My Test Manuscript

Abstract

Hier kommt das Abstract

# Preface

# Abstract

(Knuth 1984)

# Introduction

## Complexity of Phosphorous

Phosphorous displays a wide range of behaviours in soils, in places where organic, mineral and aqueous phases interface. In phases that contain oxygen Phosphorous is almost exclusively present as several derivates of Orthophosphate It can be found as organic molecules as anhydric- and ester-groups, being needed by all known species as a constituent of DNA and energy transfer-processes. It can be present as anorganic Phosphate either as mono-orthophosphate or poly-orthophosphate , where it can strongly interact with water, forming, depending on pH or . The dissolved species of phosphate are subject to adsorption to clay- and oxide-surfaces of the solid soil-phase, they also form fallout-products such as Apatite, Vivianite etc. With the present metal-cations in the solution. While the solubility constant of most phosphate-salts are comparably low (Wert eingeben), meaning that the fallout and formation of minerals happens at low chemical activities of phosphate, phosphate often is leached from soil-surface-layers, heavily reducing the efficacy of P-fertilization and presenting a disturbance to P-limited ecosystems. Those phenomena, many of them being physicochemically controlled, are influenced by parameters such as pH, ionic-strength, clay-content, specific-surface of the solid phase, amorphous -content amorphous -content, in short the phenomena depend heavily on the composition, distribution and geometry of the soil. Those properties are considered to be stable respectively long-term properties of a soil, when looked at it with the interest of modelling the transport processes of Phosphate in soils. Factors such as water-content, temperature, vegetation and precipitation are factors that temporally can vary fast and to a certain degree unpredictably. Organic forms of phosphates, prominently DNA or oligonucleotides and phytate are also subject to physicochemical reactions, mainly decomposition, but are foremost controlled in their presence by enzymatic processes, where i.e. plants form phytates in seeds to provide the embryo a compact and specific reserve of phosphate, but many bacteria possess via Phytases the ability to hydrolyse phytate and use it for their own means. To assess and cover those phenomena, models, dynamically describing the motion of Phosphorous in soils, differentiate several pools of Phosphorous, most prominently the organic-P, dissolved-P, adsorbed-P, mineral-P, where the difference in temporal behaviour, such as the mean-reside-time can lead to a differentiation between labile-P, semi-labile-P and so on.

# Plants as Phosphate sinks

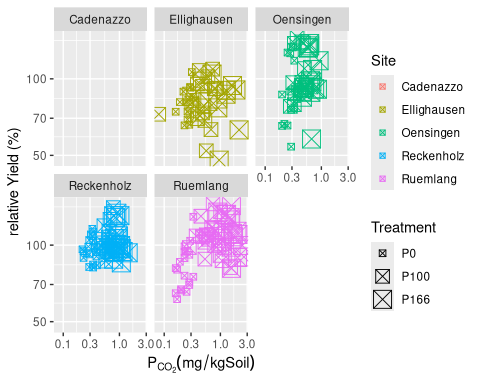
When a soil is used agronomically, P-sinks such as leaching and plant P-uptake

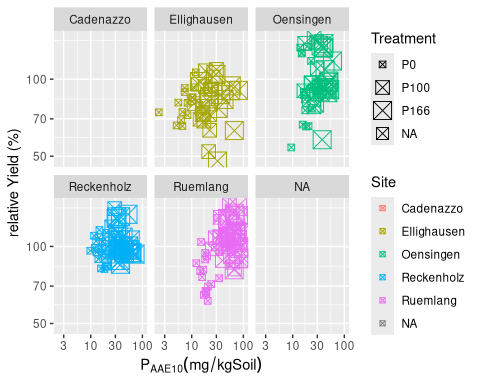
Source: [Article Notebook](https://Andrapodon.github.io/Master-Thesis-P-kinetics/index.qmd.html)

