LakeN

Yoav Ben Dor

6.12.2016

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

$$NO_3$$

Nitrite

$$NO_2^-$$

ammonia

$$NH_3$$

ammonium

$$NH_4^+$$

Hypolimion

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

Epilimion

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 nitrate by nitrobacteria. The process can be summarized as:

$$NH_4^+ ß NH_3 ß NO_2^- ß NO_3$$

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 places 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 fuul 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 buildsup 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 specie 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 measurment process provides a “snapshot” of lake conditions in a specific time, and that all coocuring 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 arithmatically 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 cycanobacteria and N recycling through consumption of primary producer up the food chasin. 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 inherintly 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-ammonioum transitions:

1. Nitrate build-up during lake stratification in the epylimnion
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 oppertunity to examine wether 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 measurments. The depths of the measurments are not constant, and the time intervals between measurments are also not constant, and range from several days to several weeks.

read the data and load relevant libraries

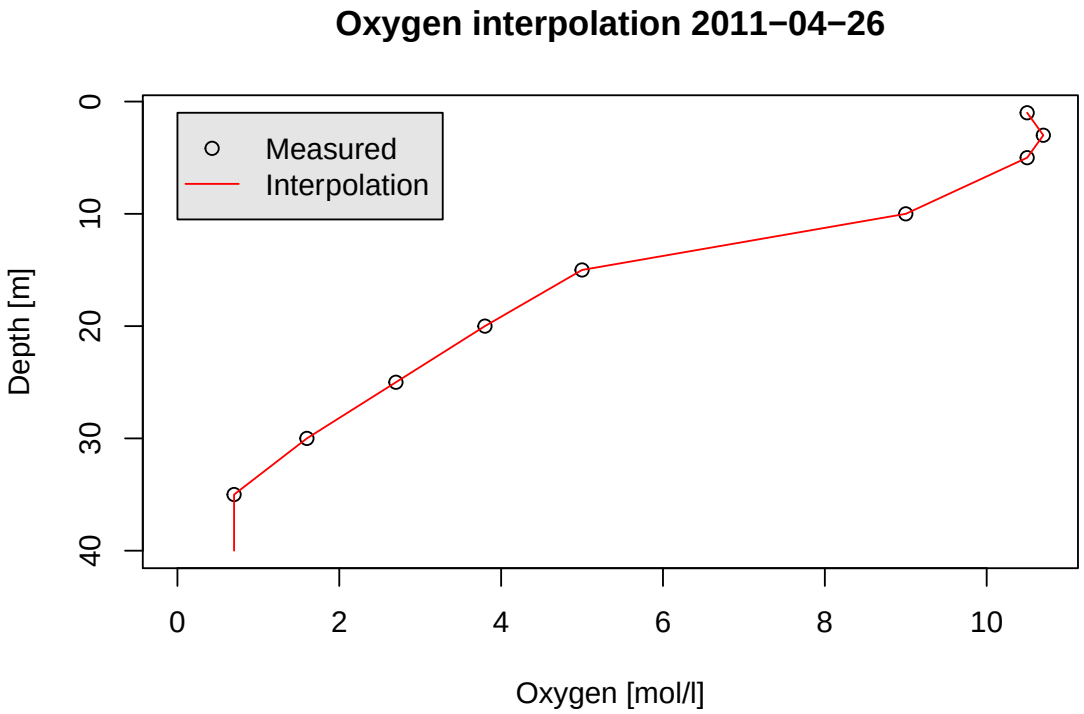
```
##          Date          Depth            NH4             Nitrit
##  2012-06-03:  13   Min.   : 1.00   Min.   :0.0030   Min.   :0.00200
```

