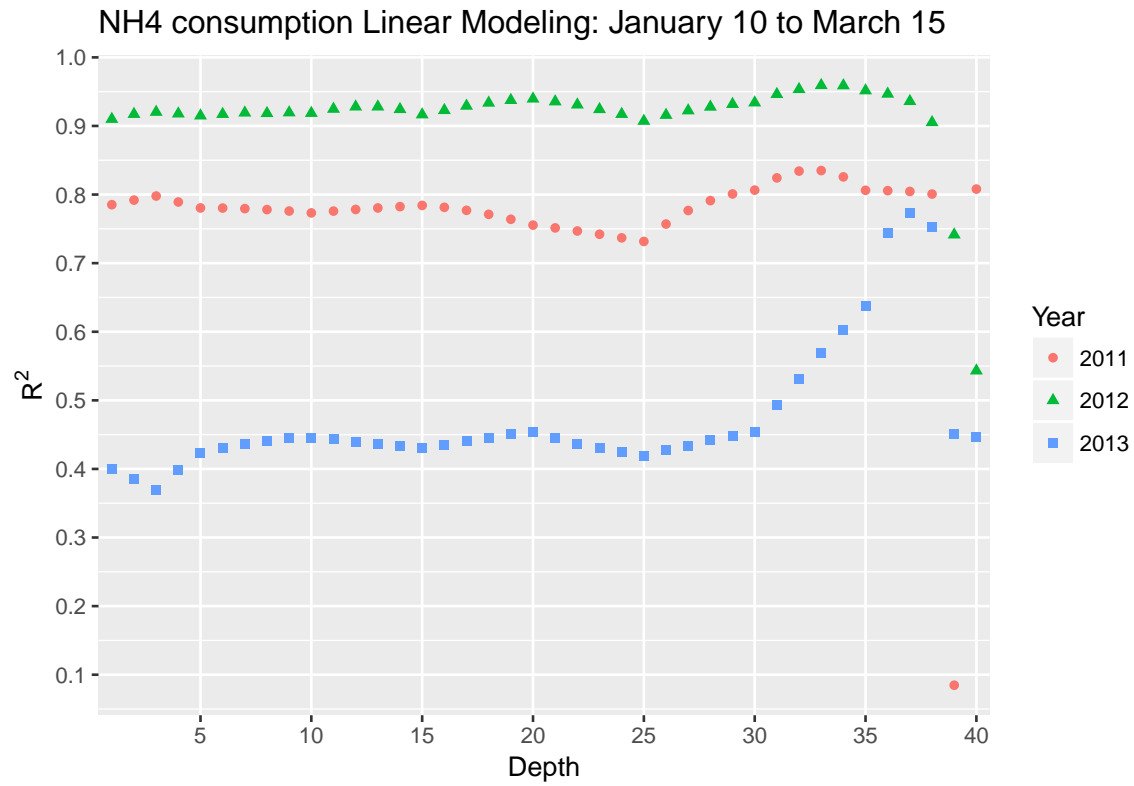
b parameter for NH4 build-up: April 30 to December 1