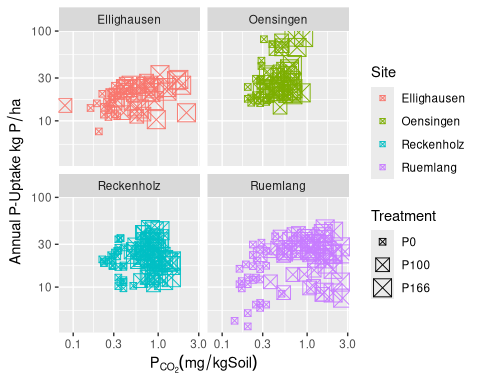
## Research Questions:

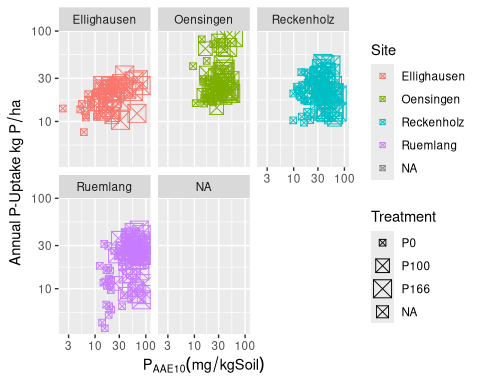
### How well can current GRUD measurements of predict the relative Yield, P-Uptake and P-Balance?

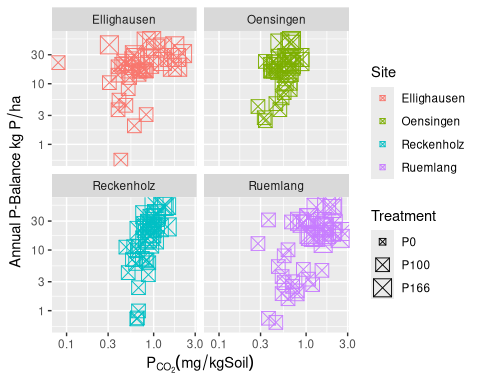
* Hypothesis I: The measurements of the equlibrium concentrations of Phosphorus in a solvent do not display significant effects on relative Yield and consequently P-Uptake, since it is strongly dependent on yield. relates strongly to the amount of Phosphorus applied, the P-balance might well be siginificantly correlated to but not explain a lot of variance.

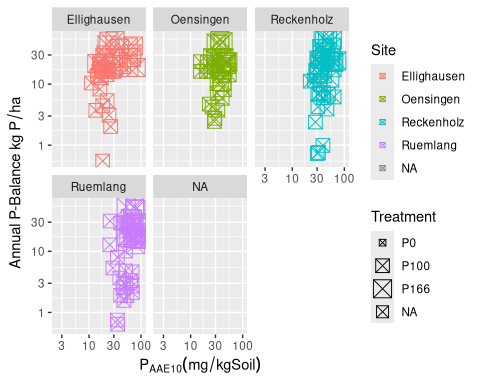












Source: [Article Notebook](https://Andrapodon.github.io/Master-Thesis-P-kinetics/index.qmd.html)

Now we want to check the strength of the models in terms of and the significance of the effects in terms of p-values:

We fitted a linear mixed model (estimated using REML and nloptwrap optimizer)  
to predict Ymain\_rel with soil\_0\_20\_P\_CO2, soil\_0\_20\_P\_AAE10 and Treatment  
(formula: Ymain\_rel ~ log(soil\_0\_20\_P\_CO2) + log(soil\_0\_20\_P\_AAE10) +  
Treatment). The model included year as random effects (formula: list(~1 | year,  
~1 | Site, ~1 | Site:block, ~1 | Site:Treatment)). The model's total  
explanatory power is substantial (conditional R2 = 0.58) and the part related  
to the fixed effects alone (marginal R2) is of 0.10. The model's intercept,  
corresponding to soil\_0\_20\_P\_CO2 = 0, soil\_0\_20\_P\_AAE10 = 0 and Treatment = P0,  
is at 70.66 (95% CI [38.22, 103.10], t(202) = 4.30, p < .001). Within this  
model:  
  