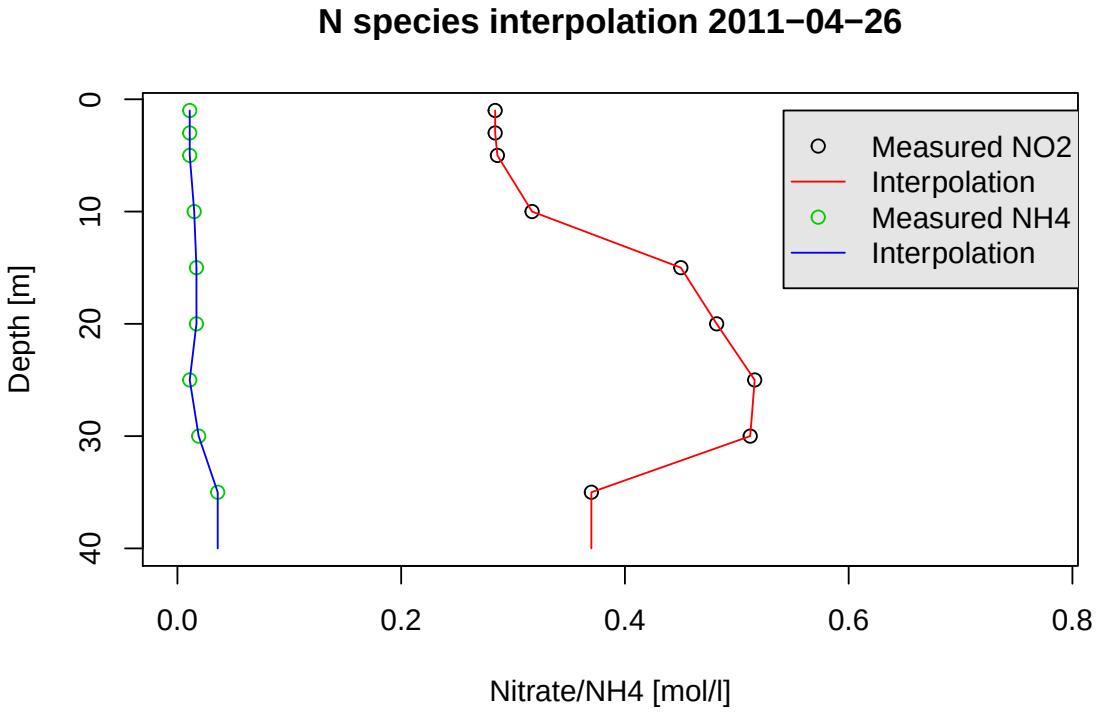
```
##  2012-06-24:  13   1st Qu.: 5.00   1st Qu.:0.0210   1st Qu.:0.00200
##  2012-07-08:  13   Median :16.00   Median :0.0850   Median :0.00300
##  2012-09-23:  13   Mean   :16.91   Mean   :0.2125   Mean   :0.01409
##  2013-06-02:  13   3rd Qu.:25.00   3rd Qu.:0.2447   3rd Qu.:0.01400
##  2013-06-23: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

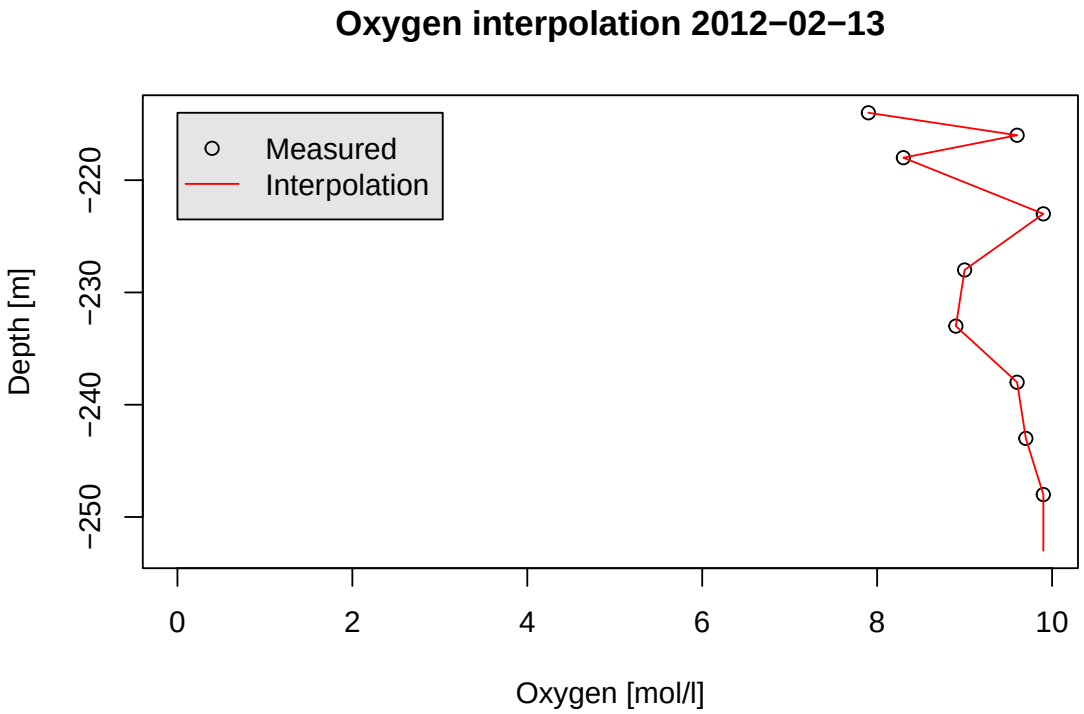


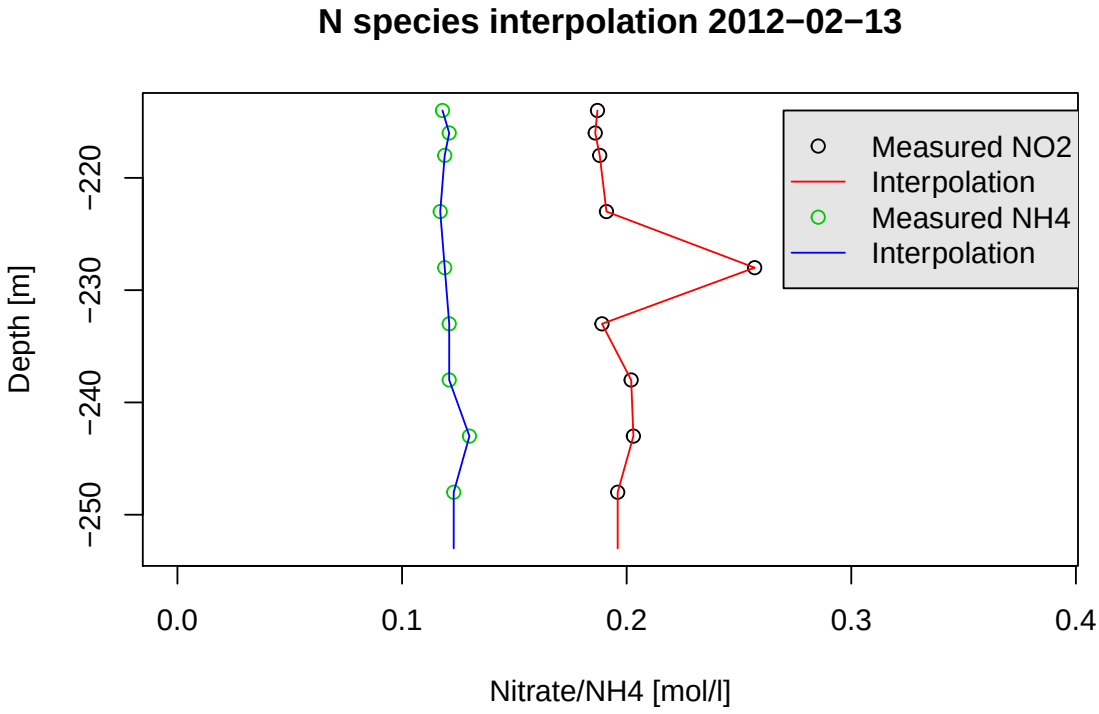


Depth and Level Corrections

Calculate the appropriate depth for each measurment using available daily level measurments. Use function "realdepth" and use closest day if no level measurment 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.

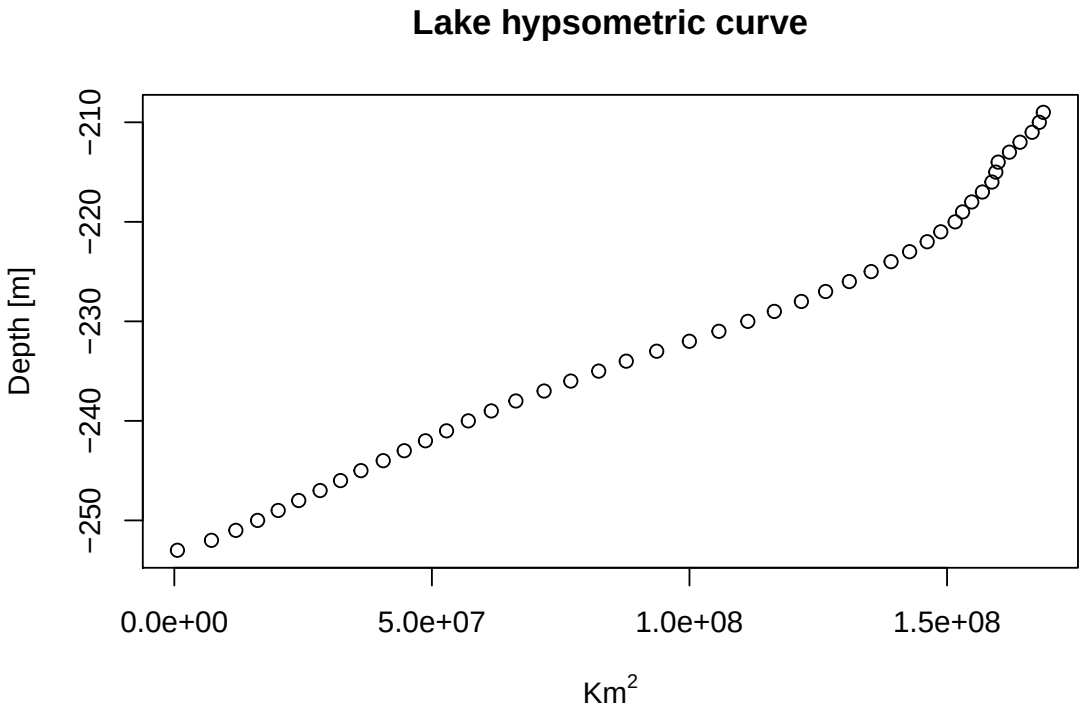
demonstrate the results according to the new depth scale of randomly selected data



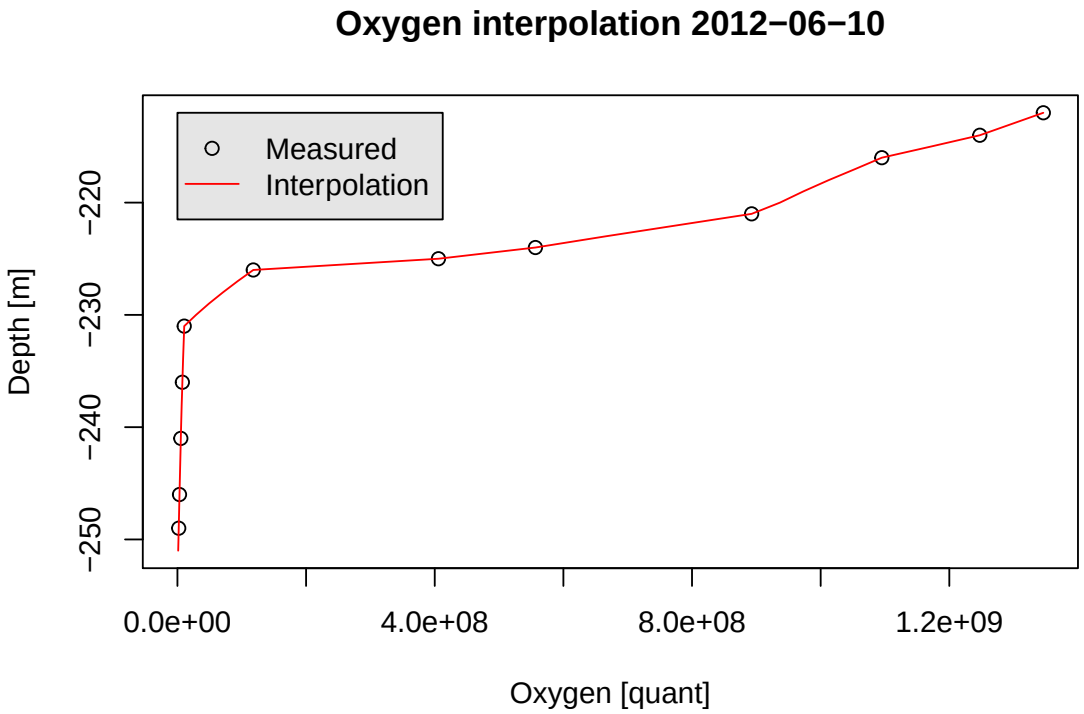


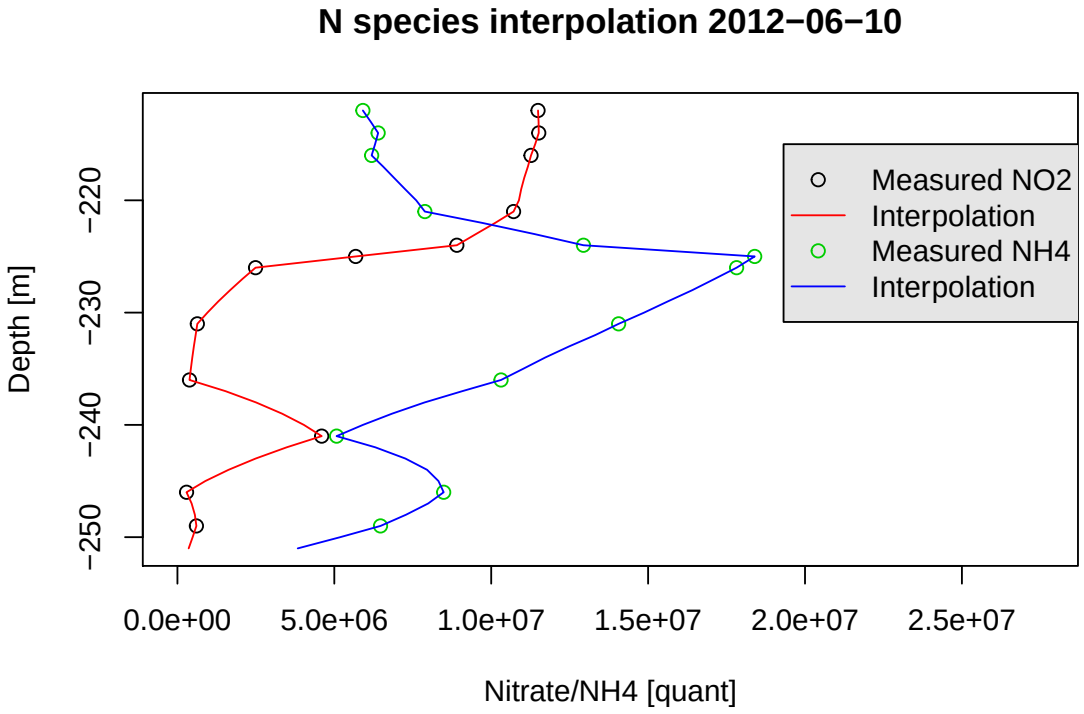
Quantify the data using lake hypsometric curve

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



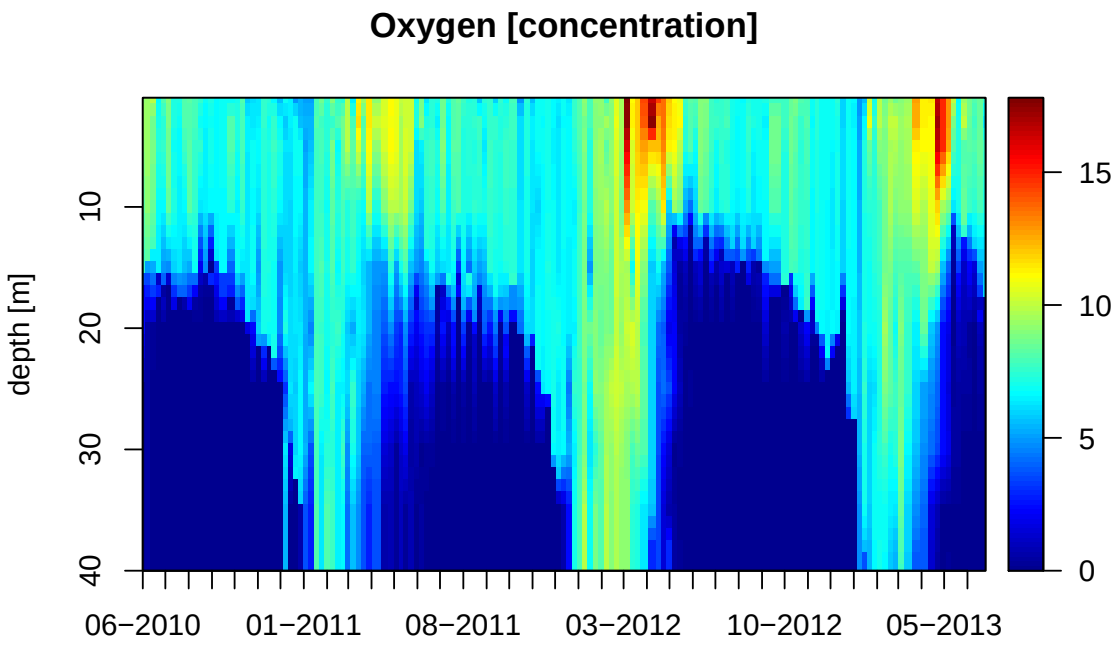
demonstrate the results according to the new depth scale of randomly selected data

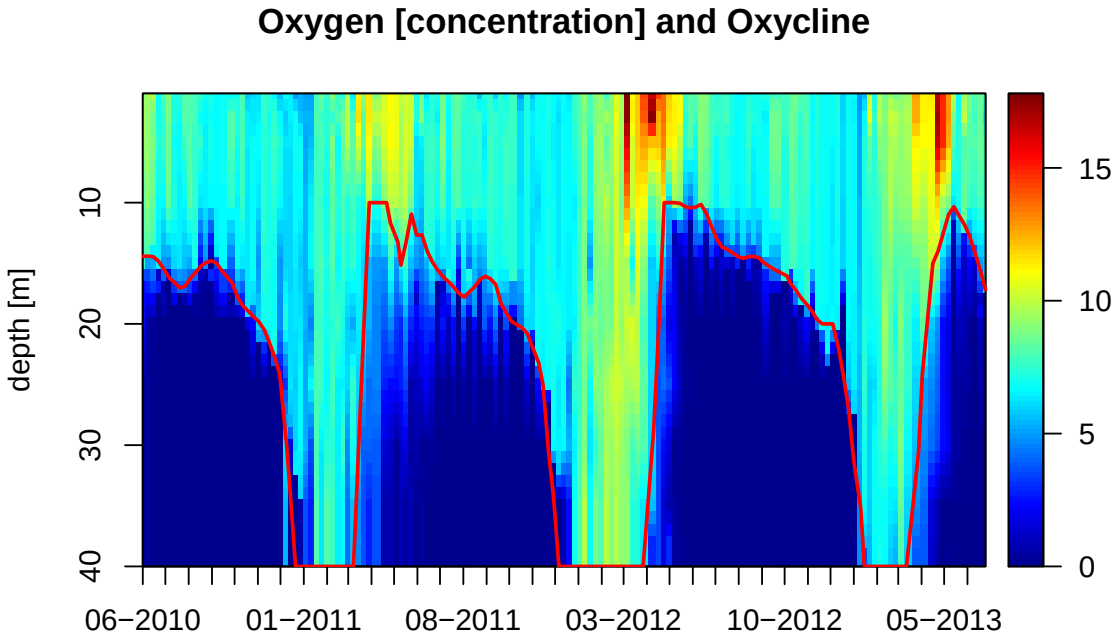


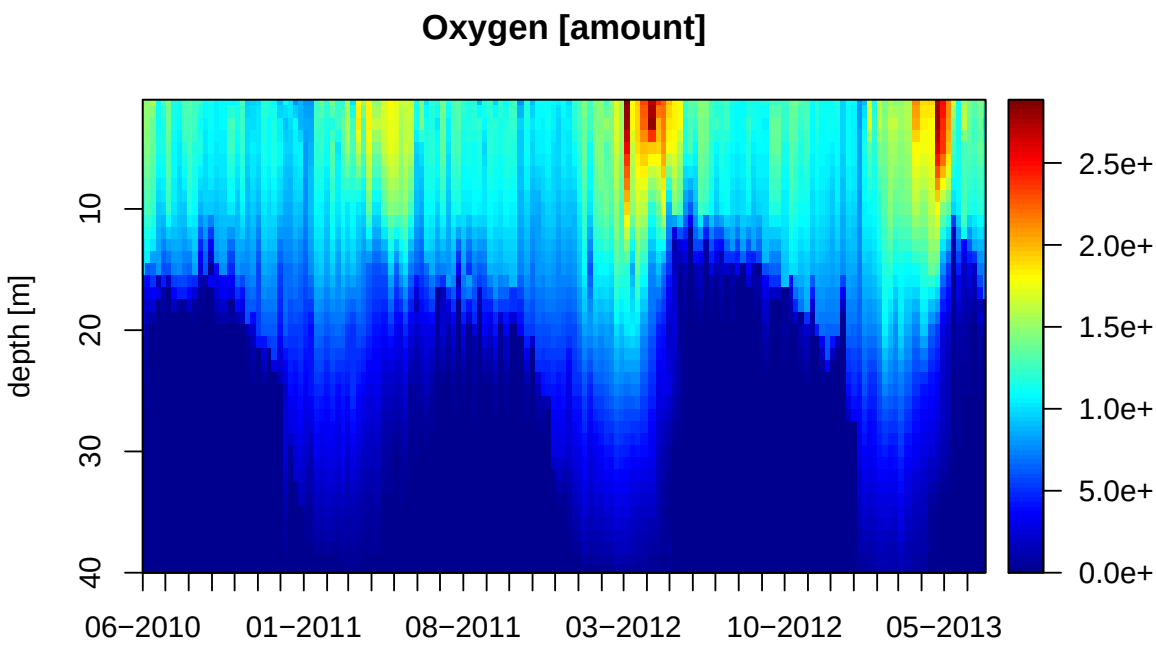


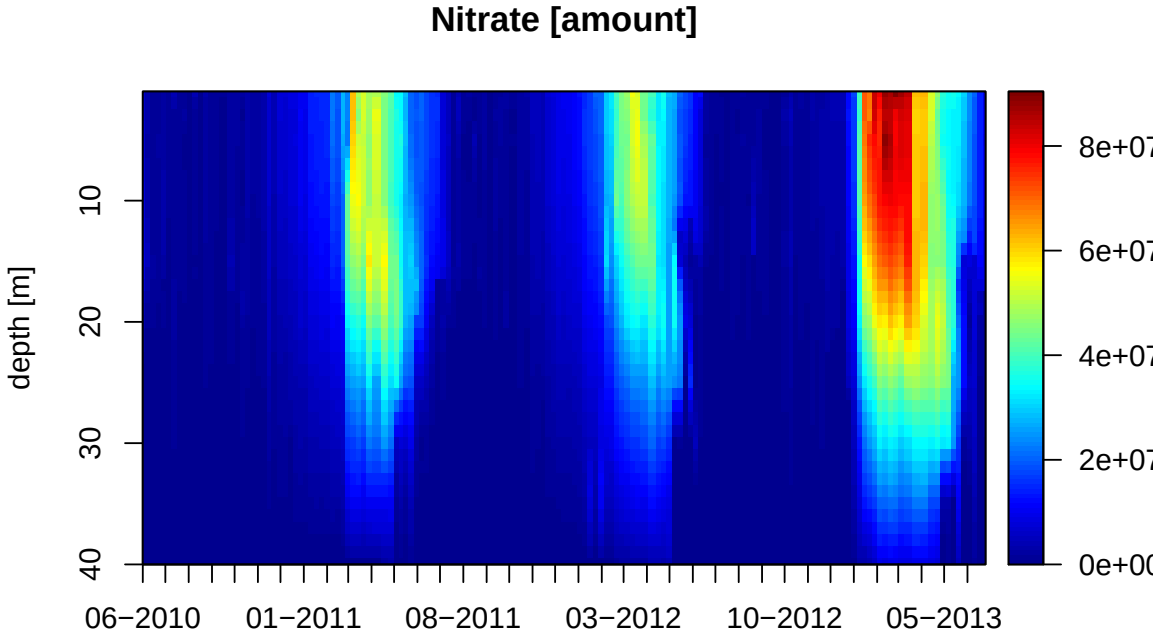
Time series plots

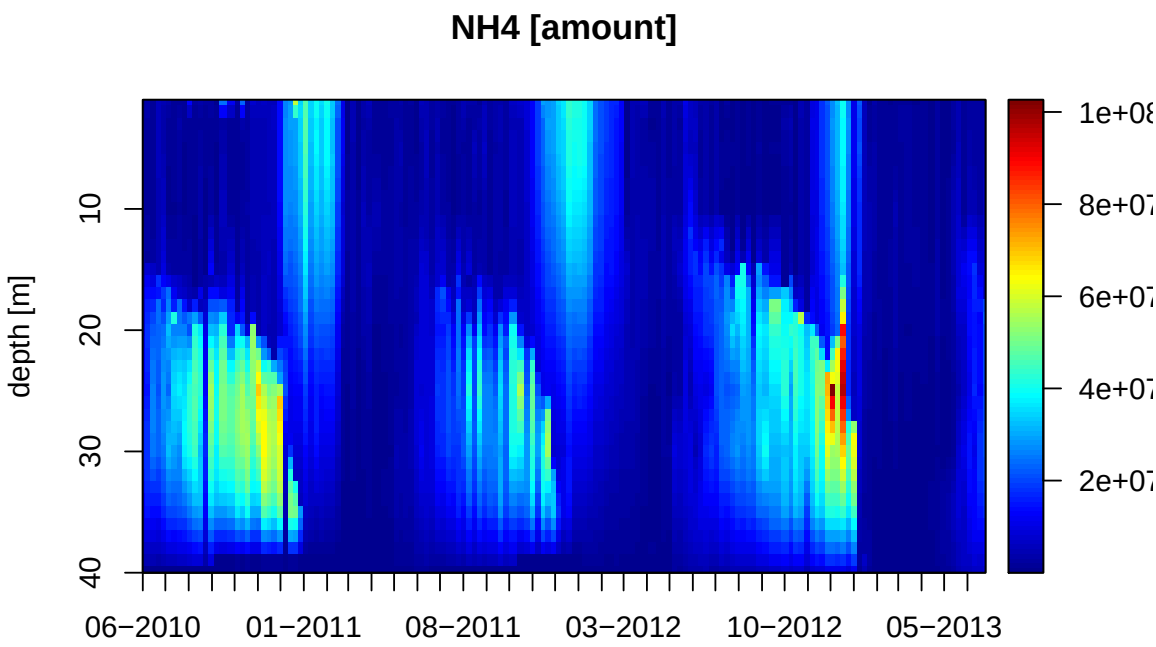
The following plots provide some visual estimation of the data to visualize time-depth processes for further considerations for the modelling of the processes

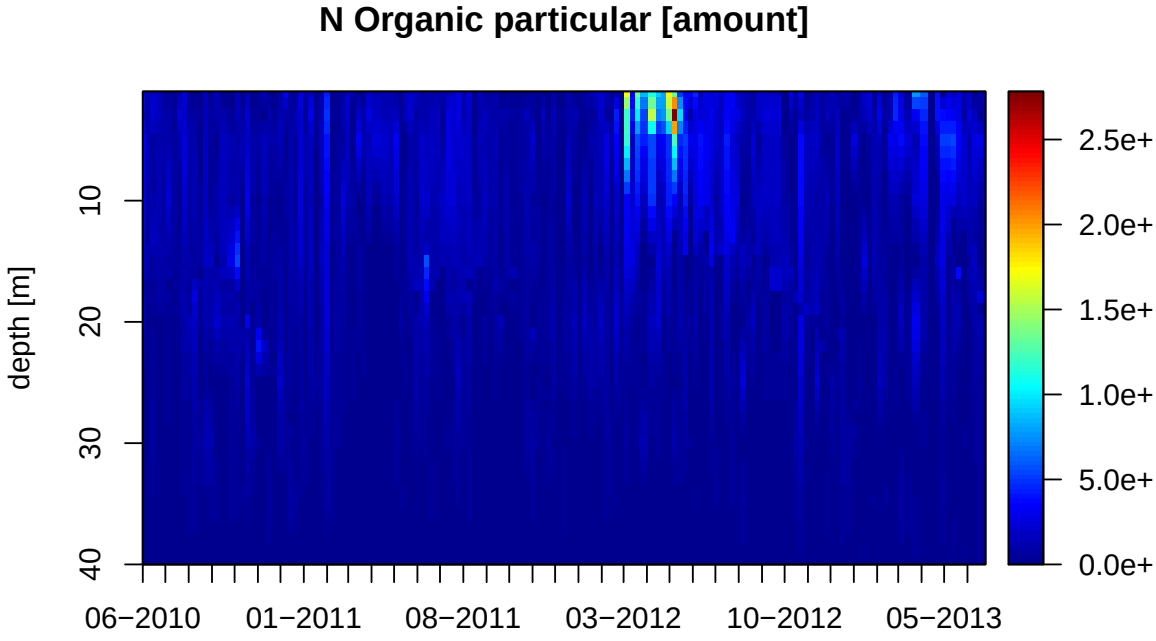

Oxygen [concentration]
depth [m]
10
20
30
40
06−2010
01−2011
08−2011
03−2012
10−2012
05−2013
15
10
5
0

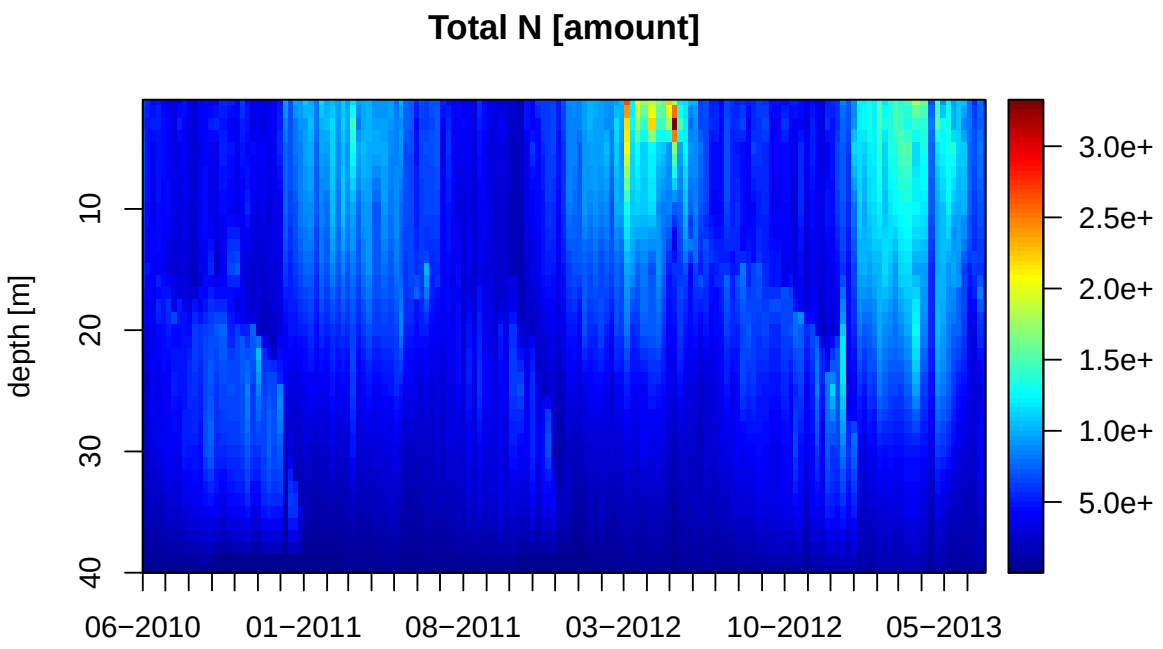

Oxygen [concentration] and Oxycline
depth [m]
10
20
30
40
06−2010
01−2011
08−2011
03−2012
10−2012
05−2013
15
10
5
0


Oxygen [amount]
depth [m]
10
20
30
40
06−2010
01−2011
08−2011
03−2012
10−2012
05−2013
2.5e+
2.0e+
1.5e+
1.0e+
5.0e+
0.0e+

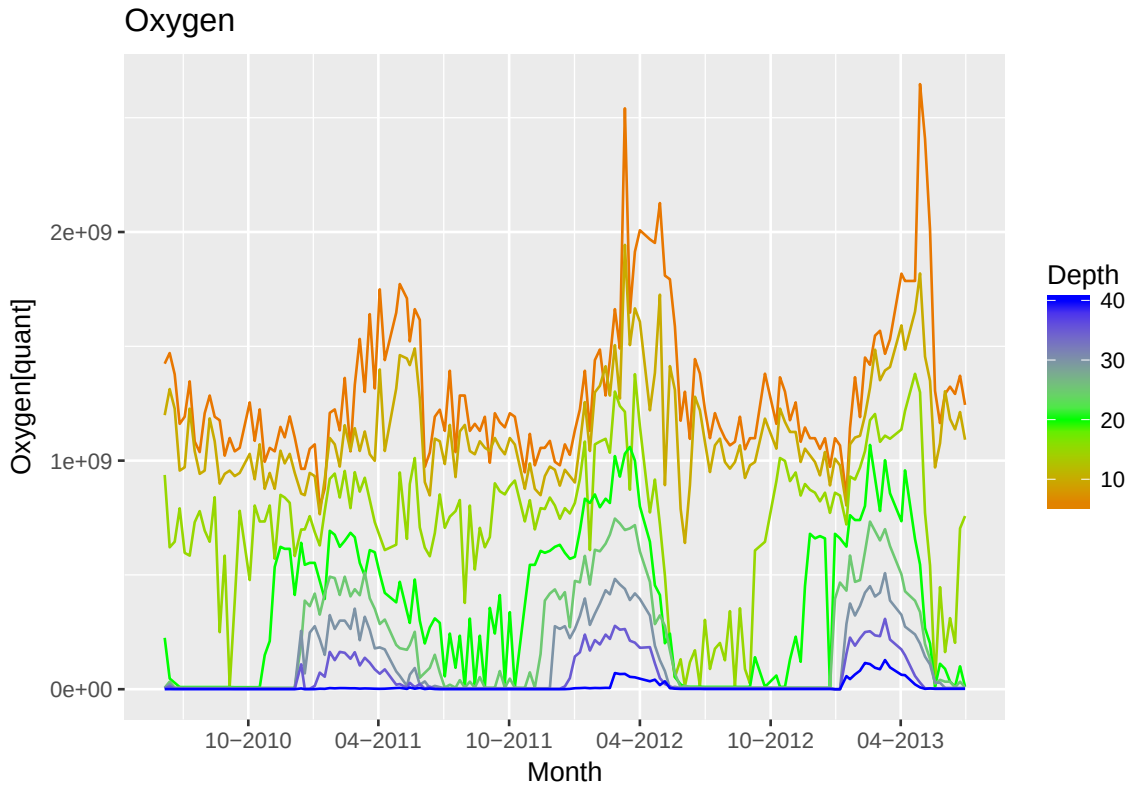

Nitrate [amount]
depth [m]
10
20
30
40
06−2010
01−2011
08−2011
03−2012
10−2012
05−2013
8e+07
6e+07
4e+07
2e+07
0e+00

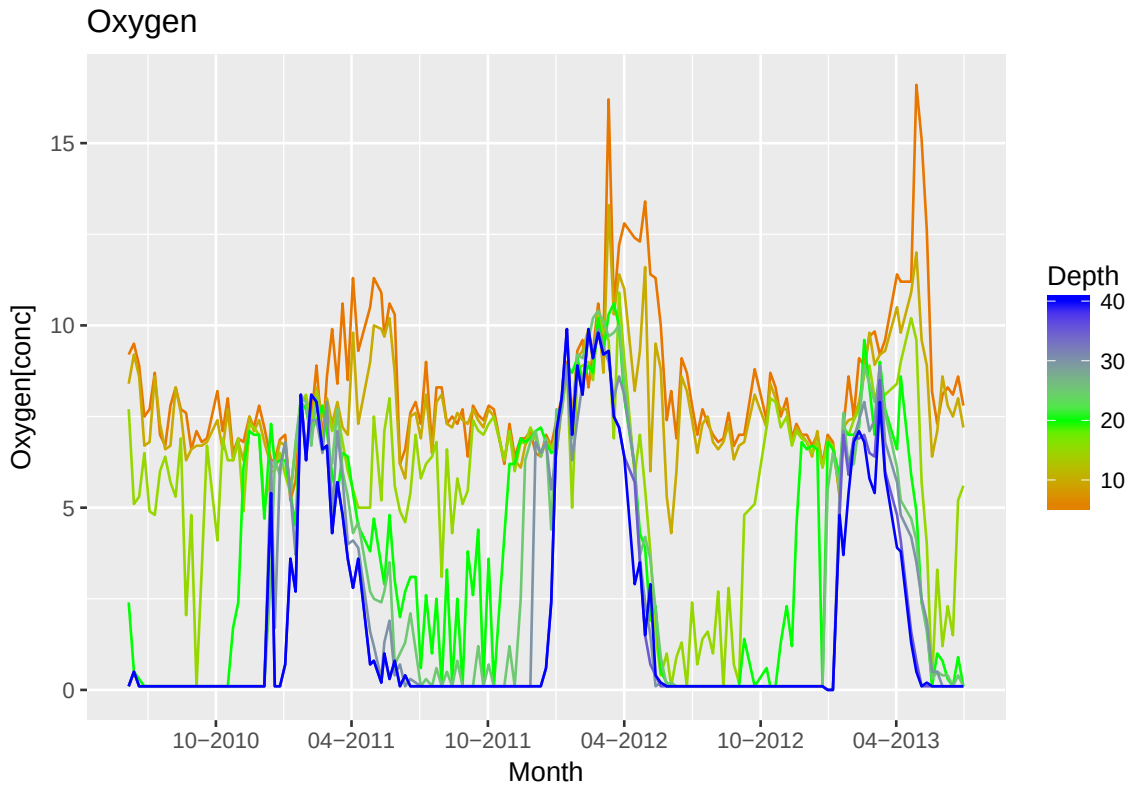

NH4 [amount]
depth [m]
10
20
30
40
06−2010
01−2011
08−2011
03−2012
10−2012
05−2013
1e+08
8e+07
6e+07
4e+07
2e+07

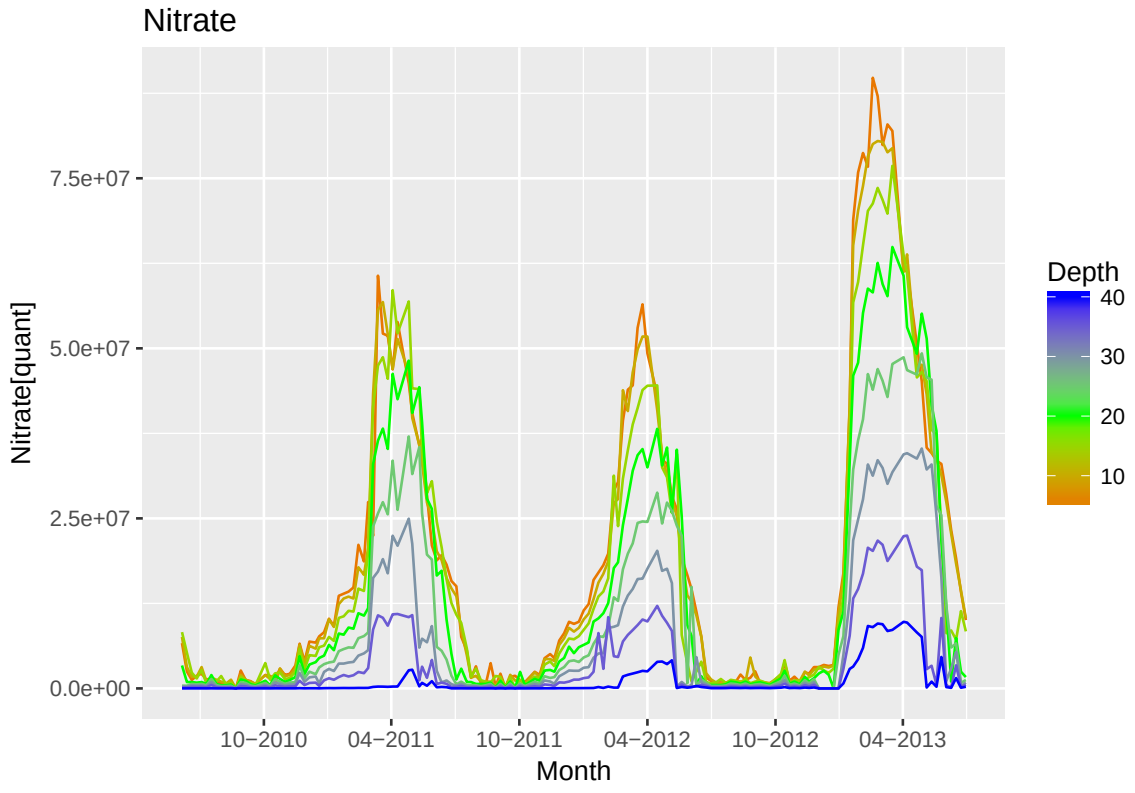

N Organic particular [amount]
depth [m]
10
20
30
40
06−2010
01−2011
08−2011
03−2012
10−2012
05−2013
2.5e+
2.0e+