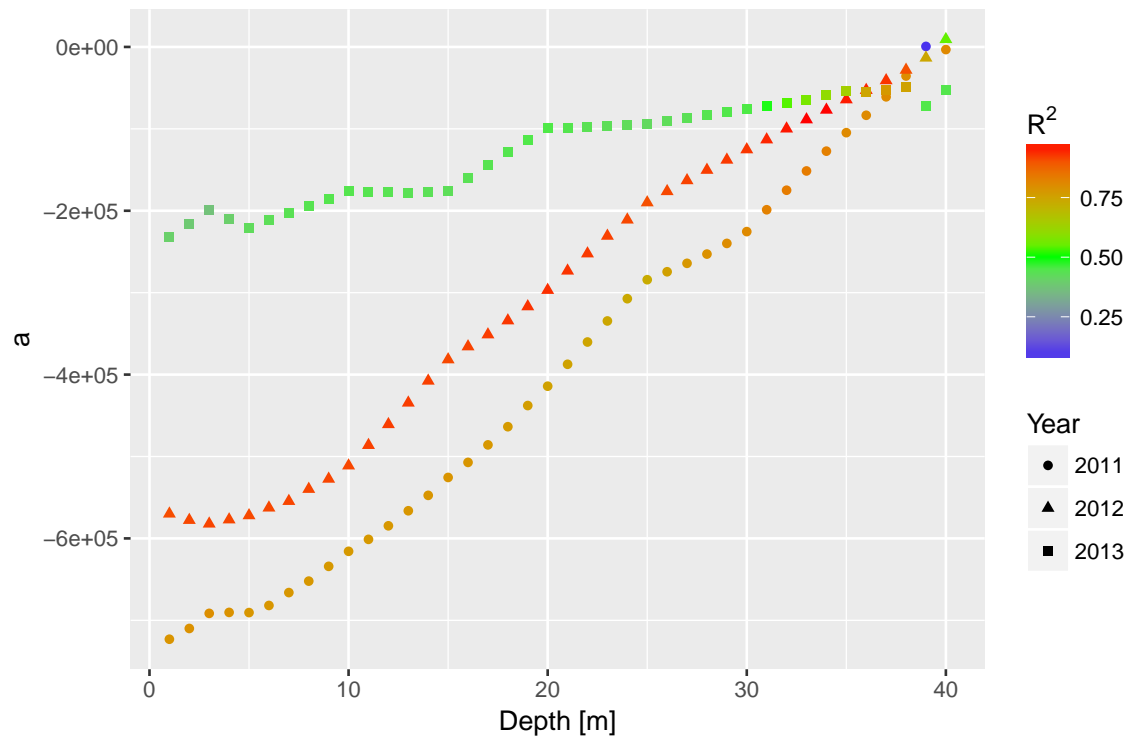


Ammonium consumption after mixing between January 10th to March 15th

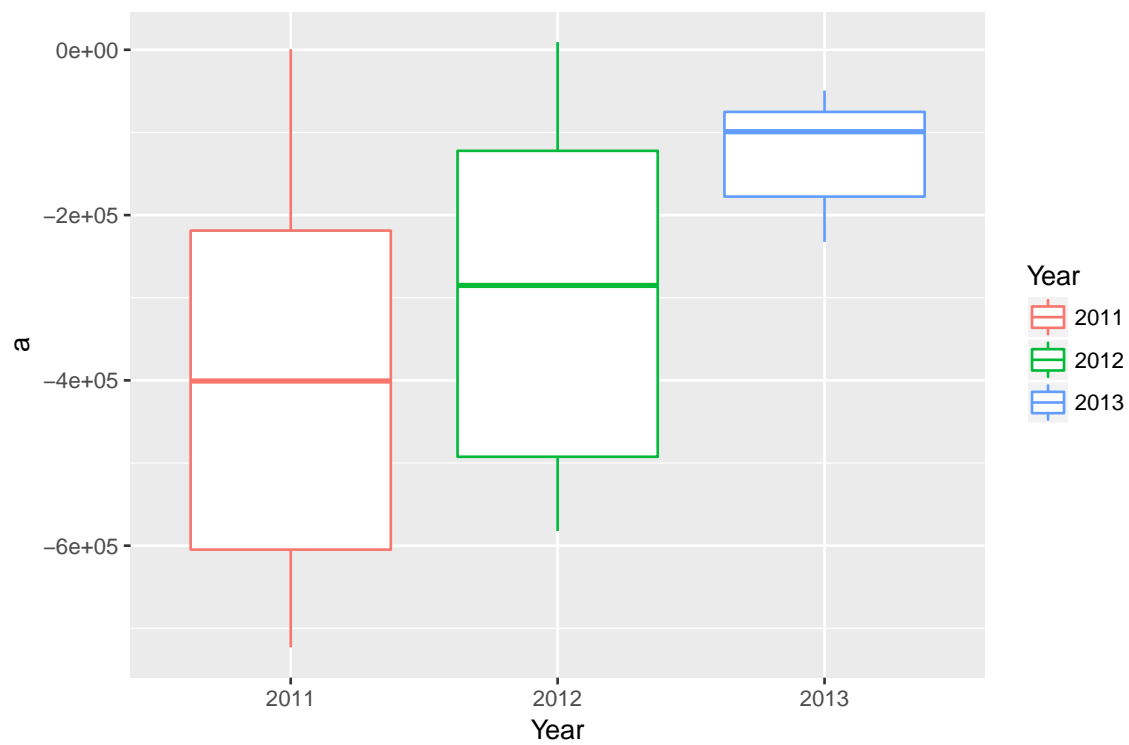
##	Depth	a	b	r2
##	Min. : 1.00	Min. : -723066	Min. : -9510	Min. : 0.08467
##	1st Qu.: 10.75	1st Qu.: -443545	1st Qu.: 5888522	1st Qu.: 0.45085
##	Median : 20.50	Median : -200589	Median : 10710844	Median : 0.77990
##	Mean : 20.50	Mean : -272712	Mean : 17447156	Mean : 0.71780
##	3rd Qu.: 30.25	3rd Qu.: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