 - The effect of soil 0 20 P CO2 [log] is statistically non-significant and  
positive (beta = 1.16, 95% CI [-6.67, 8.98], t(202) = 0.29, p = 0.771; Std.  
beta = -0.28, 95% CI [-0.97, 0.42])  
 - The effect of soil 0 20 P AAE10 [log] is statistically non-significant and  
positive (beta = 8.10, 95% CI [-0.14, 16.33], t(202) = 1.94, p = 0.054; Std.  
beta = 0.93, 95% CI [0.17, 1.68])  
 - The effect of Treatment [P100] is statistically non-significant and positive  
(beta = 4.06, 95% CI [-5.90, 14.02], t(202) = 0.80, p = 0.422; Std. beta =  
0.29, 95% CI [-0.18, 0.76])  
 - The effect of Treatment [P166] is statistically non-significant and positive  
(beta = 1.60, 95% CI [-10.64, 13.84], t(202) = 0.26, p = 0.797; Std. beta =  
0.20, 95% CI [-0.39, 0.80])  
  
Standardized parameters were obtained by fitting the model on a standardized  
version of the dataset. 95% Confidence Intervals (CIs) and p-values were  
computed using a Wald t-distribution approximation.

Random effect variances not available. Returned R2 does not account for random effects.

Random effect variances not available. Returned R2 does not account for random effects.

We fitted a linear mixed model (estimated using REML and nloptwrap optimizer)  
to predict annual\_P\_uptake with soil\_0\_20\_P\_CO2, soil\_0\_20\_P\_AAE10 and  
Treatment (formula: annual\_P\_uptake ~ log(soil\_0\_20\_P\_CO2) +  
log(soil\_0\_20\_P\_AAE10) + Treatment). The model included year as random effects  
(formula: list(~1 | year, ~1 | Site, ~1 | Site:block, ~1 | Site:Treatment)).  
The model's explanatory power related to the fixed effects alone (marginal R2)  
is 0.05. The model's intercept, corresponding to soil\_0\_20\_P\_CO2 = 0,  
soil\_0\_20\_P\_AAE10 = 0 and Treatment = P0, is at 14.25 (95% CI [-3.31, 31.81],  
t(402) = 1.59, p = 0.112). Within this model:  
  
 - The effect of soil 0 20 P CO2 [log] is statistically non-significant and  
positive (beta = 2.08, 95% CI [-1.75, 5.92], t(402) = 1.07, p = 0.286; Std.  
beta = 0.15, 95% CI [-0.29, 0.60])  
 - The effect of soil 0 20 P AAE10 [log] is statistically non-significant and  
positive (beta = 0.82, 95% CI [-3.27, 4.91], t(402) = 0.40, p = 0.693; Std.  
beta = 0.16, 95% CI [-0.35, 0.66])  
 - The effect of Treatment [P100] is statistically non-significant and positive  
(beta = 1.52, 95% CI [-2.04, 5.09], t(402) = 0.84, p = 0.401; Std. beta = 0.12,  
95% CI [-0.10, 0.35])  
 - The effect of Treatment [P166] is statistically non-significant and positive  
(beta = 1.18, 95% CI [-3.83, 6.19], t(402) = 0.46, p = 0.643; Std. beta = 0.10,  
95% CI [-0.22, 0.42])  
  
Standardized parameters were obtained by fitting the model on a standardized  
version of the dataset. 95% Confidence Intervals (CIs) and p-values were  
computed using a Wald t-distribution approximation.

Random effect variances not available. Returned R2 does not account for random effects.

Random effect variances not available. Returned R2 does not account for random effects.