1.5e+
1.0e+
5.0e+
0.0e+

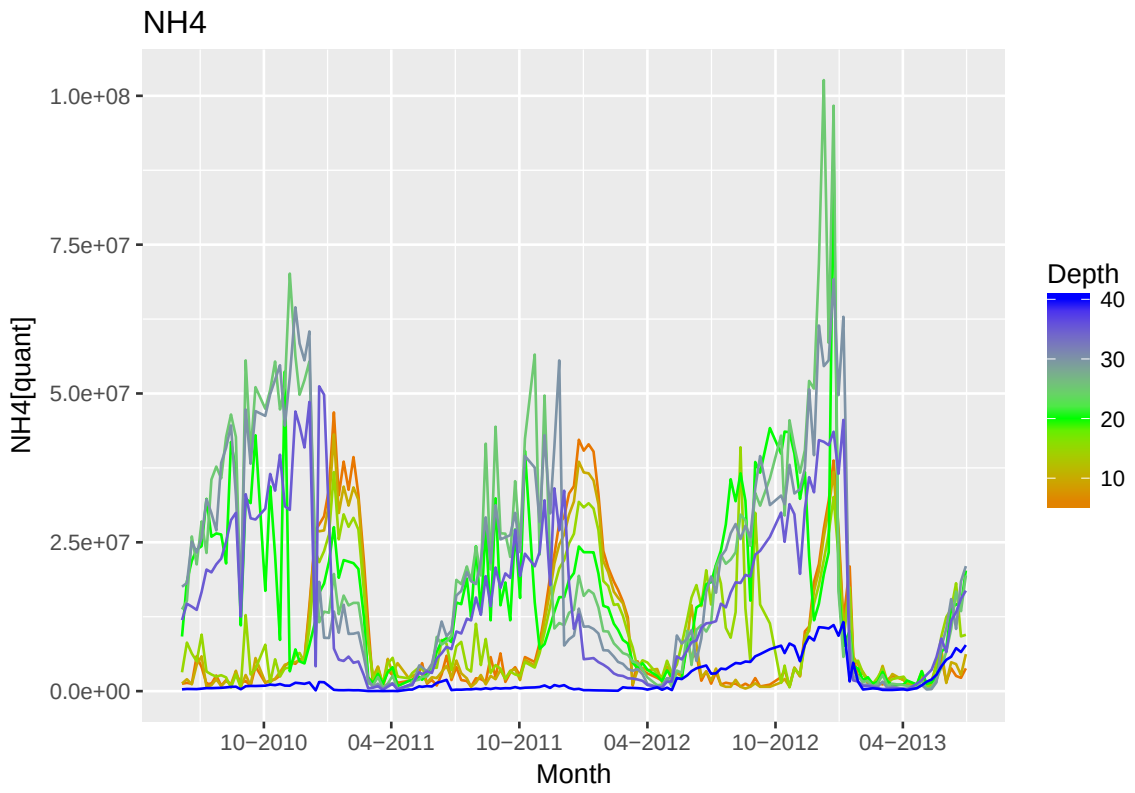

Total N [amount]
depth [m]
10
20
30
40
06−2010
01−2011
08−2011
03−2012
10−2012
05−2013
3.0e+
2.5e+
2.0e+
1.5e+
1.0e+
5.0e+

Time-depth cross sections



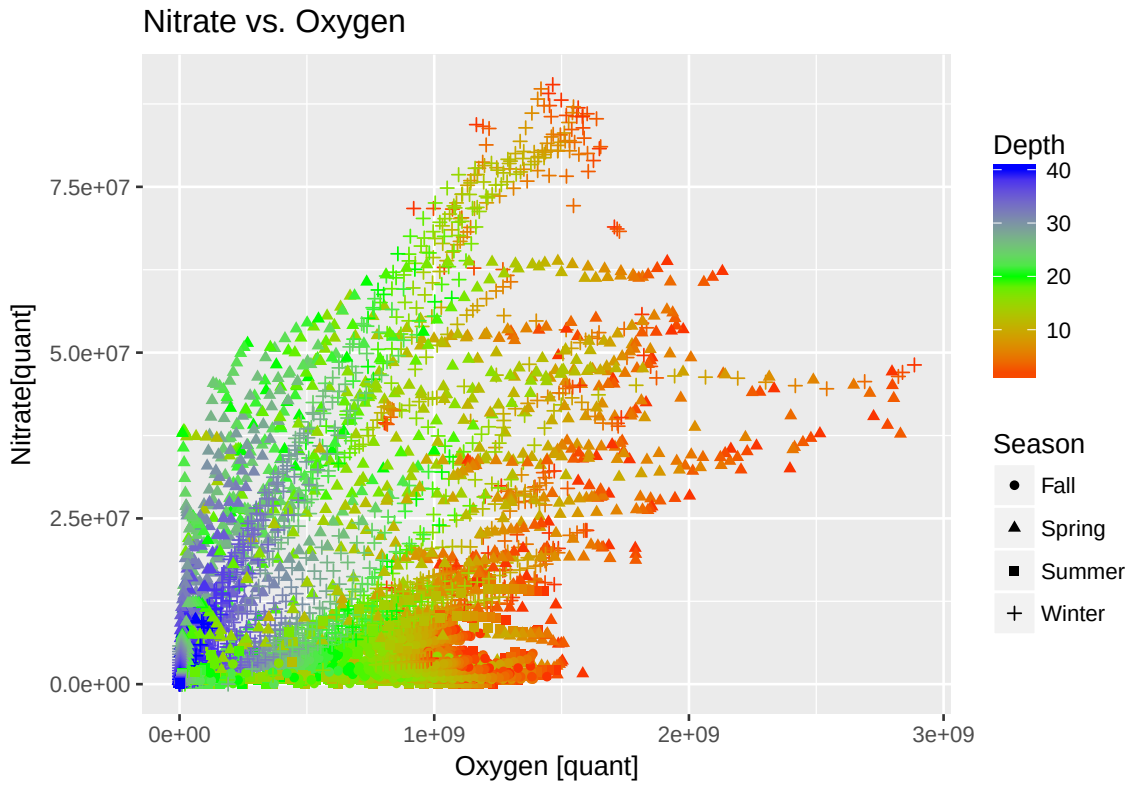


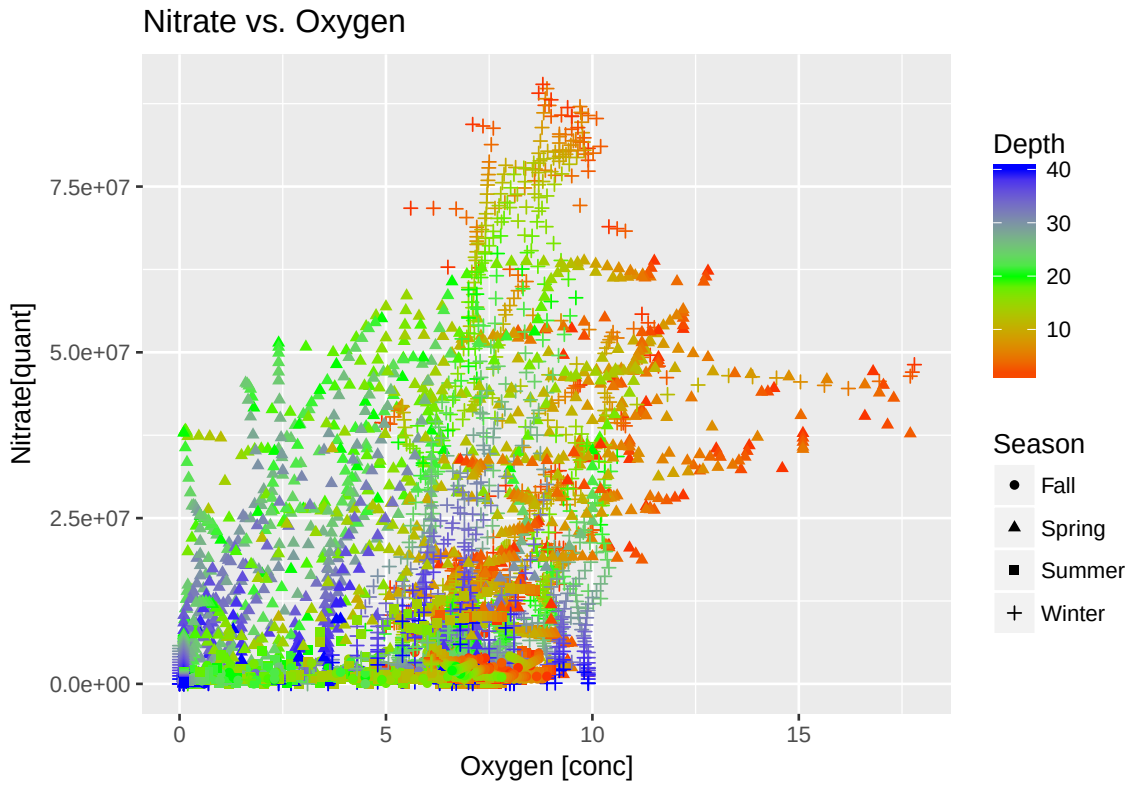

Nitrate
Nitrate[quant]
7.5e+07
5.0e+07
2.5e+07
0.0e+00
10−2010
04−2011
10−2011
04−2012
10−2012
04−2013
Month
Depth
40
30
20
10

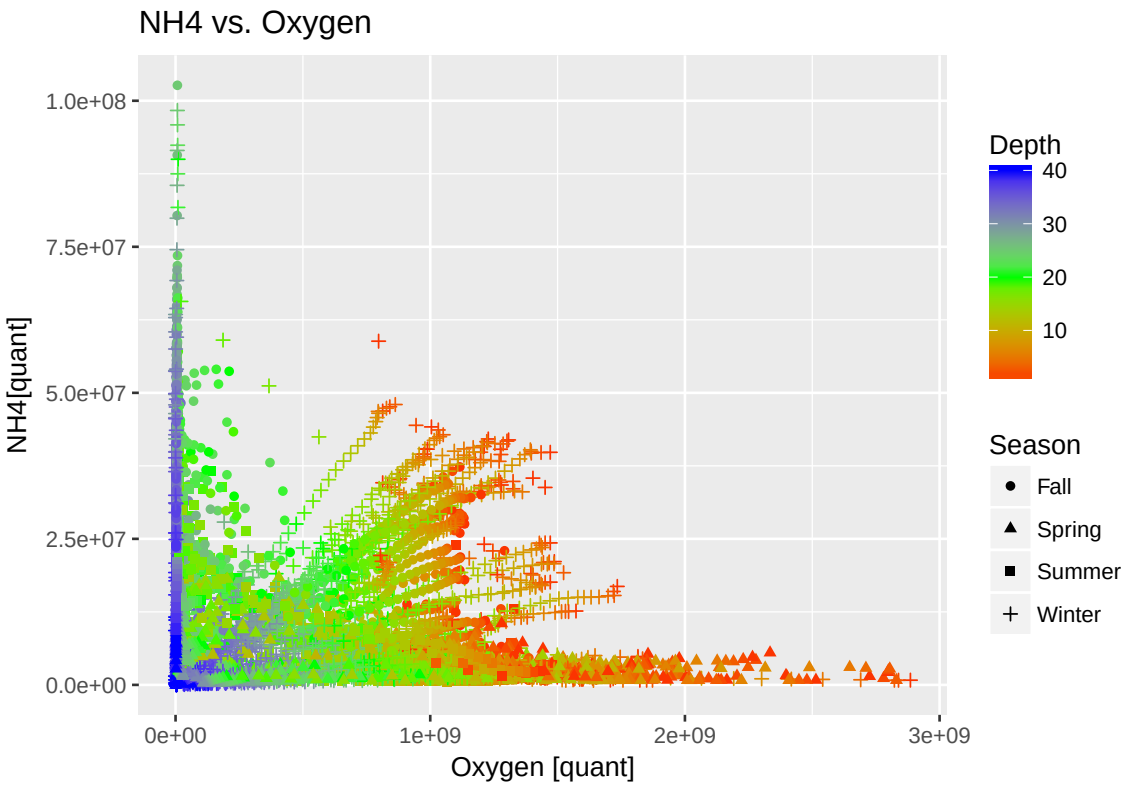

NH4
NH4[quant]
1.0e+08
7.5e+07
5.0e+07
2.5e+07
0.0e+00
10−2010
04−2011
10−2011
04−2012
10−2012
04−2013
Month
Depth
40
30
20
10

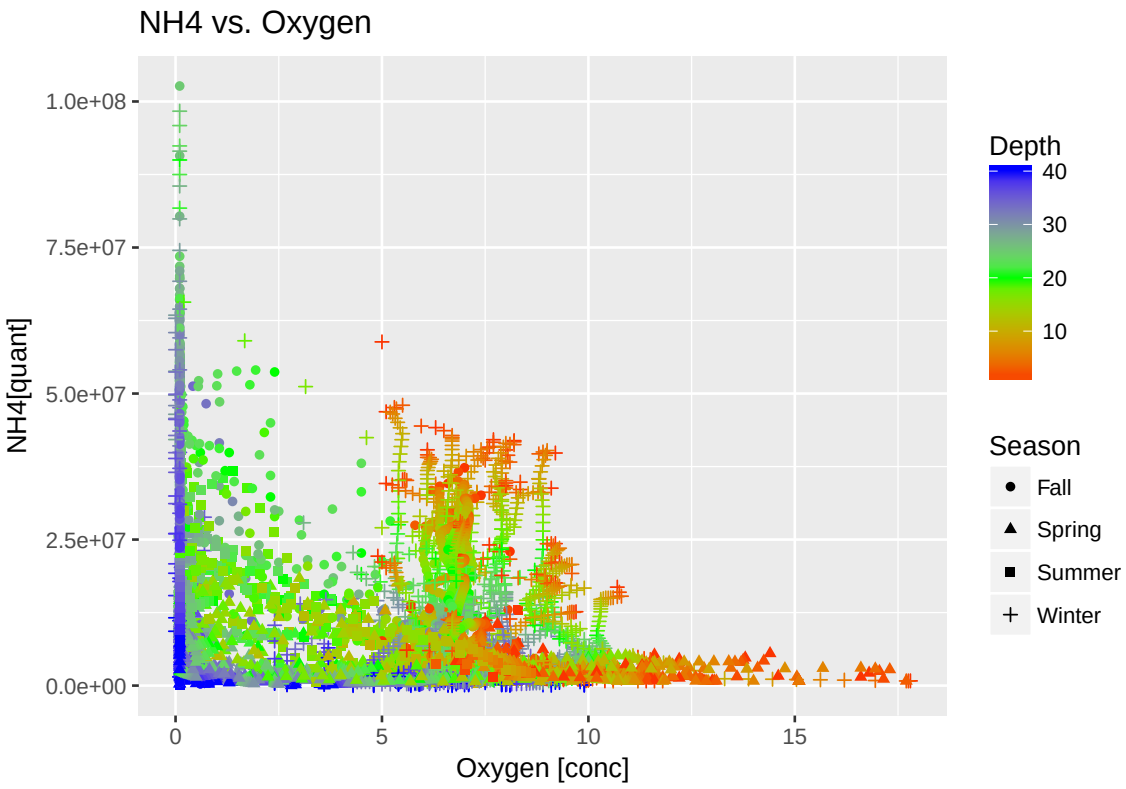
Correlation plots

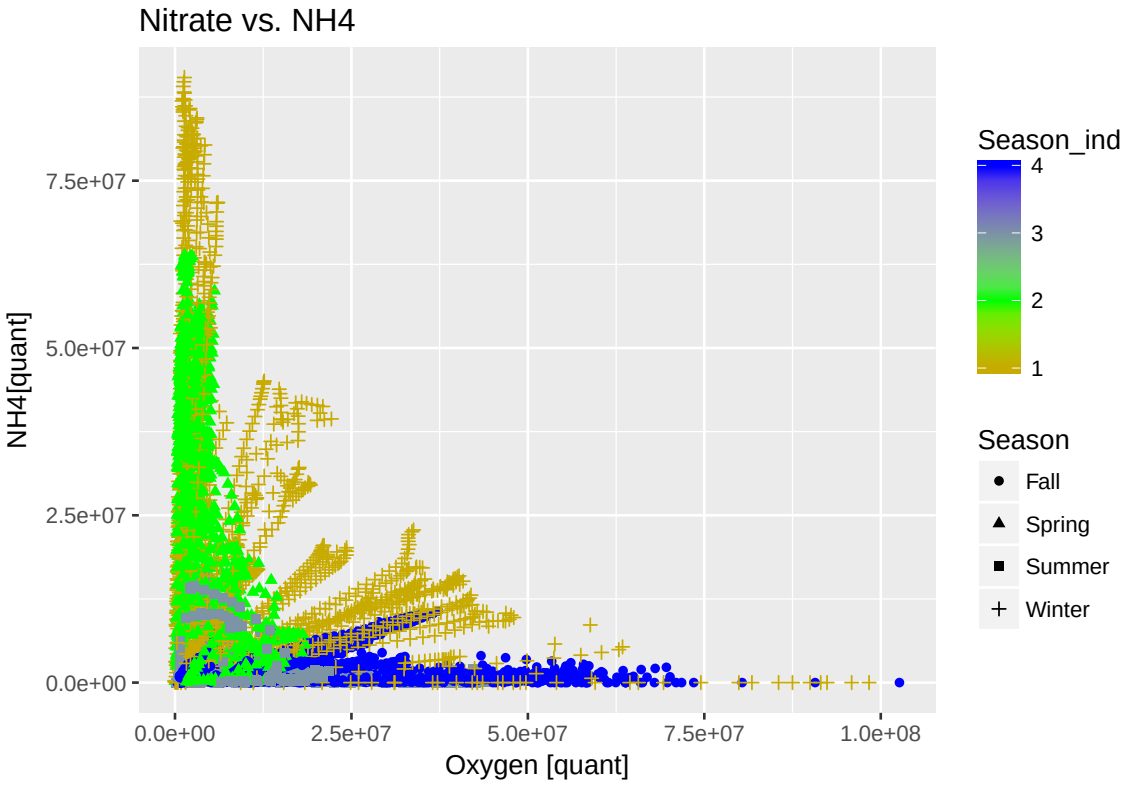
The following plots provide some visual estimation of data correlation

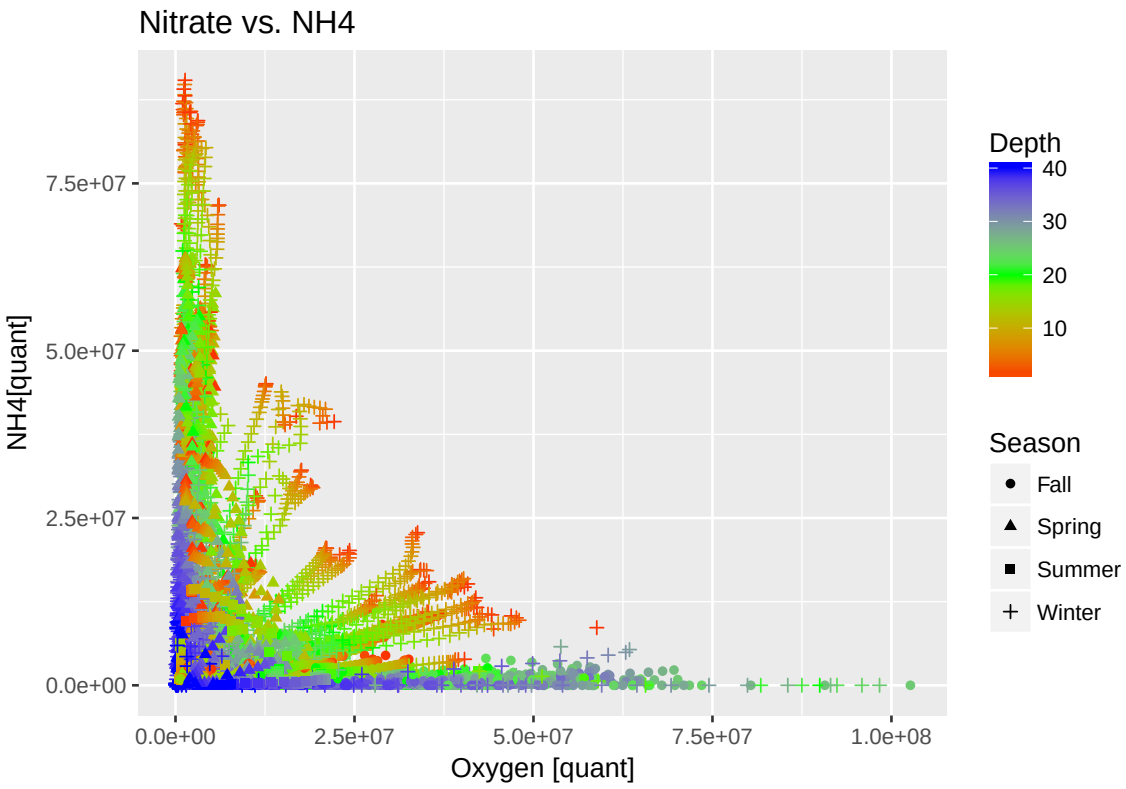





NH4 vs. Oxygen
1.0e+08
7.5e+07
5.0e+07
2.5e+07
0.0e+00
NH4[quant]
0e+00
1e+09
2e+09
3e+09
Oxygen [quant]
Depth
40
30
20
10
Season
Fall
Spring
Summer
Winter

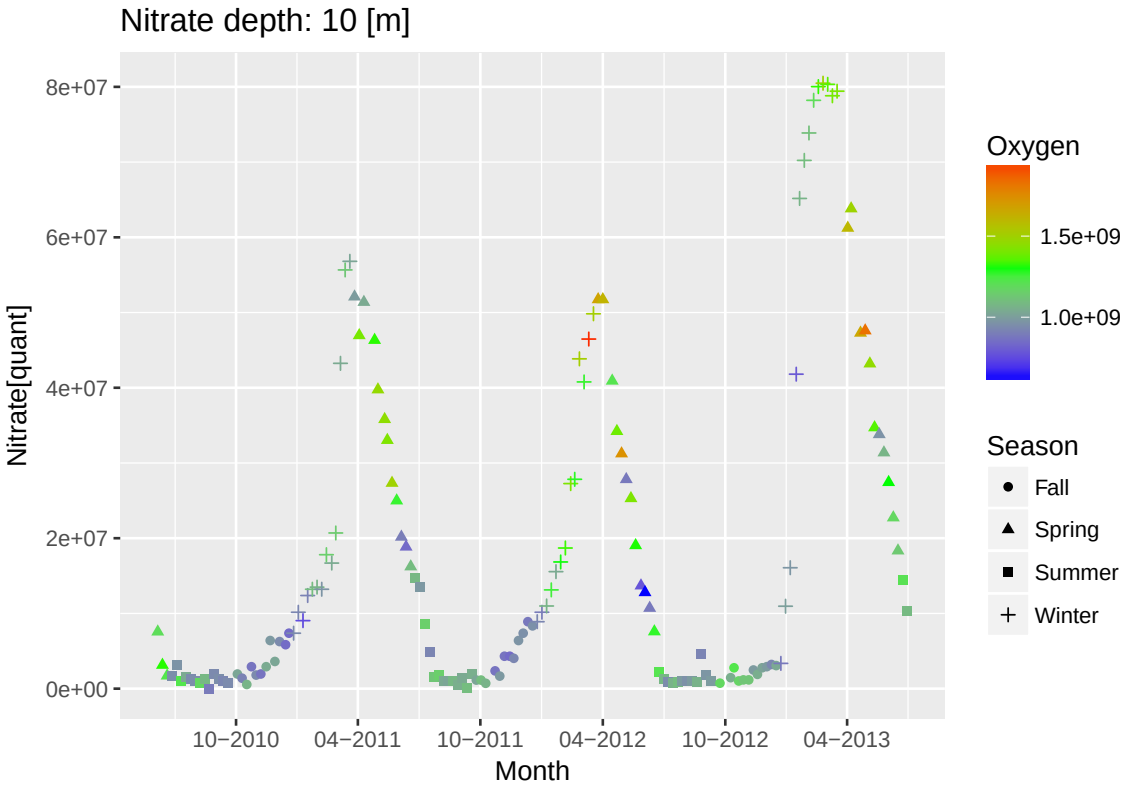

NH4 vs. Oxygen
1.0e+08
7.5e+07
5.0e+07
2.5e+07
0.0e+00
NH4[quant]
0
5
10
15
Oxygen [conc]
Depth
40
30
20
10
Season
Fall
Spring
Summer
Winter

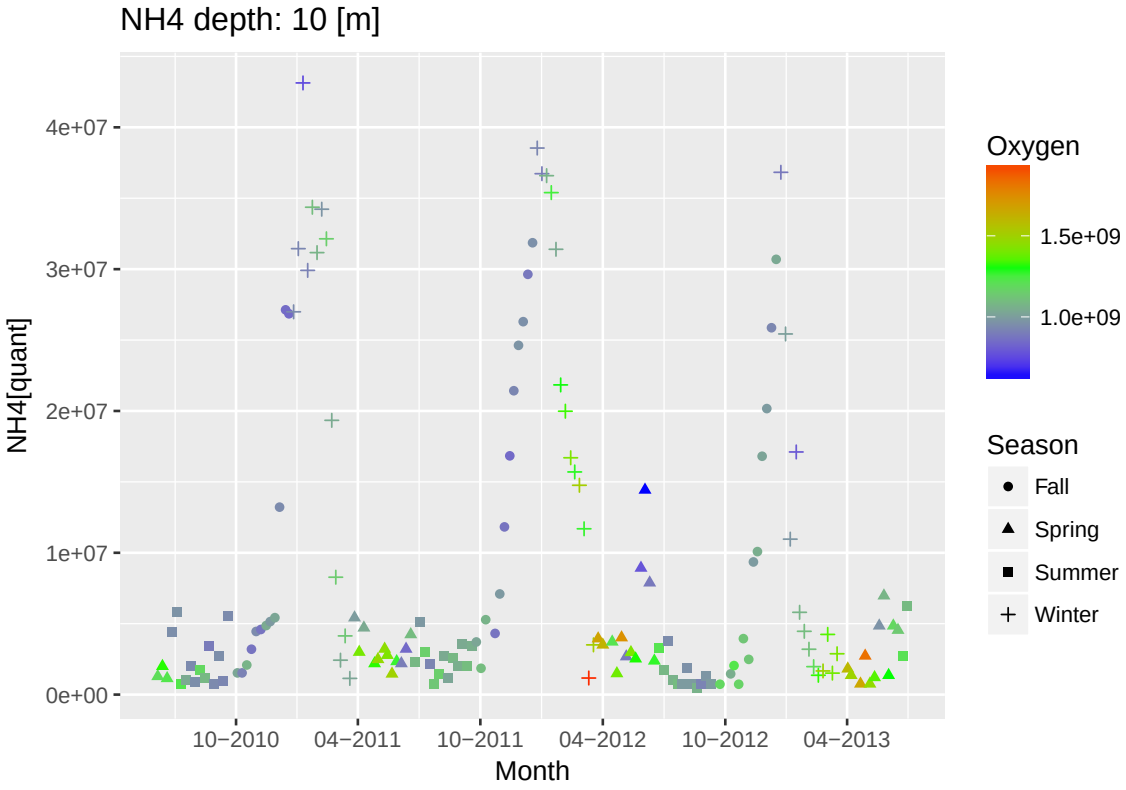

Nitrate vs. NH4
NH4[quant]
7.5e+07
5.0e+07
2.5e+07
0.0e+00
0.0e+00
2.5e+07
5.0e+07
7.5e+07
1.0e+08
Oxygen [quant]
Season_ind
4
3
2
1
Season
Fall
Spring
Summer
Winter

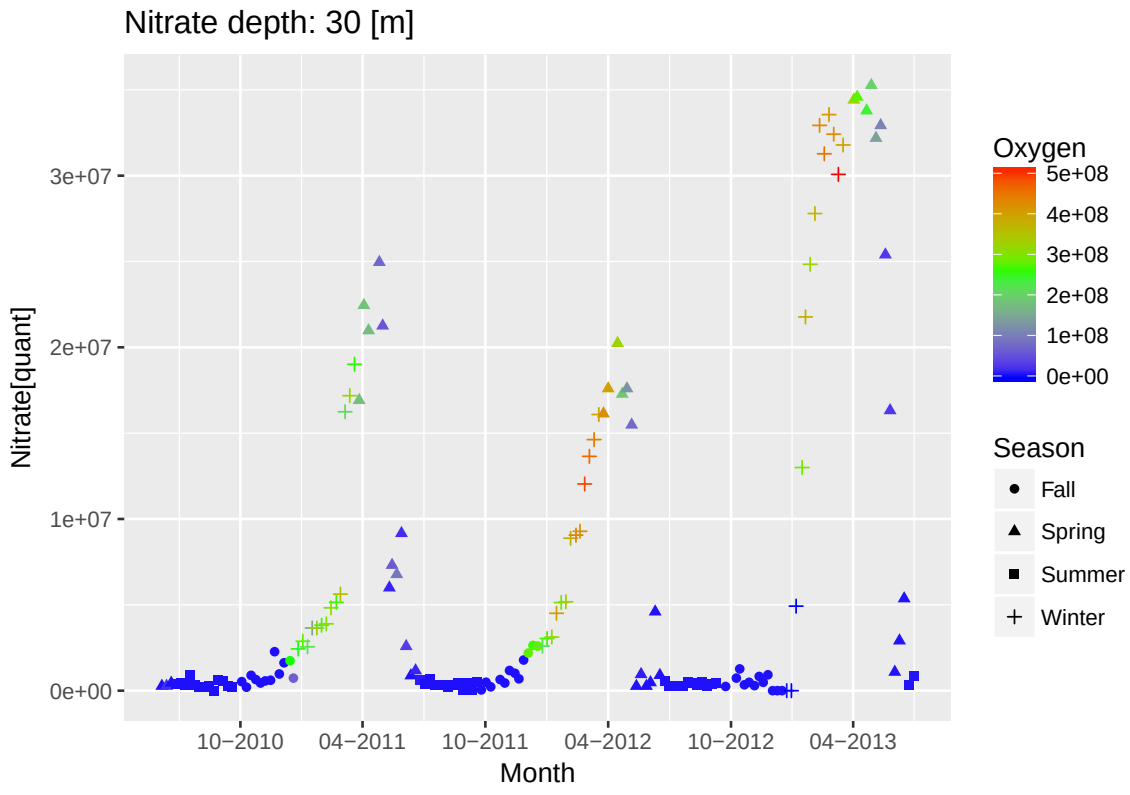

Nitrate vs. NH4
NH4[quant]
7.5e+07
5.0e+07
2.5e+07
0.0e+00
0.0e+00
2.5e+07
5.0e+07
7.5e+07
1.0e+08
Oxygen [quant]
Depth
40
30
20
10
Season
Fall
Spring
Summer
Winter

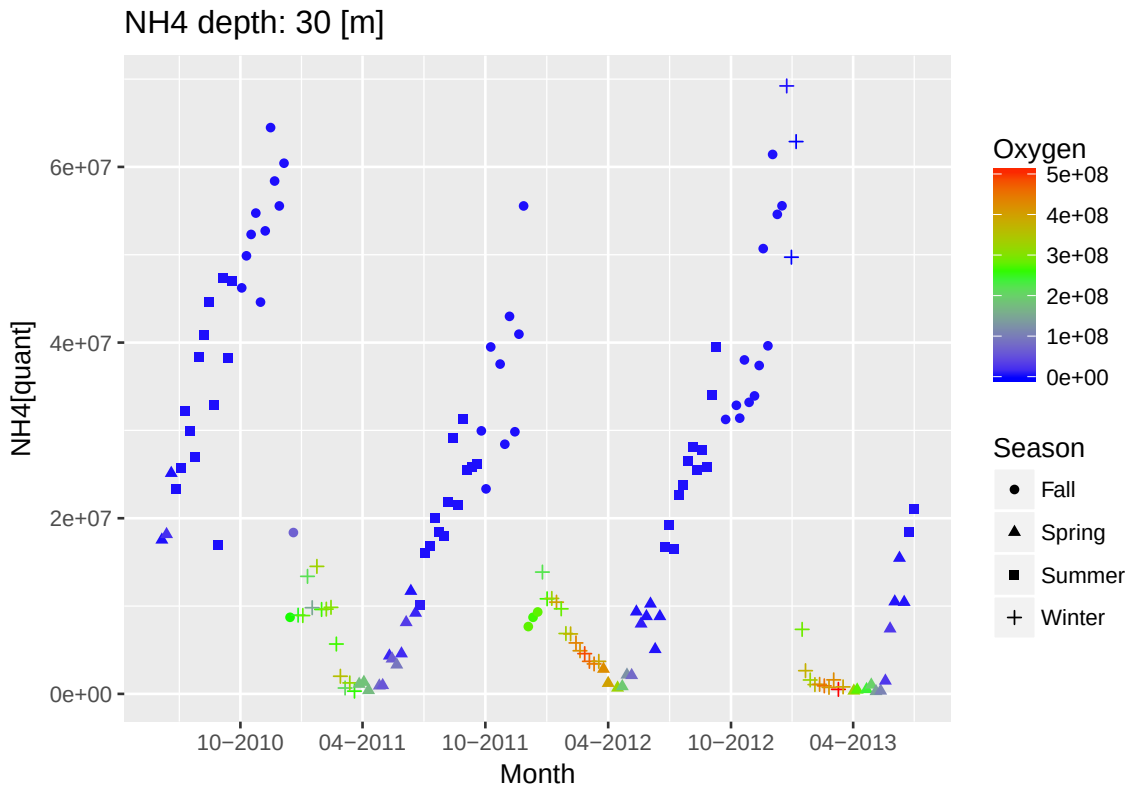
Model fitting estimation

Nitrification and denitrification are two oposing processes that take place in the present 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 assumprion that their development depends on the presence of oxygen and the time available for their accumulation. Lake mixing, which takes place during winter, disrupts thier build-up, and uniformly distribute them across the lake, and mixing propagates towards the lake bottom. These two proceeses (stratification and mixing)can be examined in detail in two representative depths of 10m (nitrification) and 30m (denitrification).


Nitrate depth: 10 [m]
Nitrate[quant]
8e+07
6e+07
4e+07
2e+07
0e+00
10−2010
04−2011
10−2011
04−2012
10−2012
04−2013
Month
Oxygen
1.5e+09
1.0e+09
Season
Fall
Spring
Summer
Winter


NH4 depth: 10 [m]