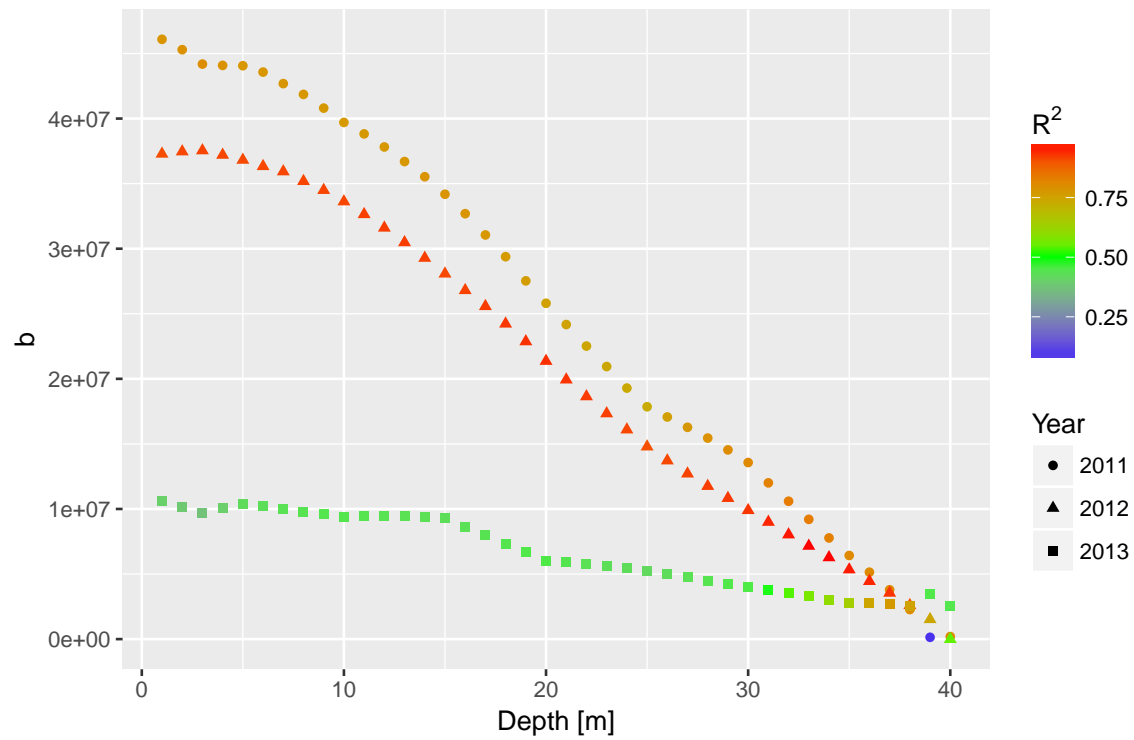
NH₄ consumption Linear Modeling: January 10 to March 15



a NH₄ consumption: January 10 to March 15



NH₄ consumption Linear Modeling: January 10 to March 15



b NH₄ consumption : January 10 to March 15