NH4[quant]
4e+07
3e+07
2e+07
1e+07
0e+00
10−2010
04−2011
10−2011
04−2012
10−2012
04−2013
Month
Oxygen
1.5e+09
1.0e+09
Season
Fall
Spring
Summer
Winter

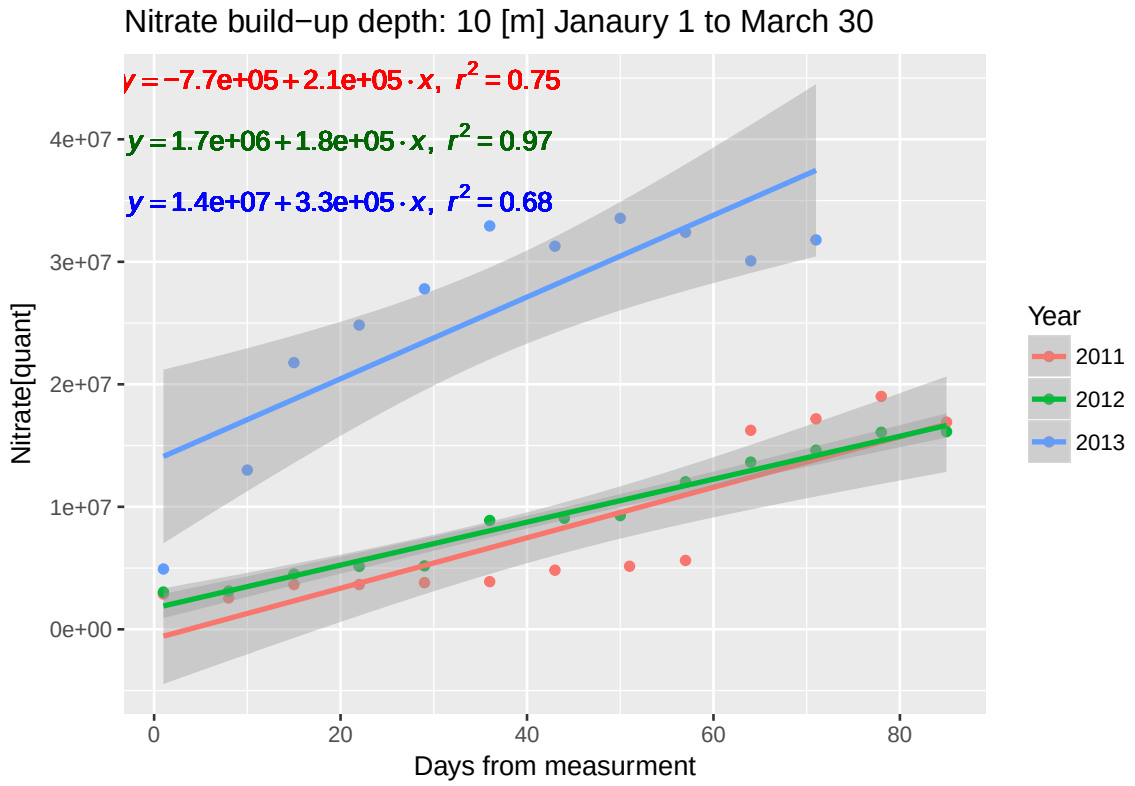

Nitrate depth: 30 [m]
Nitrate[quant]
3e+07
2e+07
1e+07
0e+00
10−2010
04−2011
10−2011
04−2012
10−2012
04−2013
Month
Oxygen
5e+08
4e+08
3e+08
2e+08
1e+08
0e+00
Season
Fall
Spring
Summer
Winter


NH4 depth: 30 [m]
NH4[quant]
6e+07
4e+07
2e+07
0e+00
10−2010
04−2011
10−2011
04−2012
10−2012
04−2013
Month
Oxygen
5e+08
4e+08
3e+08
2e+08
1e+08
0e+00
Season
Fall
Spring
Summer
Winter

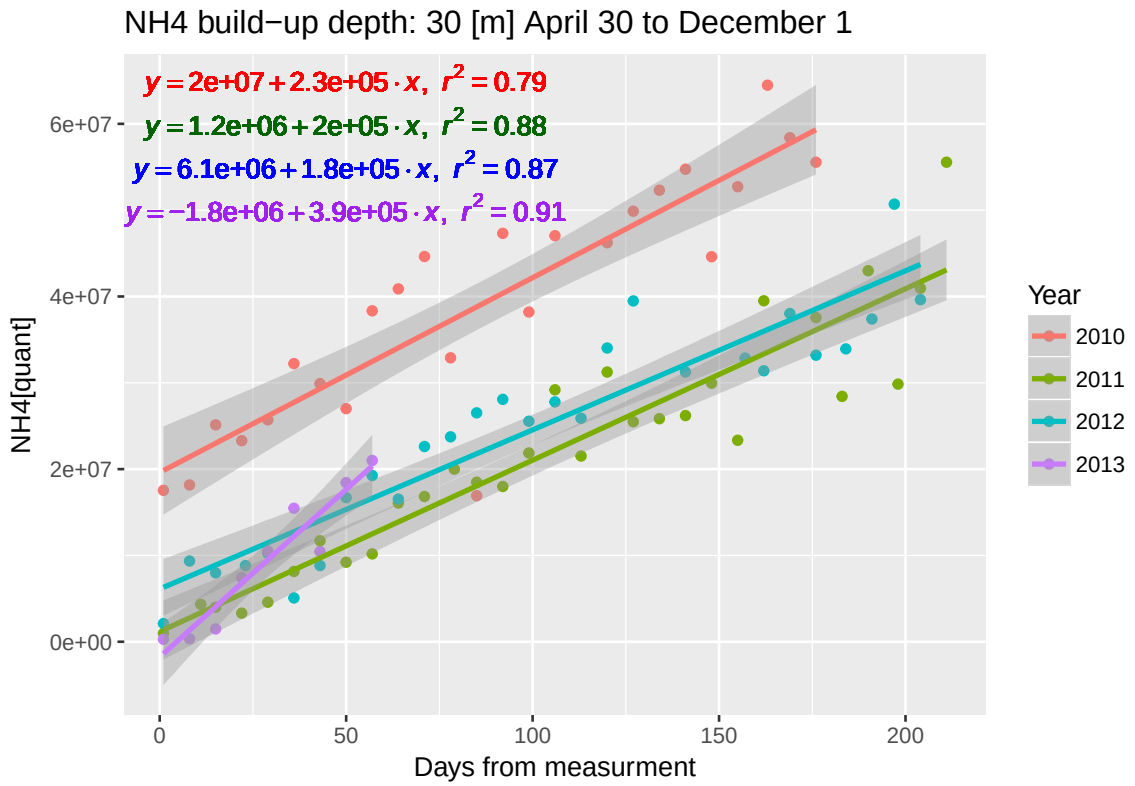
Process rate estimation

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 thtough 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 epiliomnion 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 build-up and consumption processes.

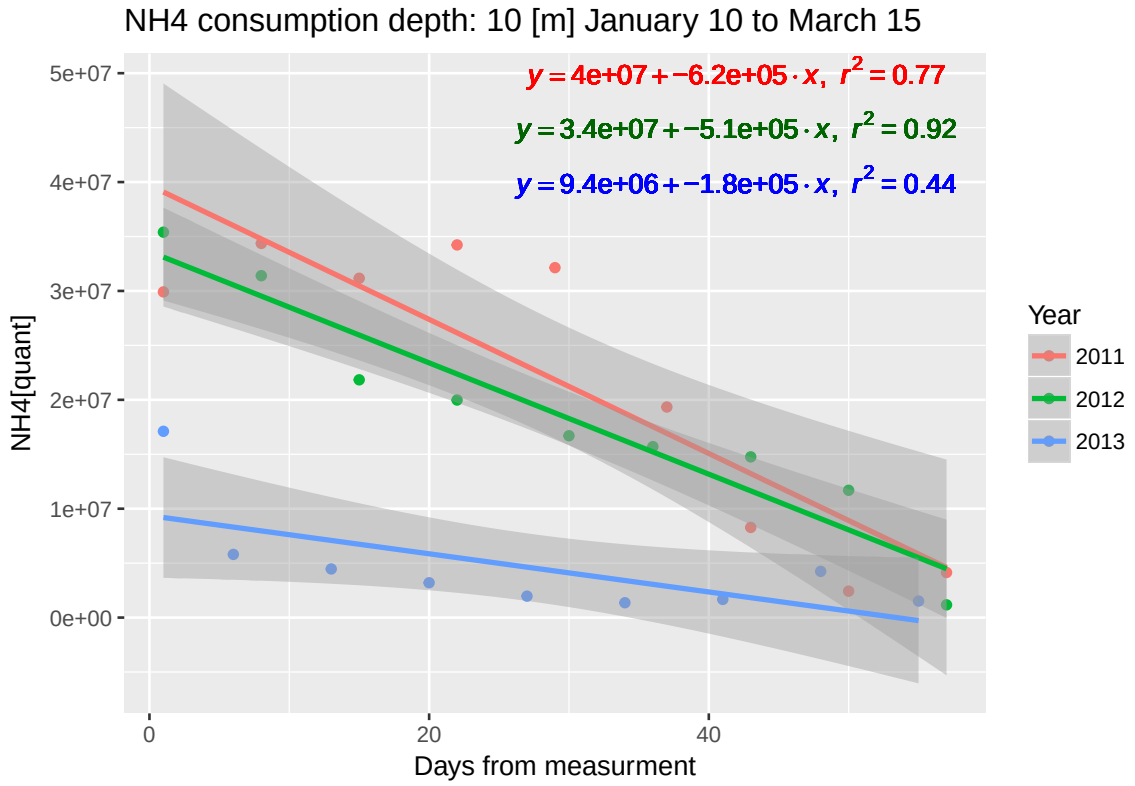
Simulate nitrate build-up between January 1^{st} and March 30^{th} in 10m depth in order to estimate processes rate



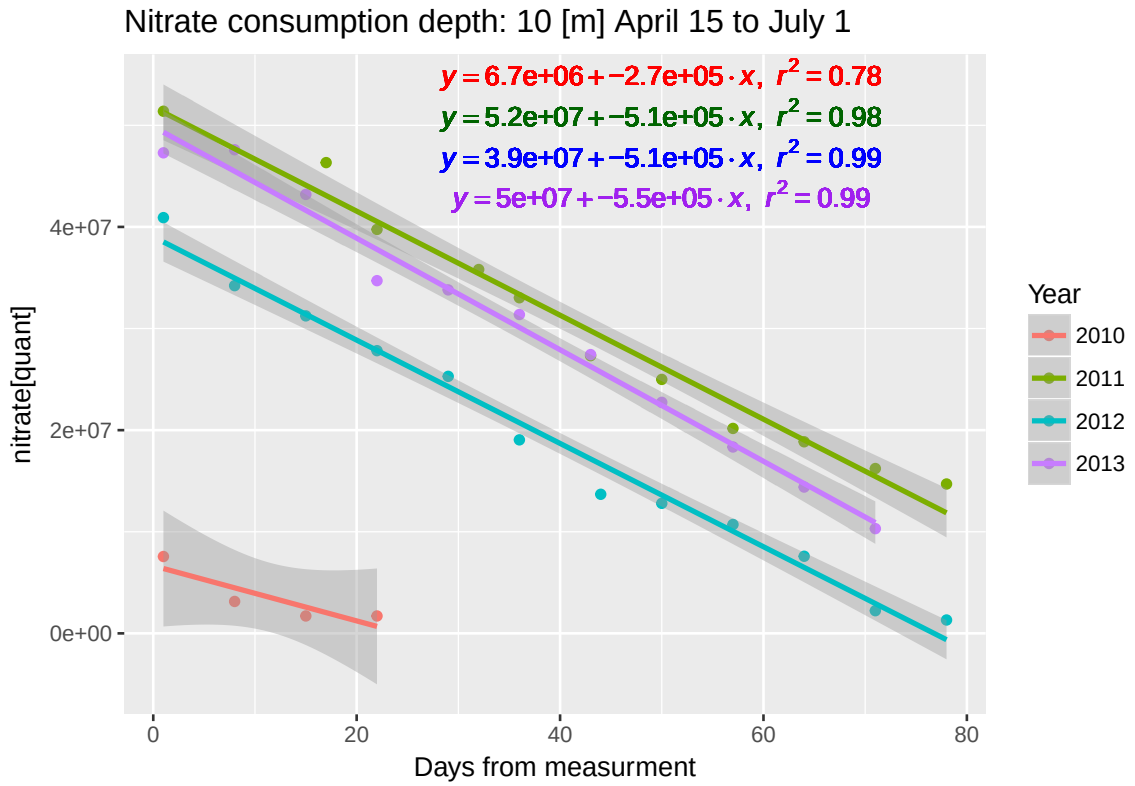
simulate NH4 build-up between April 30^{th} and December 1^{st} in 30m depth in order to estimate reaction rate



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



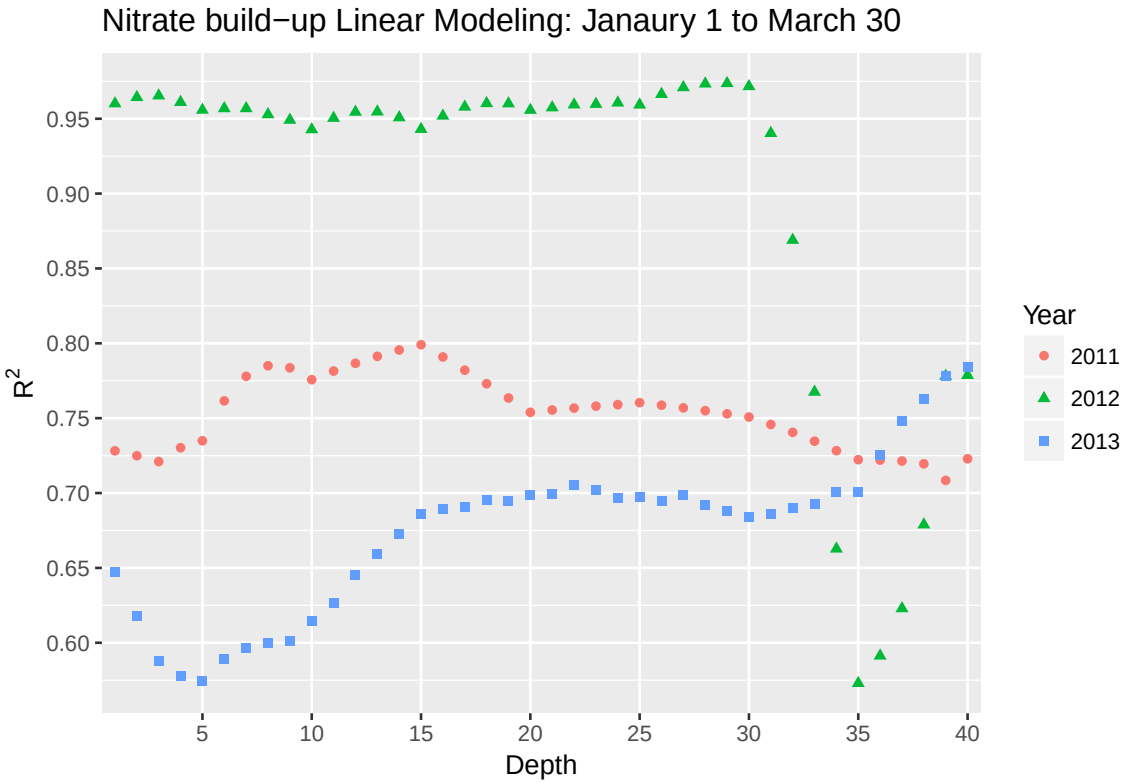
simulate nitrate consumption between April 10^{th} and July 1^{st} in 10m depth in order to estimate reaction rate

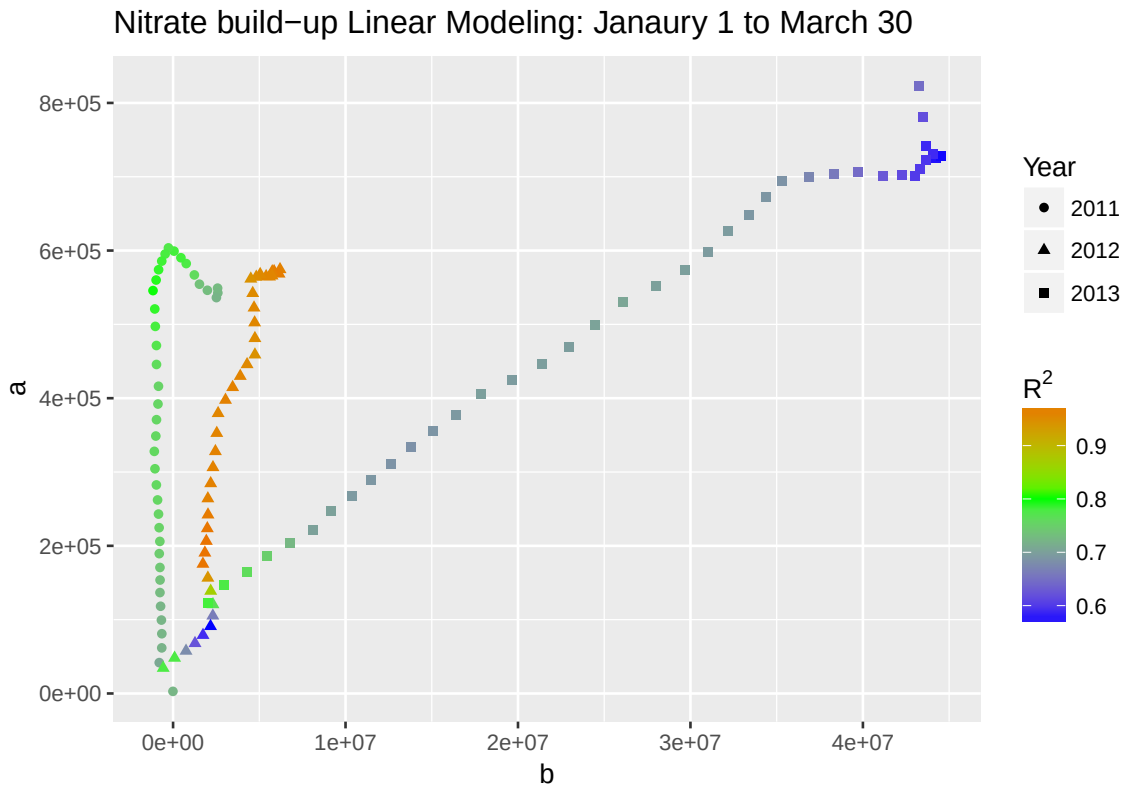


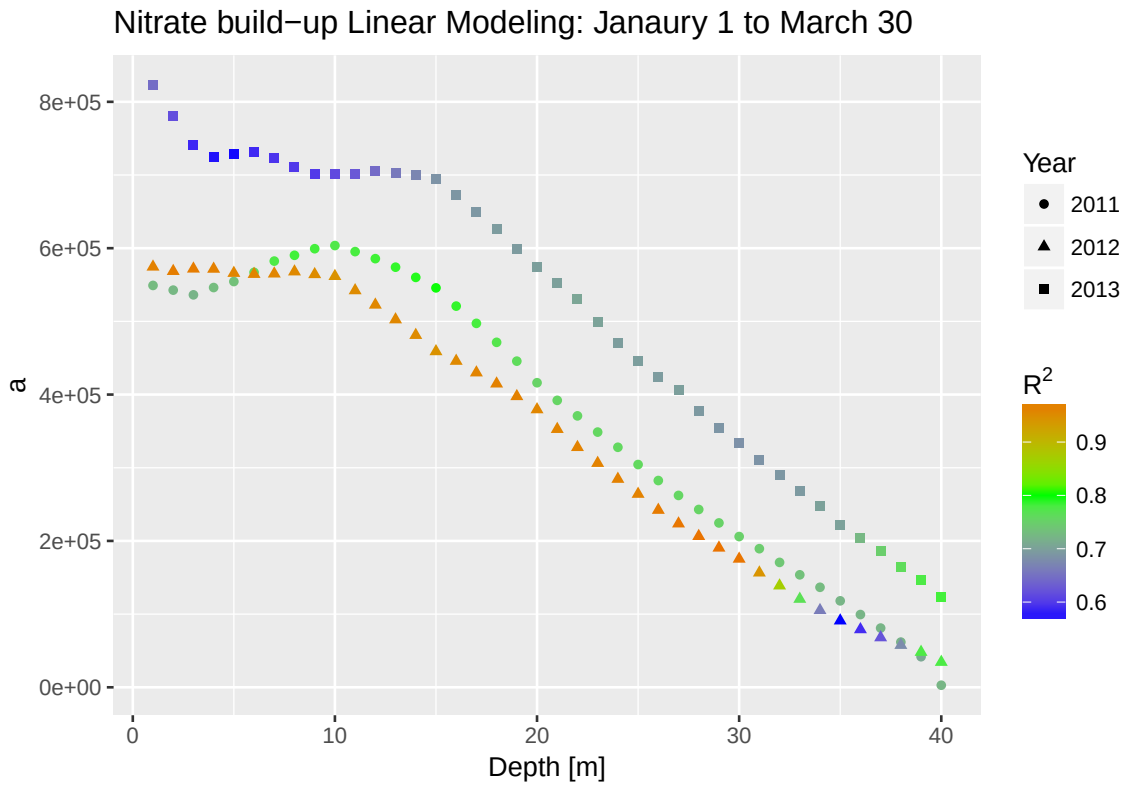
Coeffiecients assement for all depths

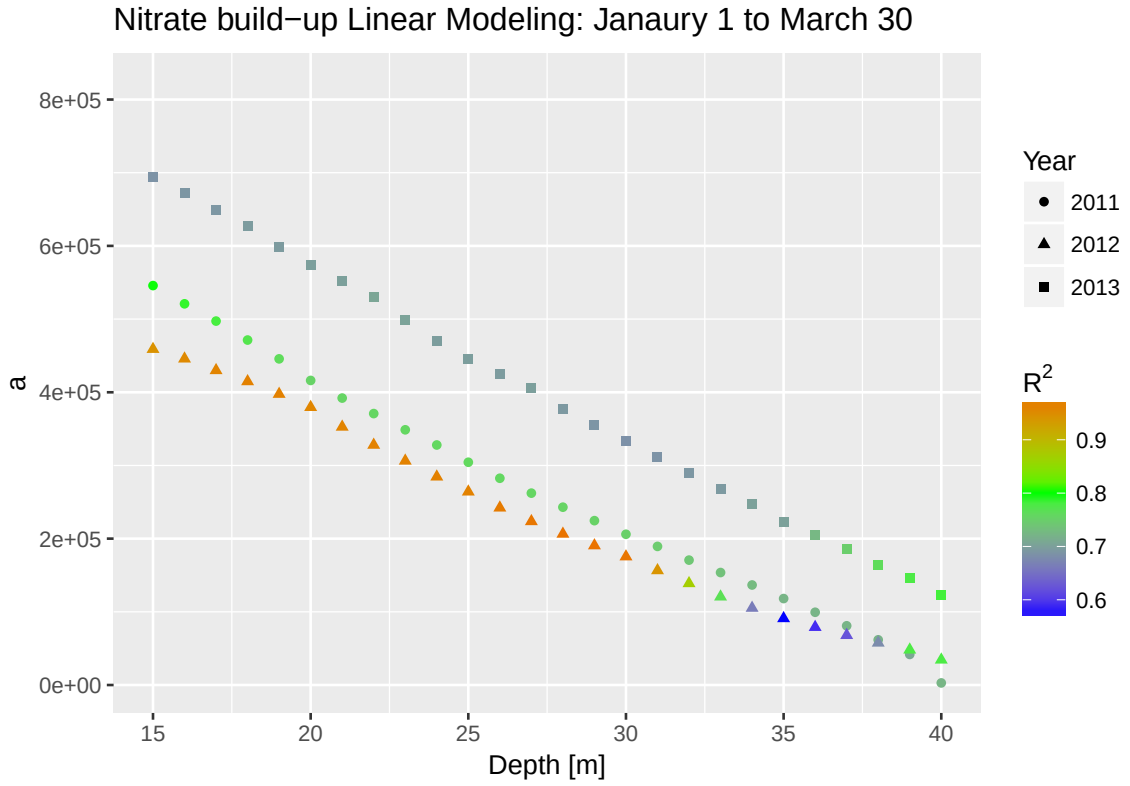
After consideration of the dominant processes that control nitrate and ammonium content in the lake, the following section provides an assesment of the processes and their fit to a linear model separately for each depth. The R^2 value can be used to asses the best fit of the model for each depth. It can be observed that the quality of the fit varries greatly amongst different years. This elucidates the effect of 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.

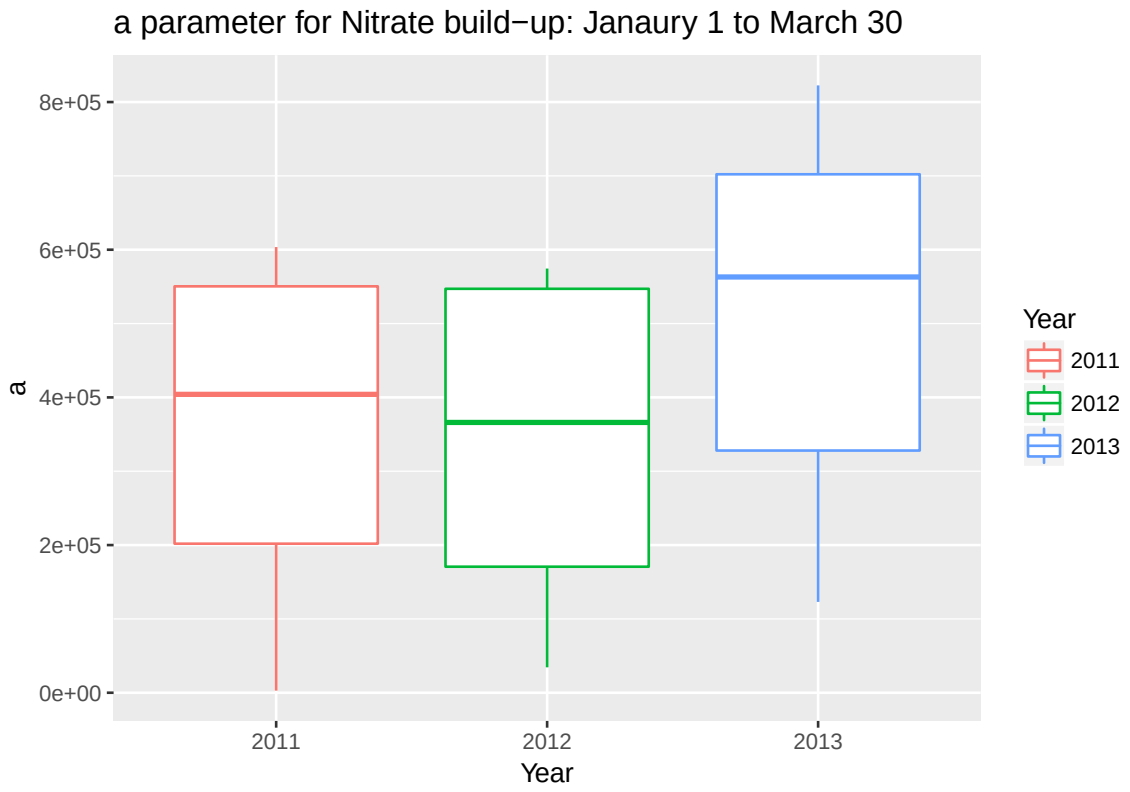
```
##      Depth             a                b                 r2        
##  Min.   : 1.00   Min.   :  2837   Min.   :-1163352   Min.   :0.5730  
##  1st Qu.:10.75   1st Qu.:223195   1st Qu.: -315929   1st Qu.:0.6953  
##  Median :20.50   Median :437797   Median : 2589163   Median :0.7545  
##  Mean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

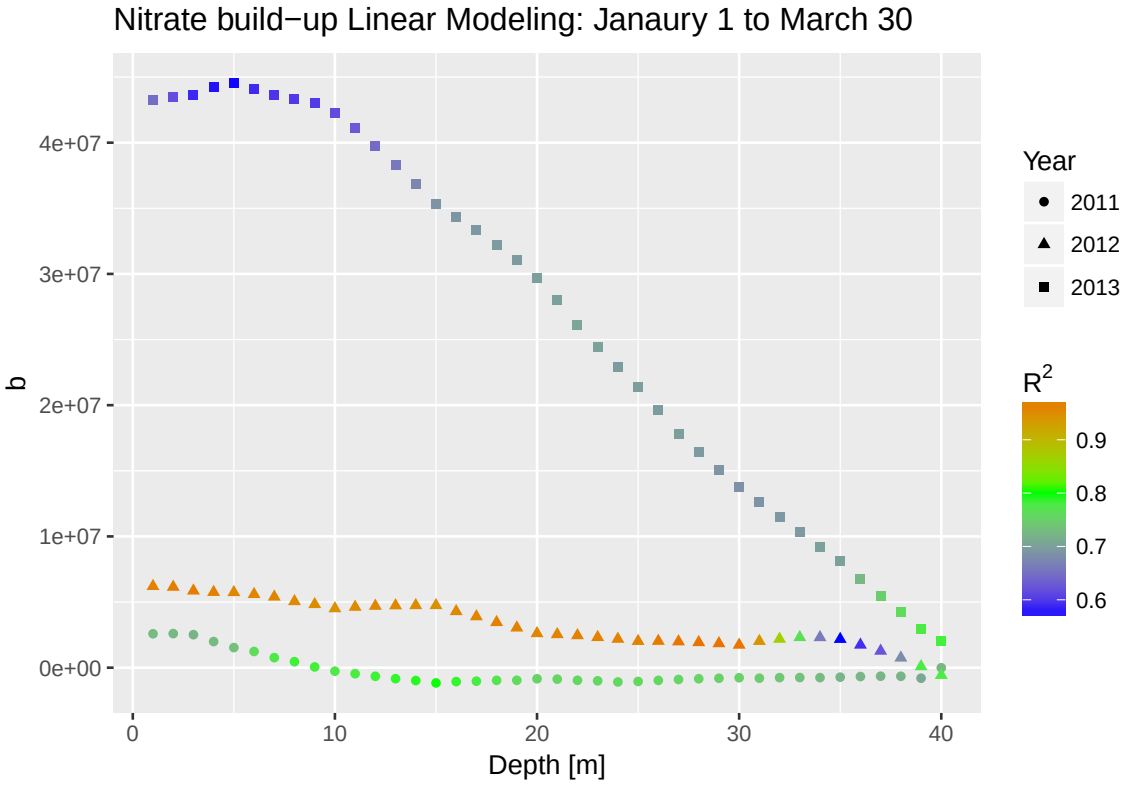

Nitrate build−up Linear Modeling: Janaury 1 to March 30
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
R2
5
10
15
20
25
30
35
40
Depth
Year
2011
2012
2013

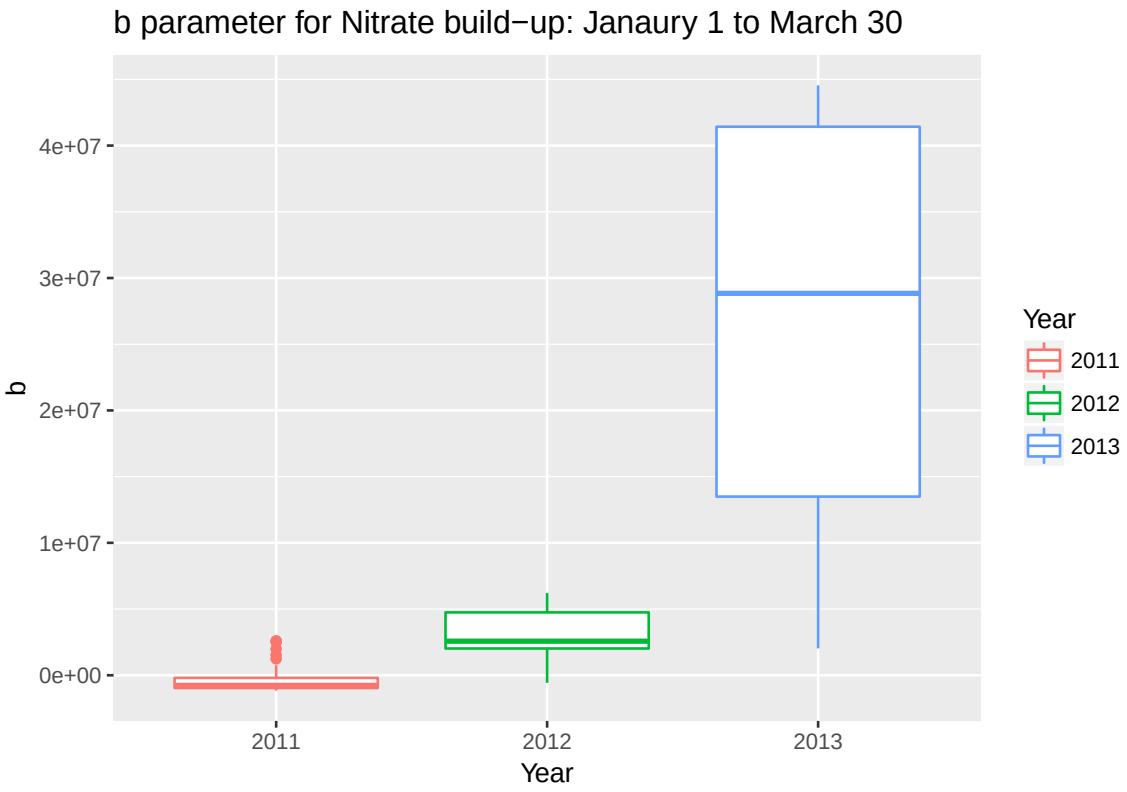

Nitrate build−up Linear Modeling: Janaury 1 to March 30
8e+05
6e+05
4e+05
2e+05
0e+00
a
0e+00
1e+07
2e+07
3e+07
4e+07
b
Year
2011
2012
2013
R2
0.9
0.8
0.7
0.6

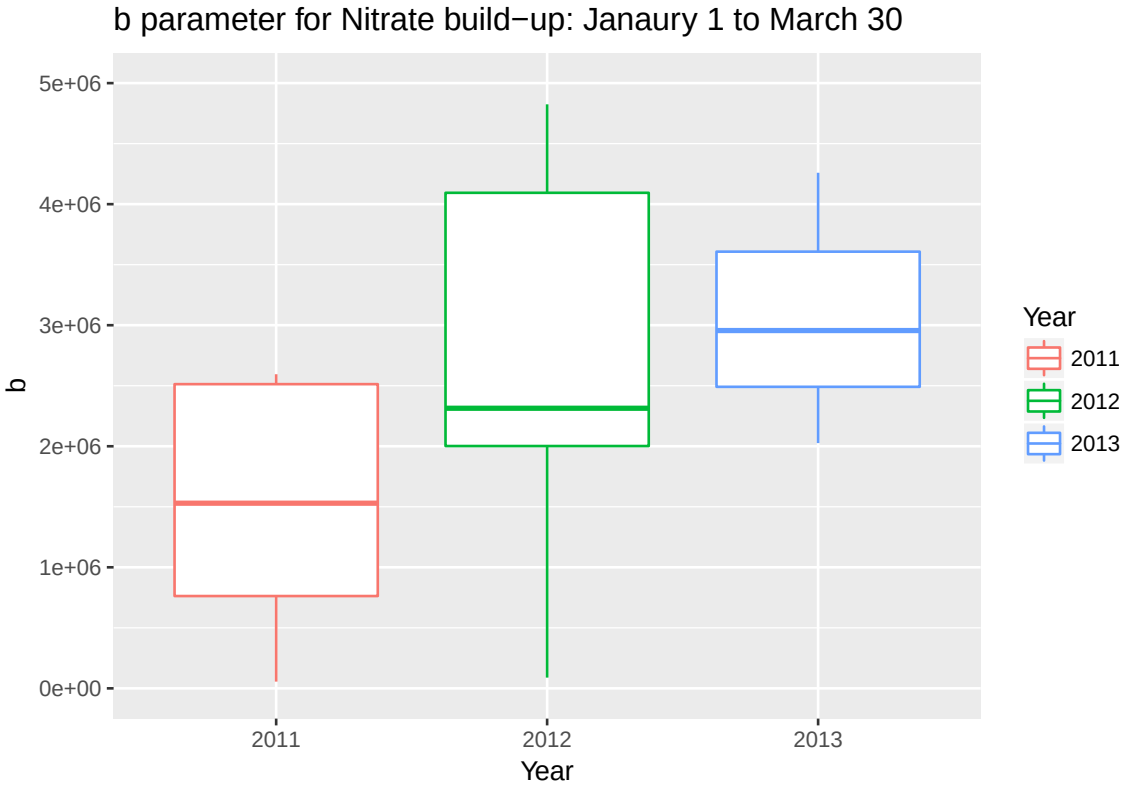

Nitrate build−up Linear Modeling: Janaury 1 to March 30
8e+05
6e+05
4e+05
2e+05
0e+00
a
0
10
20
30
40
Depth [m]
Year
2011
2012
2013
R2
0.9
0.8
0.7
0.6


Nitrate build−up Linear Modeling: Janaury 1 to March 30
8e+05
6e+05
4e+05
2e+05
0e+00
a
15
20
25
30
35
40
Depth [m]
Year
2011
2012
2013
R2
0.9
0.8
0.7
0.6


a parameter for Nitrate build−up: Janaury 1 to March 30
8e+05
6e+05
4e+05
2e+05
0e+00
a
2011
2012
2013
Year
Year
2011
2012
2013


Nitrate build−up Linear Modeling: Janaury 1 to March 30
4e+07
3e+07
2e+07
1e+07
0e+00
b
0
10
20
30
40
Depth [m]
Year
2011
2012
2013
R2
0.9
0.8
0.7
0.6

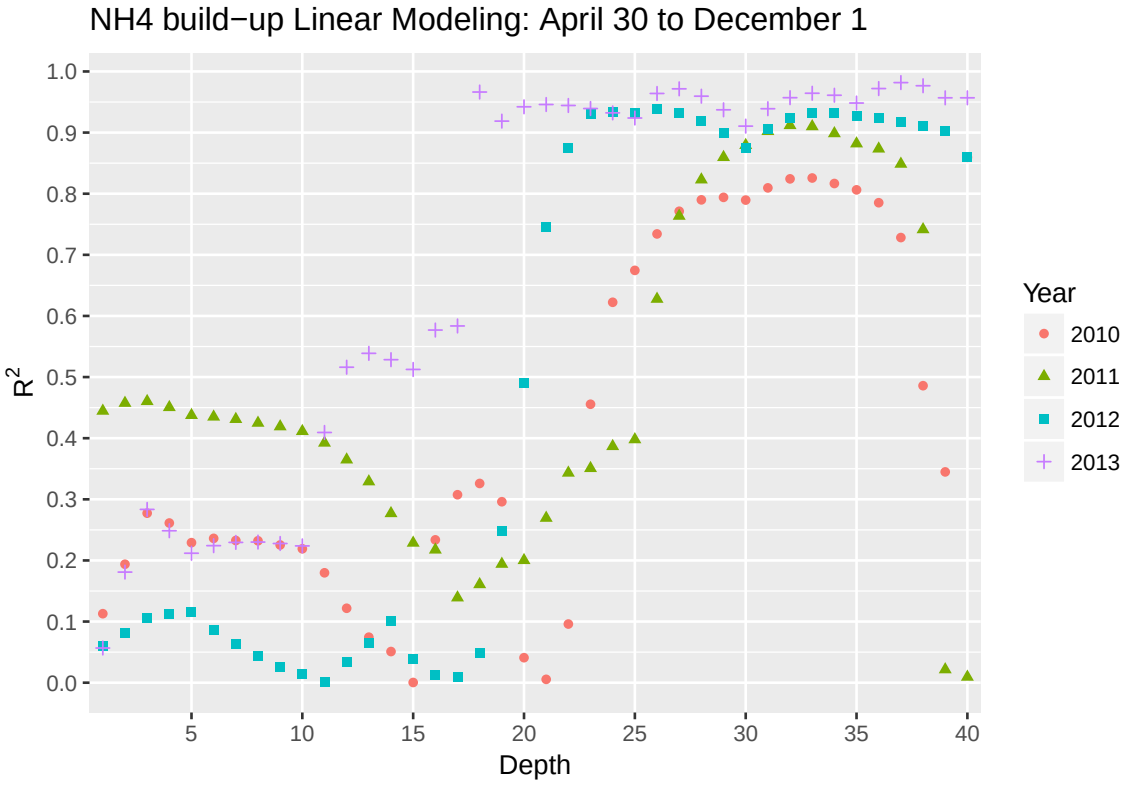


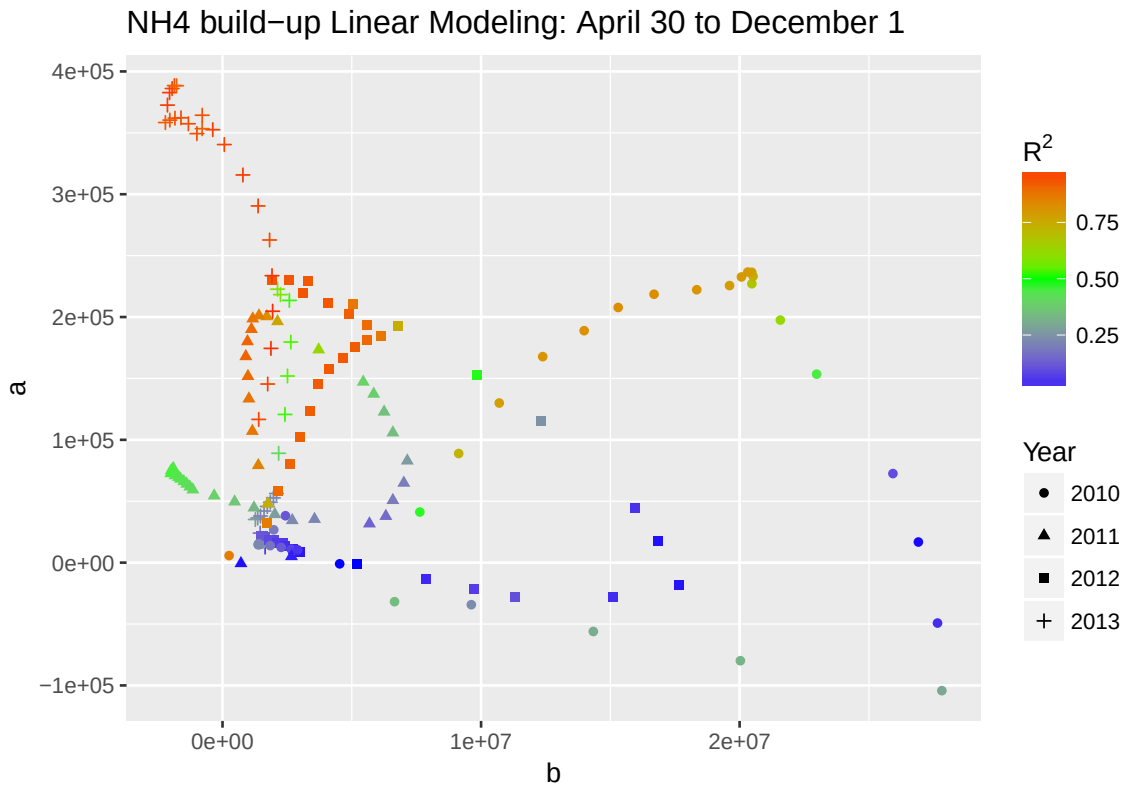


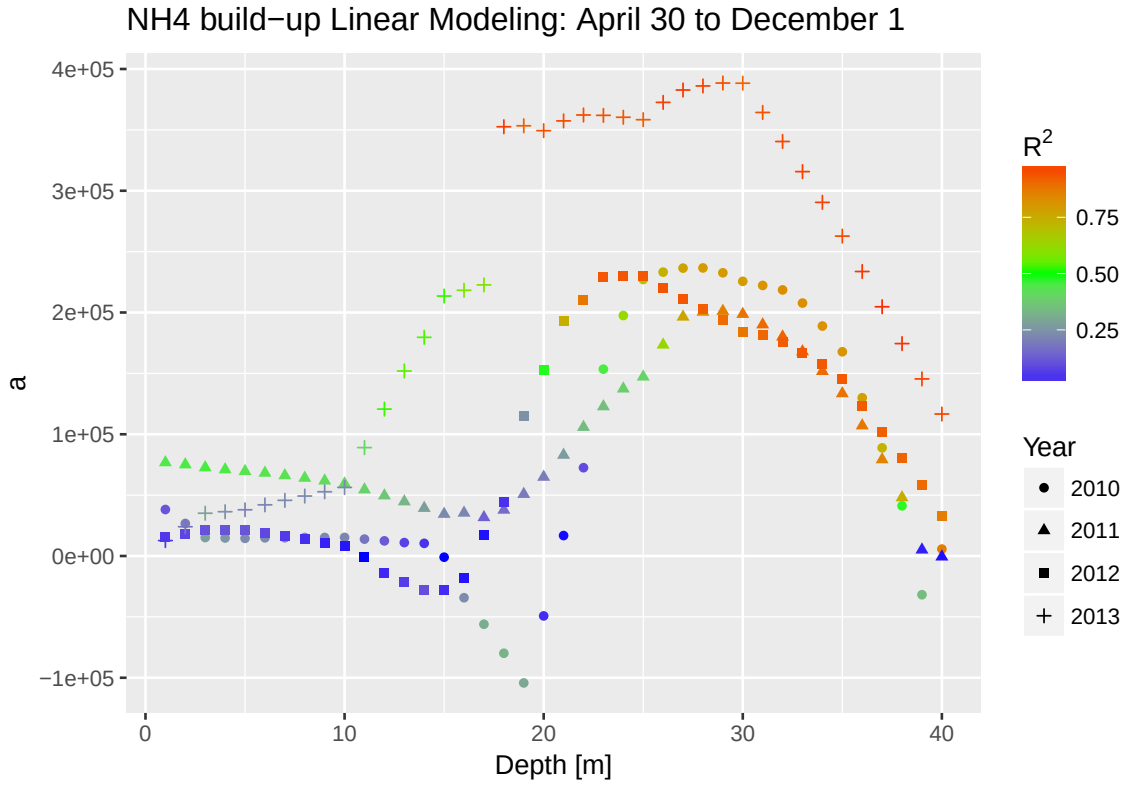
It can be observed that ammonium buildup does fit the linear model in most depths as nicely as nitrate. Intraannual changes are significatn, and once more illustrate the complexity of the system and its divergence from linearity. Unsurprisingly, the model has the best fit for depths of 20 to 35m, where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

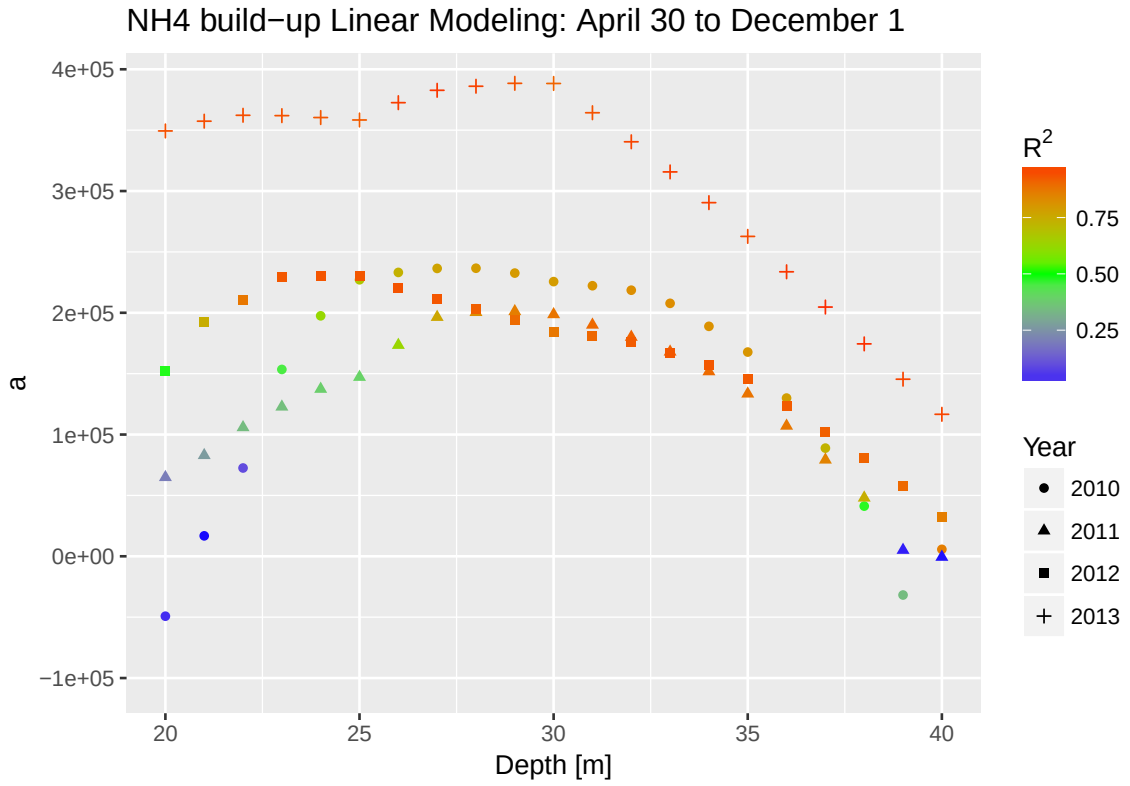
depends on annual stratification and mixing.

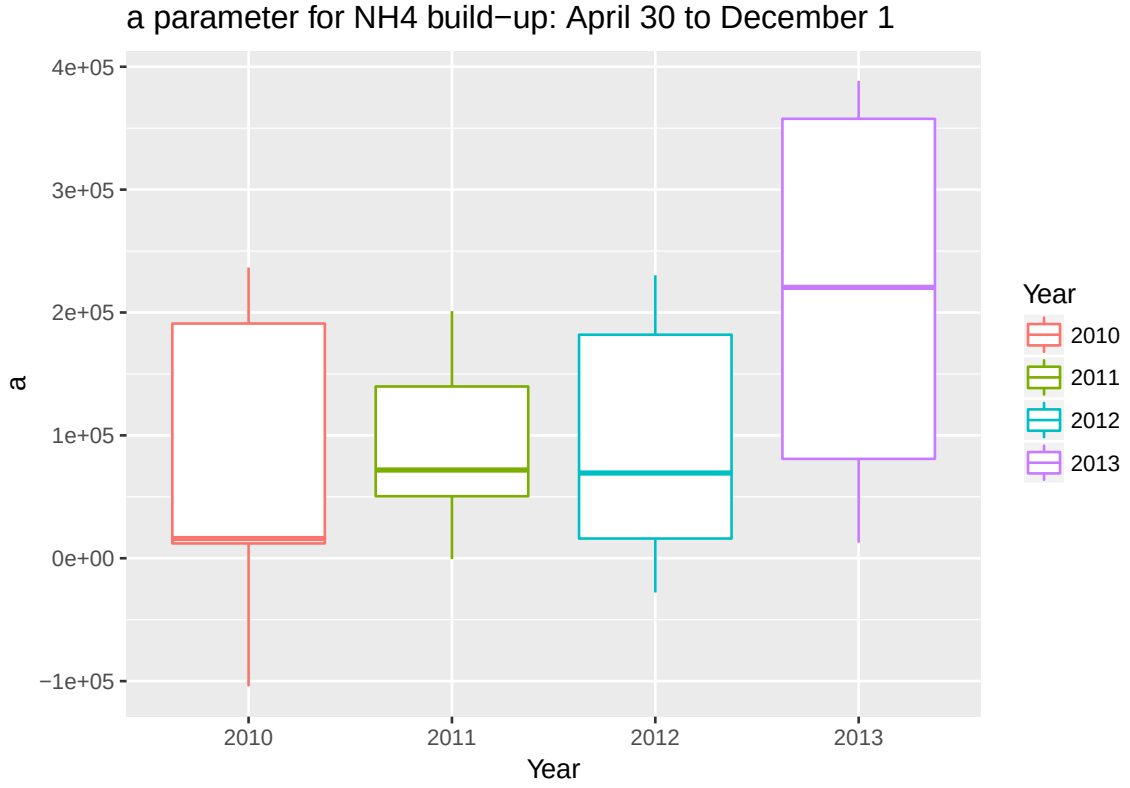
```
##      Depth             a                  b                  r2
##  Min.   : 1.00   Min.   :-104262   Min.   :-2209182   Min.   :0.0003153
##  1st Qu.:10.75   1st Qu.:  21419   1st Qu.: 1373549   1st Qu.:0.2240937
##  Median :20.50   Median :  81791   Median : 2140742   Median :0.4588809
##  Mean   :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
```

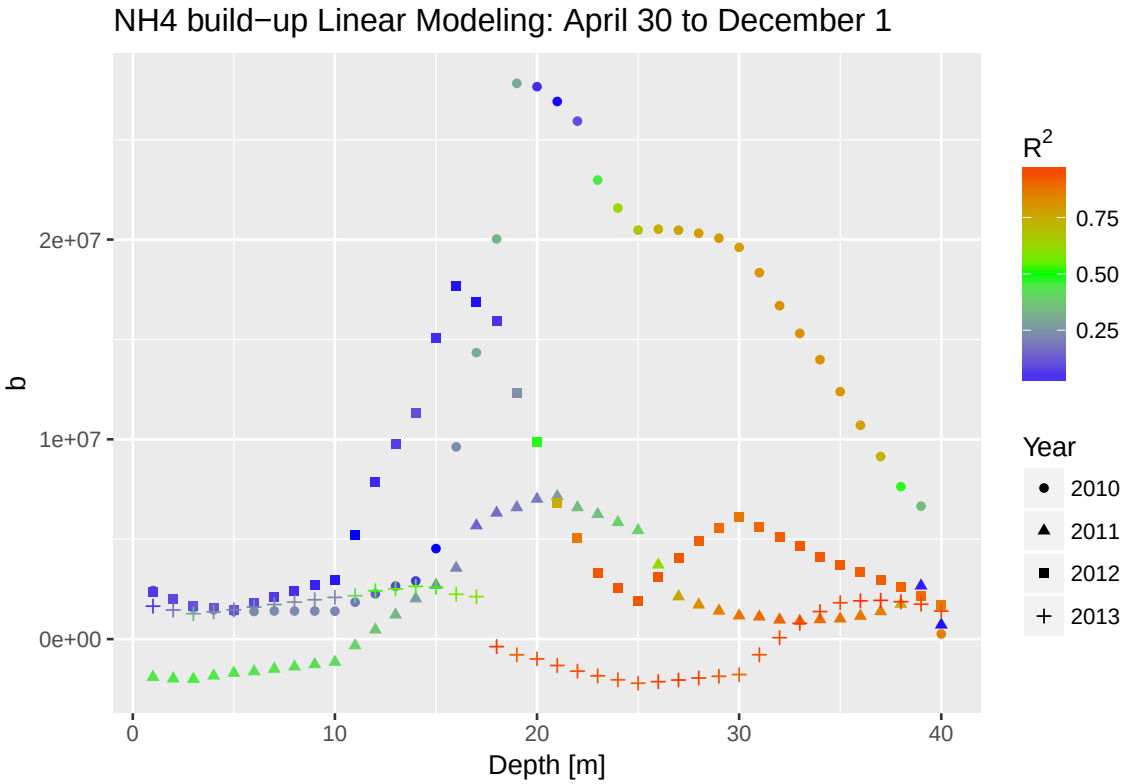


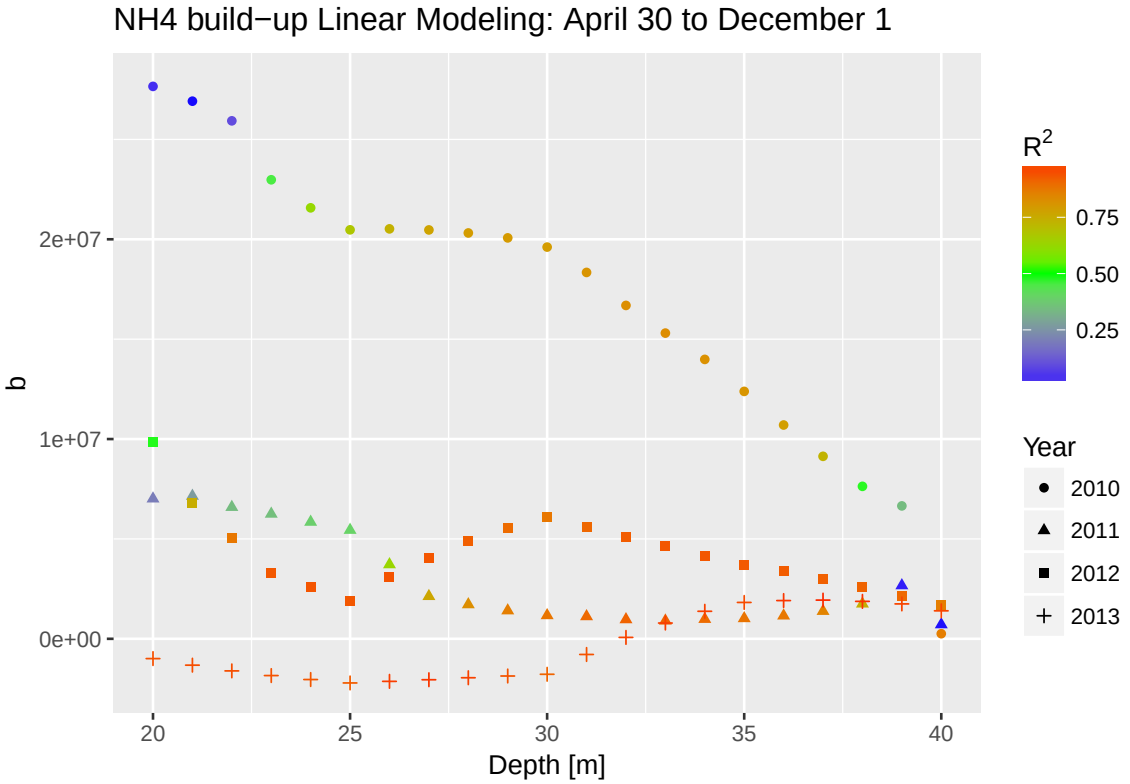

NH4 build−up Linear Modeling: April 30 to December 1
4e+05
3e+05
2e+05
1e+05
0e+00
−1e+05
a
0e+00
1e+07
2e+07
b
R2
0.75
0.50
0.25
Year
2010
2011
2012
2013

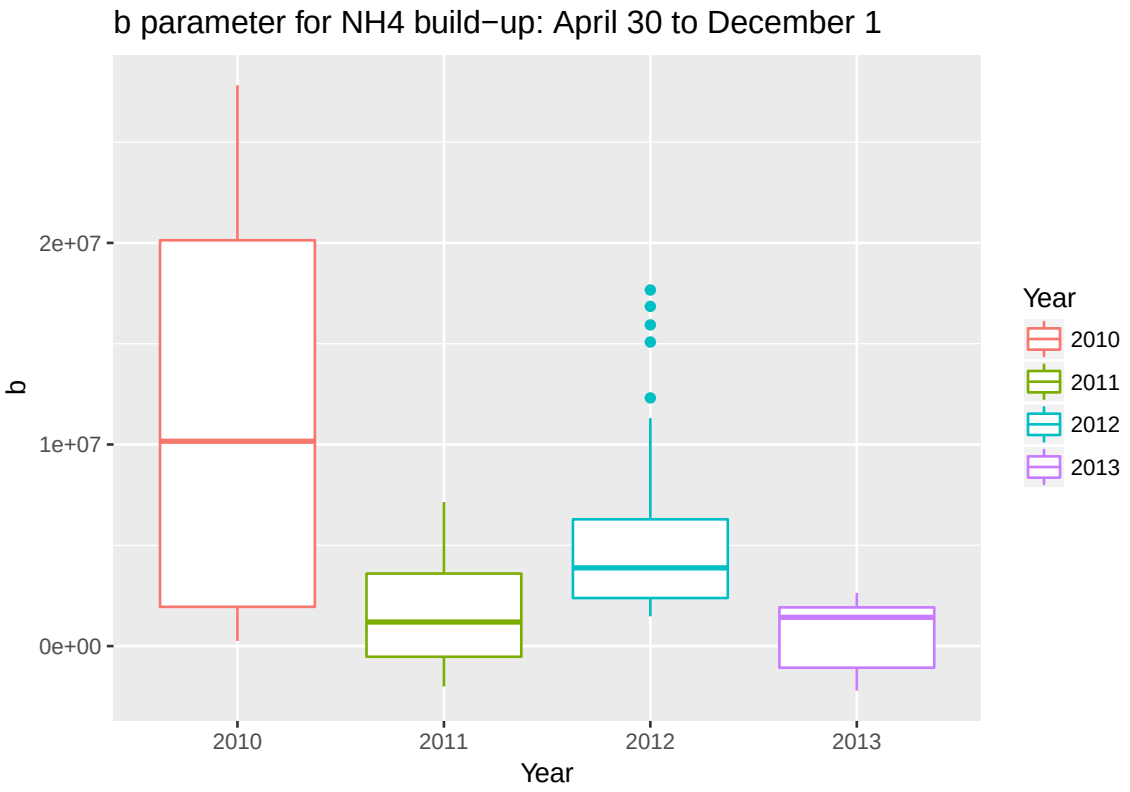

NH4 build−up Linear Modeling: April 30 to December 1
4e+05
3e+05
2e+05
1e+05
0e+00
−1e+05
a
0
10
20
30
40
Depth [m]
R2
0.75
0.50
0.25
Year
2010
2011
2012
2013

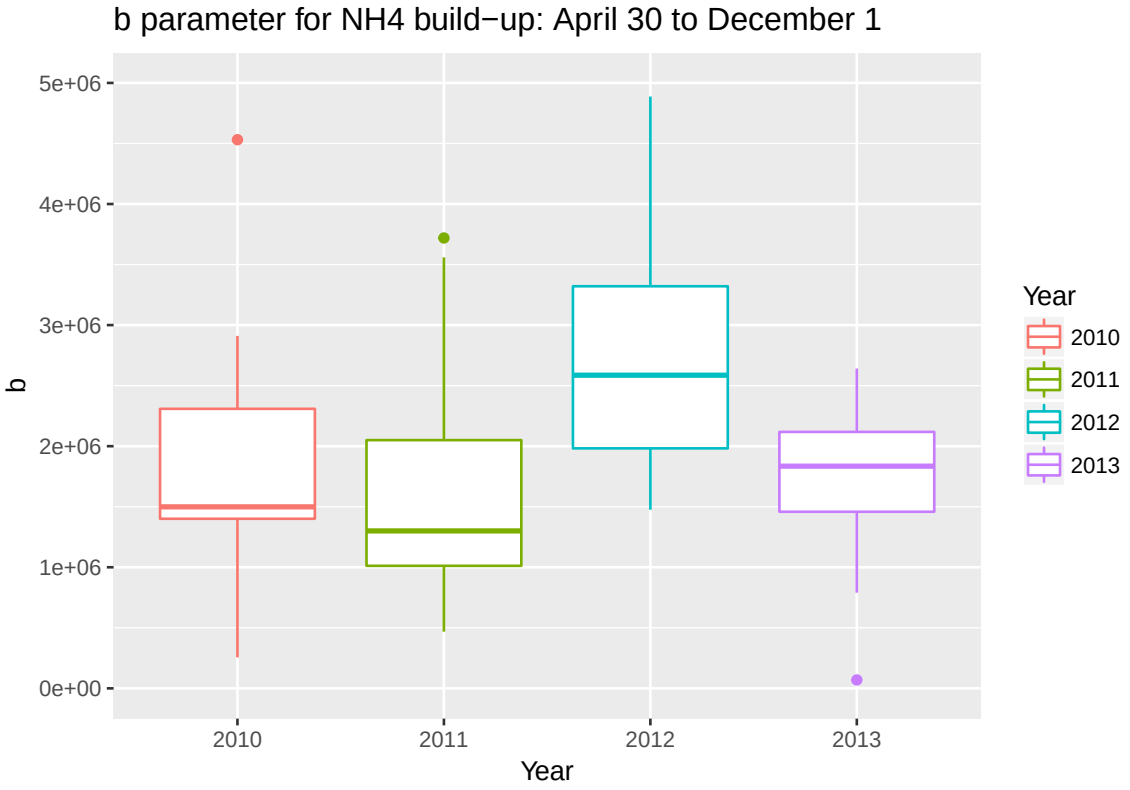

NH4 build−up Linear Modeling: April 30 to December 1
4e+05
3e+05
2e+05
1e+05
0e+00
−1e+05
a
20
25
30
35
40
Depth [m]
R2
0.75
0.50
0.25
Year
2010
2011
2012
2013


a parameter for NH4 build−up: April 30 to December 1
4e+05
3e+05
2e+05
1e+05
0e+00
−1e+05
a
2010
2011
2012
2013
Year
Year
2010
2011
2012
2013


NH4 build−up Linear Modeling: April 30 to December 1
b
2e+07
1e+07
0e+00
0
10
20
30
40
Depth [m]
R2
0.75
0.50
0.25
Year
2010
2011
2012
2013


NH4 build−up Linear Modeling: April 30 to December 1
b
2e+07
1e+07
0e+00
20
25
30
35
40
Depth [m]
R2
0.75
0.50
0.25
Year
2010
2011
2012
2013

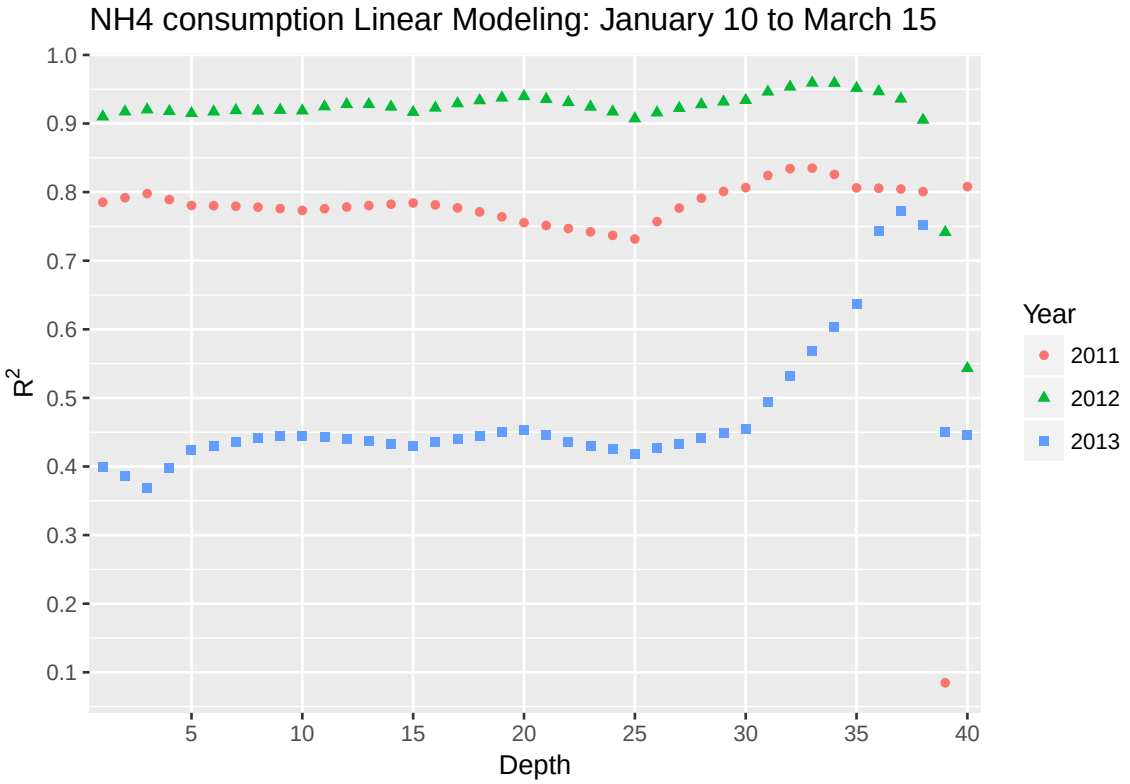


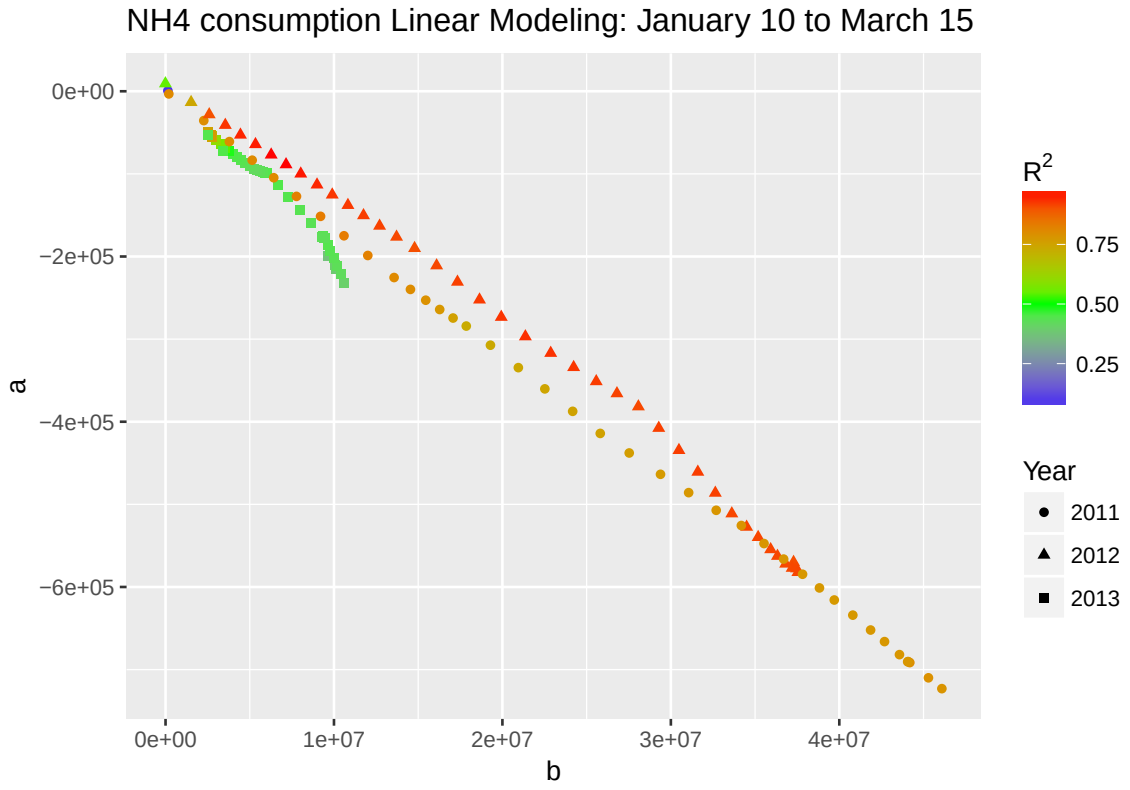


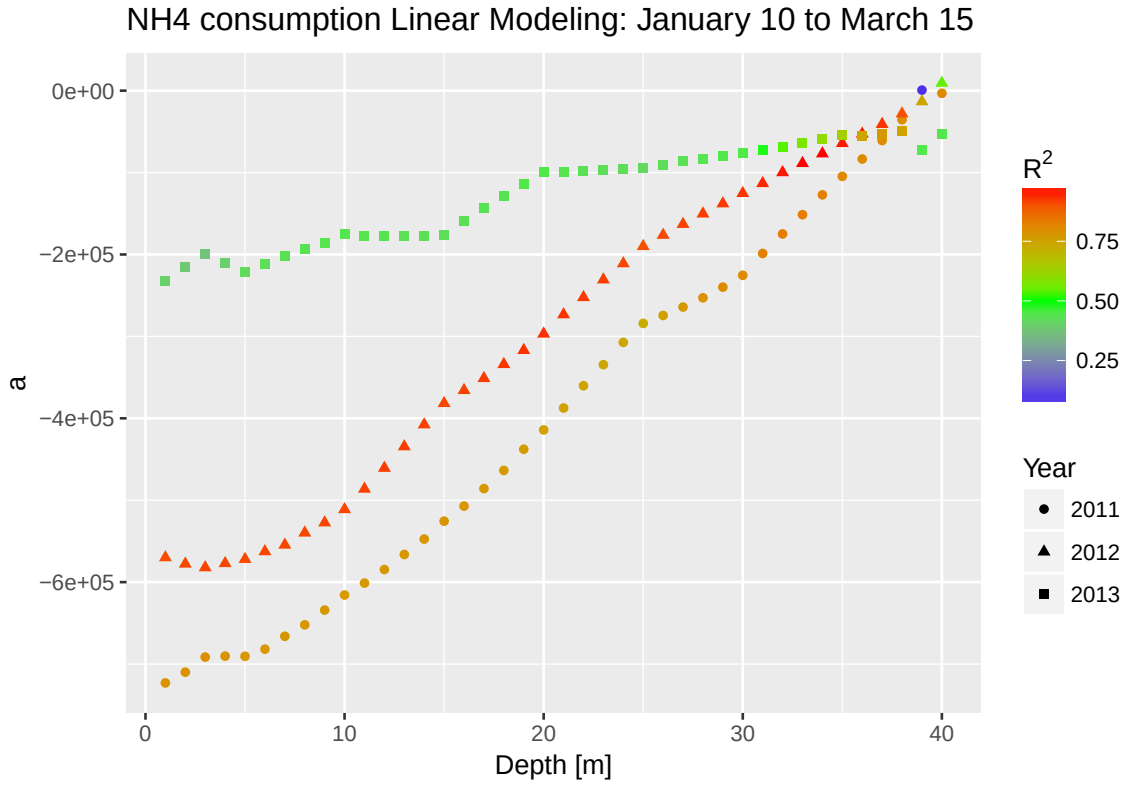
Ammonium consumption after mixing between January 15^{th} to March 15^{th}

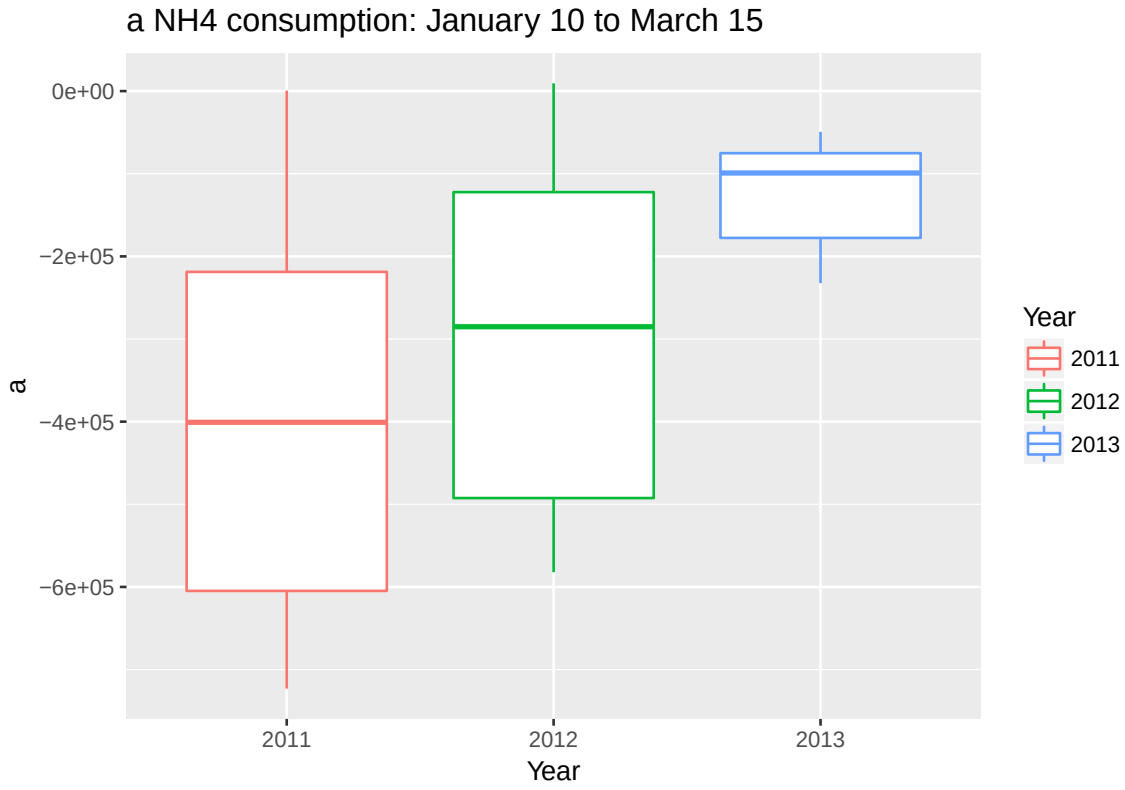
```
##       Depth                a                    b                   r2
```

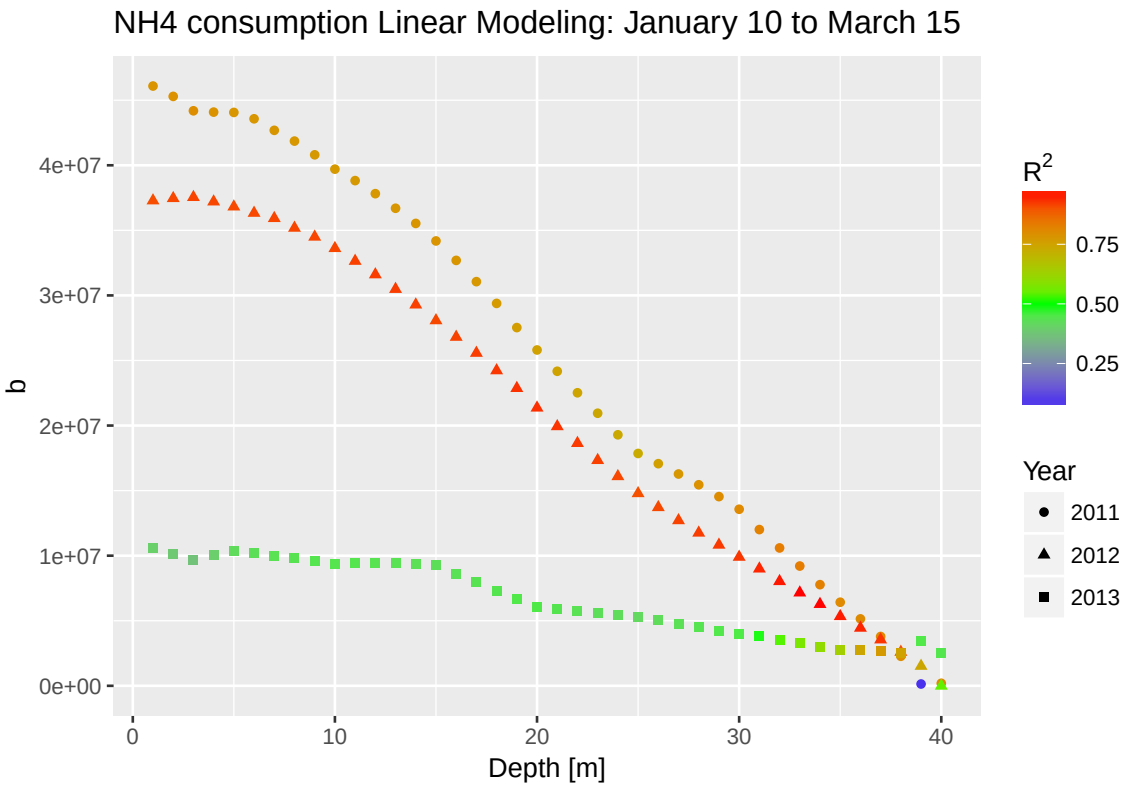
```
##  Min.   : 1.00   Min.   :-723066   Min.   :   -9510   Min.   :0.08467
##  1st Qu.:10.75   1st Qu.:-443545   1st Qu.: 5888522   1st Qu.:0.45085
##  Median :20.50   Median :-200589   Median :10710844   Median :0.77990
##  Mean   :20.50   Mean   :-272712   Mean   :17447156   Mean   :0.71780
##  3rd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

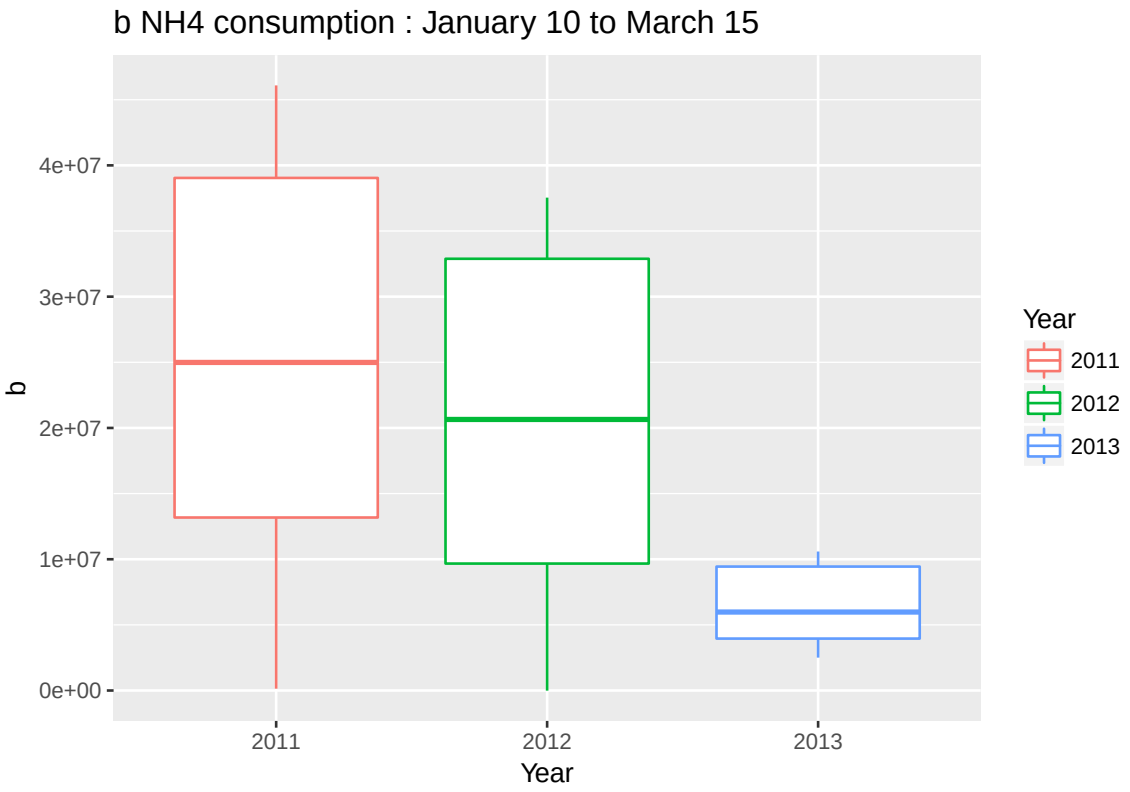



NH4 consumption Linear Modeling: January 10 to March 15
0e+00
−2e+05
−4e+05
−6e+05
a
0e+00
1e+07
2e+07
3e+07
4e+07
b
R2
0.75
0.50
0.25
Year
2011
2012
2013


NH4 consumption Linear Modeling: January 10 to March 15
0e+00
−2e+05
−4e+05
−6e+05
a
0
10
20
30
40
Depth [m]
R2
0.75
0.50
0.25
Year
2011
2012
2013

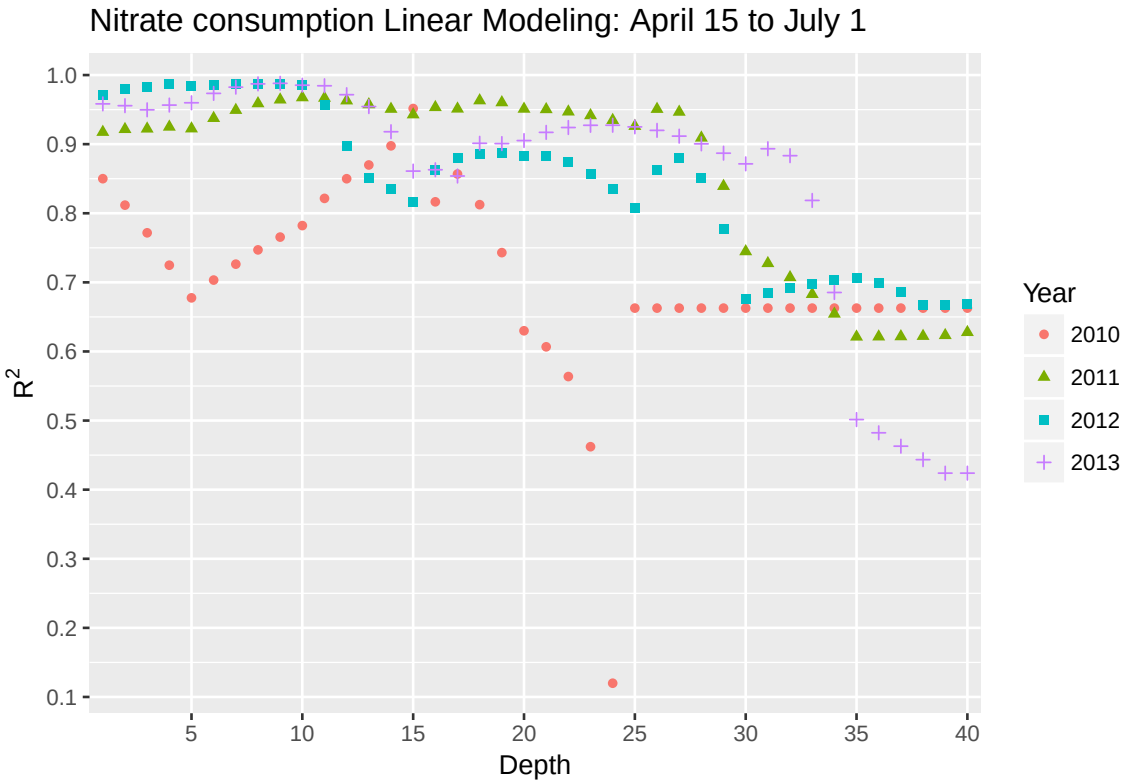

a NH4 consumption: January 10 to March 15
0e+00
−2e+05
−4e+05
−6e+05
a
2011
2012
2013
Year
Year
2011
2012
2013

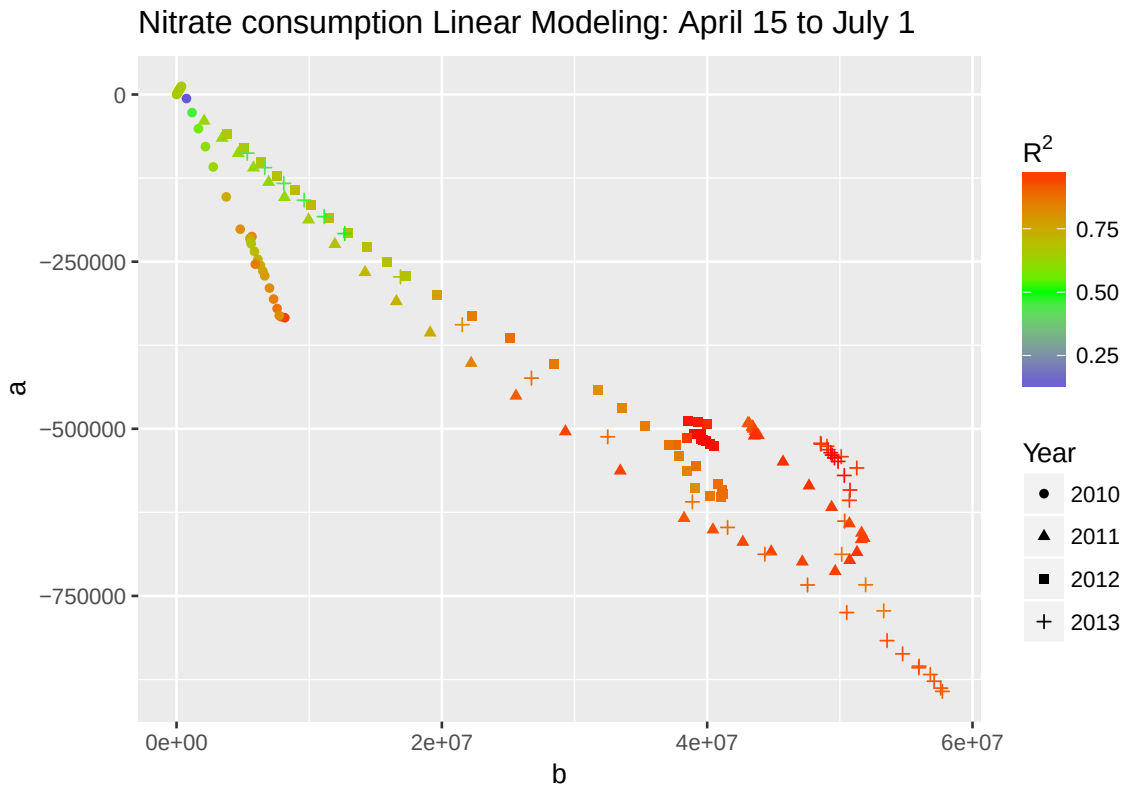

NH4 consumption Linear Modeling: January 10 to March 15
4e+07
3e+07
2e+07
1e+07
0e+00
b
0
10
20
30
40
Depth [m]
R2
0.75
0.50
0.25
Year
2011
2012
2013

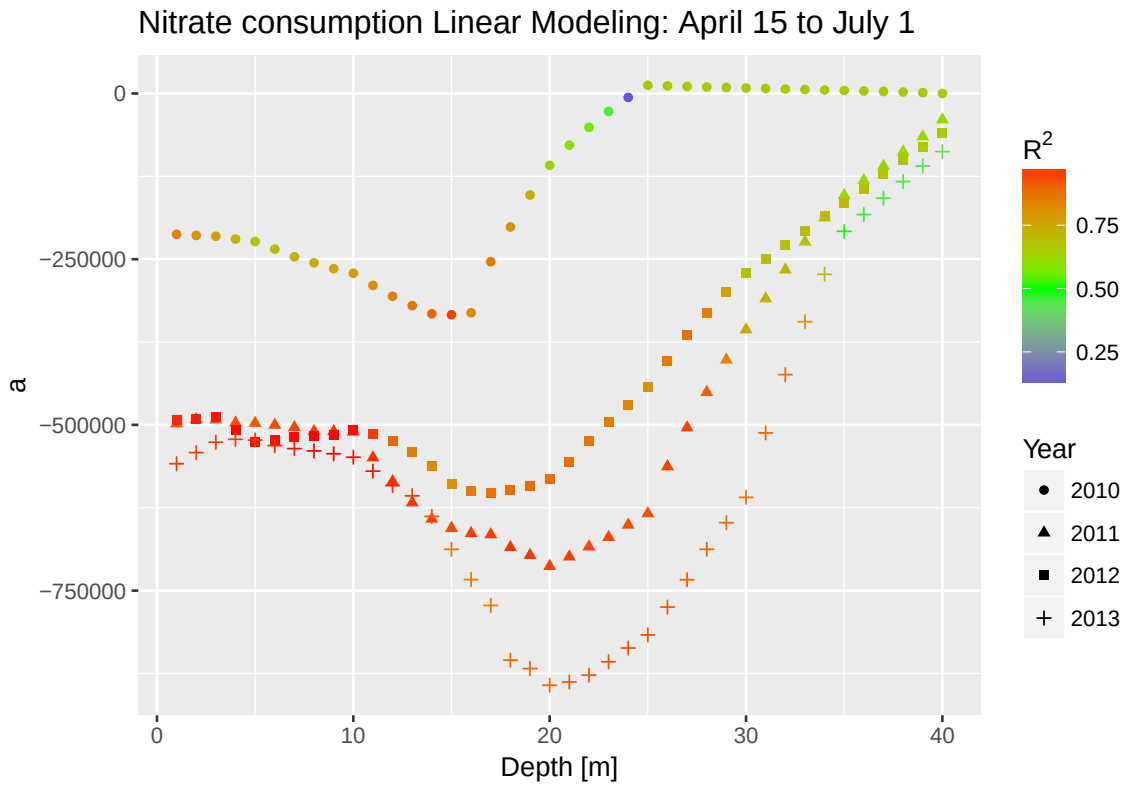


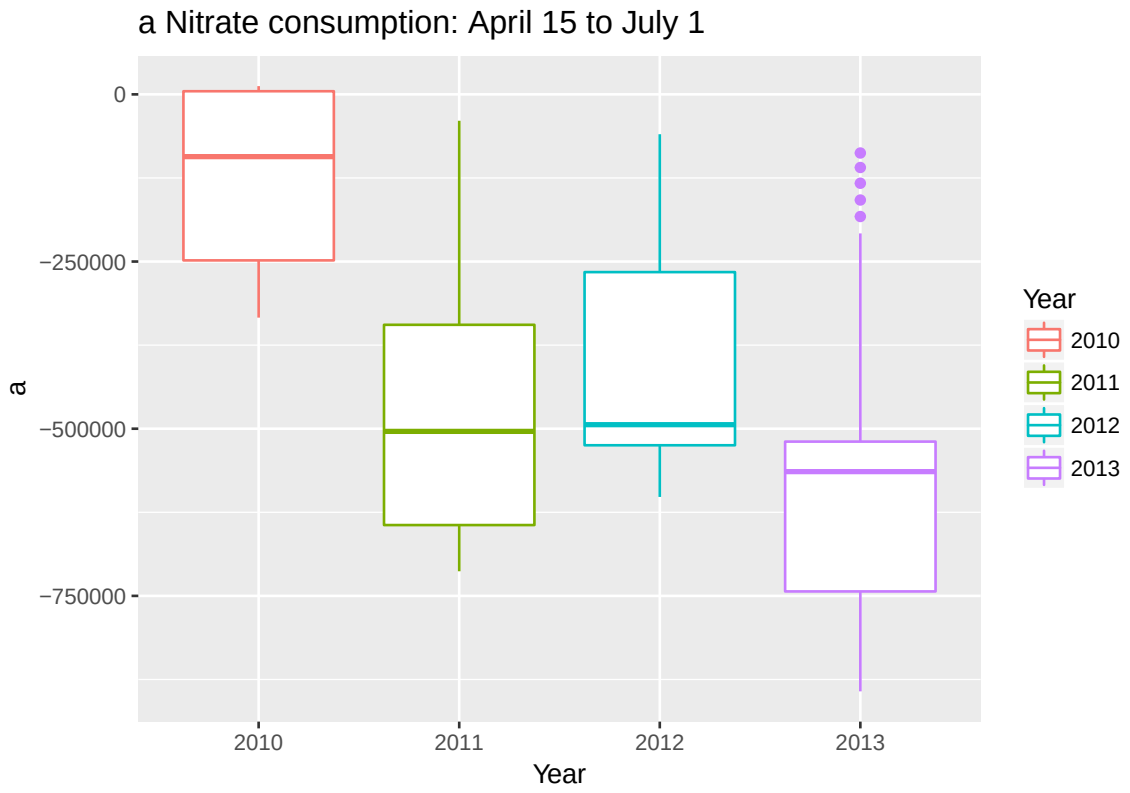
Nitrate consumption after mixing between January 10^{th} to March 15^{th}

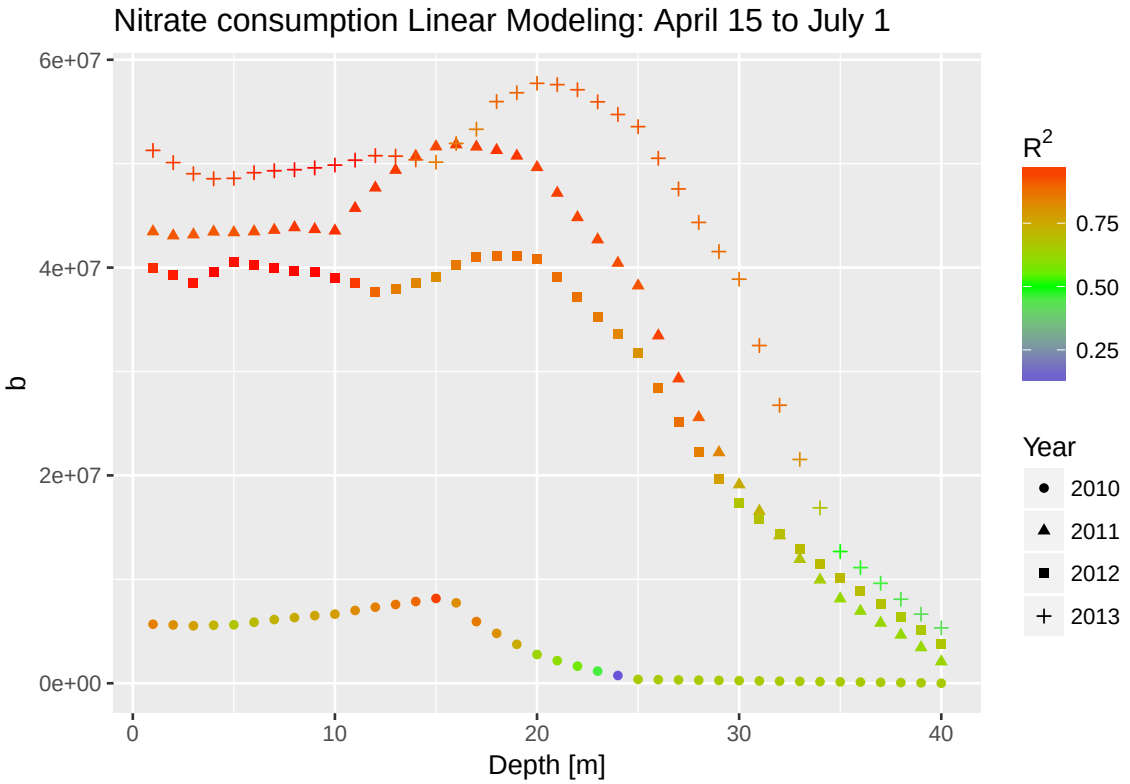
```
##      Depth             a                  b                 r2        
##  Min.   : 1.00   Min.   :-892768   Min.   :    3394   Min.   :0.1199  
##  1st Qu.:10.75   1st Qu.:-564564   1st Qu.: 6471333   1st Qu.:0.6841  
##  Median :20.50   Median :-489261   Median :32975722   Median :0.8628  
##  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
```

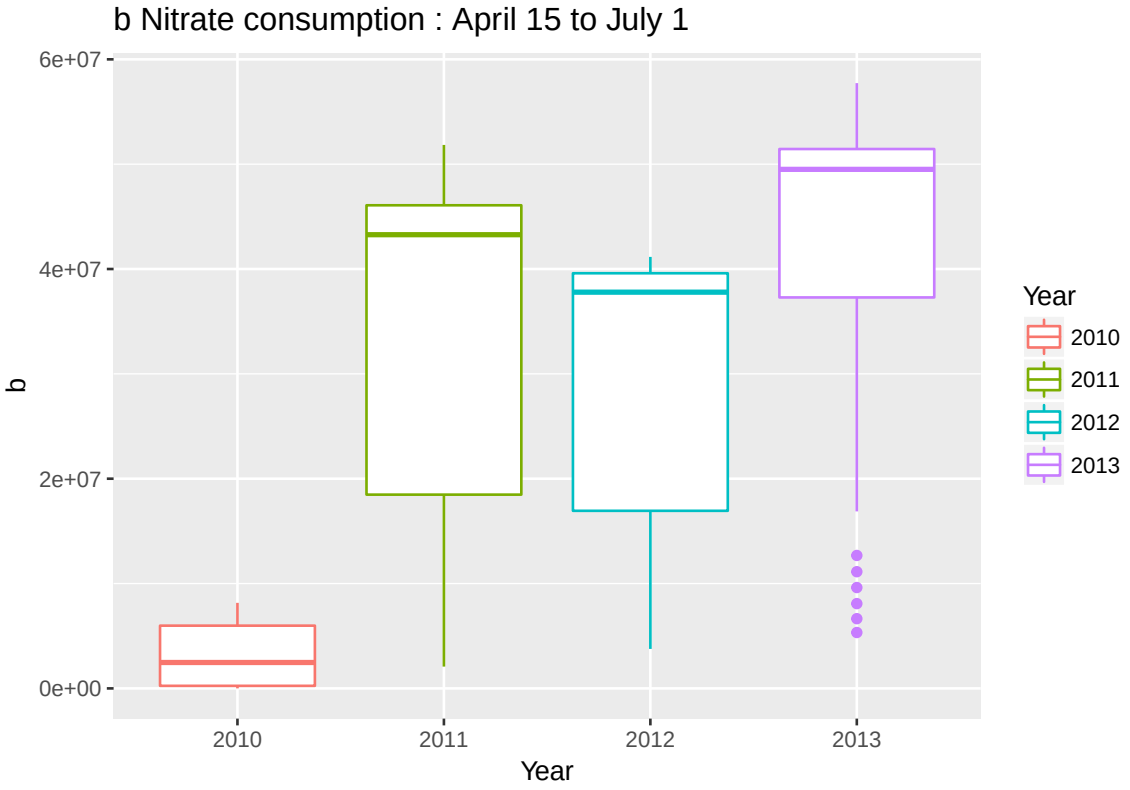

Nitrate consumption Linear Modeling: April 15 to July 1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
R2
5
10
15
20
25
30
35
40
Depth
Year
2010
2011
2012
2013


Nitrate consumption Linear Modeling: April 15 to July 1
0
−250000
−500000
−750000
a
0e+00
2e+07
4e+07
6e+07
b
R2
0.75
0.50
0.25
Year
2010
2011
2012
2013


Nitrate consumption Linear Modeling: April 15 to July 1
a
0
−250000
−500000
−750000
0
10
20
30
40
Depth [m]
R2
0.75
0.50
0.25
Year
2010
2011
2012
2013


a Nitrate consumption: April 15 to July 1
a
0
−250000
−500000
−750000
2010
2011
2012
2013
Year
Year
2010
2011
2012
2013


Nitrate consumption Linear Modeling: April 15 to July 1
6e+07
4e+07
2e+07
0e+00
b
0
10
20
30
40
Depth [m]
R2
0.75
0.50
0.25
Year
2010
2011
2012
2013


b Nitrate consumption : April 15 to July 1
6e+07
4e+07
2e+07
0e+00
b
2010
2011
2012
2013
Year
Year
2010
2011
2012
2013

lake modelling

Use the estimated parameters to model the lake N cycle