We fitted a linear mixed model (estimated using REML and nloptwrap optimizer)  
to predict annual\_P\_balance with soil\_0\_20\_P\_CO2, soil\_0\_20\_P\_AAE10 and  
Treatment (formula: annual\_P\_balance ~ log(soil\_0\_20\_P\_CO2) +  
log(soil\_0\_20\_P\_AAE10) + Treatment). The model included year as random effects  
(formula: list(~1 | year, ~1 | Site, ~1 | Site:block, ~1 | Site:Treatment)).  
The model's explanatory power related to the fixed effects alone (marginal R2)  
is 0.51. The model's intercept, corresponding to soil\_0\_20\_P\_CO2 = 0,  
soil\_0\_20\_P\_AAE10 = 0 and Treatment = P0, is at -16.64 (95% CI [-35.71, 2.43],  
t(402) = -1.72, p = 0.087). Within this model:  
  
 - The effect of soil 0 20 P CO2 [log] is statistically significant and negative  
(beta = -5.00, 95% CI [-9.65, -0.35], t(402) = -2.12, p = 0.035; Std. beta =  
-0.05, 95% CI [-0.48, 0.37])  
 - The effect of soil 0 20 P AAE10 [log] is statistically non-significant and  
negative (beta = -1.12, 95% CI [-6.04, 3.80], t(402) = -0.45, p = 0.655; Std.  
beta = -0.43, 95% CI [-0.90, 0.03])  
 - The effect of Treatment [P100] is statistically significant and positive  
(beta = 22.38, 95% CI [18.03, 26.72], t(402) = 10.13, p < .001; Std. beta =  
1.12, 95% CI [0.91, 1.33])  
 - The effect of Treatment [P166] is statistically significant and positive  
(beta = 38.89, 95% CI [32.78, 44.99], t(402) = 12.52, p < .001; Std. beta =  
1.95, 95% CI [1.65, 2.26])  
  
Standardized parameters were obtained by fitting the model on a standardized  
version of the dataset. 95% Confidence Intervals (CIs) and p-values were  
computed using a Wald t-distribution approximation.

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(**Frank?**), here I also show the non linear mixed models, following the Mitscherlich saturation curve:

Nonlinear mixed-effects model fit by maximum likelihood  
 Model: Ymain\_rel ~ A \* (1 - exp(-k \* soil\_0\_20\_P\_CO2 + E))   
 Data: D   
 AIC BIC logLik  
 744.5163 792.8389 -353.2581  
  
Random effects:  
 Formula: A ~ 1 | year  
 A.(Intercept)  
StdDev: 0.001170608  
  
 Formula: A ~ 1 | Site %in% year  
 A.(Intercept)  
StdDev: 1.560869  
  
 Formula: A ~ 1 | block %in% Site %in% year  
 A.(Intercept) Residual  
StdDev: 4.988193e-05 10.27543  
  
Fixed effects: A + k + E ~ soil\_0\_20\_clay + soil\_0\_20\_pH\_H2O + ansum\_sun + ansum\_prec   
 Value Std.Error DF t-value p-value  
A.(Intercept) 193.7899 63.1614 48 3.0681695 0.0035  
A.soil\_0\_20\_clay -0.0020 0.3174 48 -0.0062559 0.9950  
A.soil\_0\_20\_pH\_H2O 2.1577 3.3046 48 0.6529475 0.5169  
A.ansum\_sun -0.0321 0.0178 48 -1.7992514 0.0783  
A.ansum\_prec -0.0582 0.0193 48 -3.0115355 0.0041  
k.(Intercept) 1052.4990 607.1499 48 1.7335077 0.0894  
k.soil\_0\_20\_clay 0.1588 0.1220 48 1.3012499 0.1994  
k.soil\_0\_20\_pH\_H2O -49.3388 28.7546 48 -1.7158575 0.0926  
k.ansum\_sun -0.2481 0.1432 48 -1.7328670 0.0895  
k.ansum\_prec -0.2283 0.1294 48 -1.7646583 0.0840  
E.(Intercept) 267.9738 165.2244 48 1.6218779 0.1114  
E.soil\_0\_20\_clay 0.2363 0.1424 48 1.6594850 0.1035  
E.soil\_0\_20\_pH\_H2O -8.7078 5.6370 48 -1.5447609 0.1290  
E.ansum\_sun -0.0690 0.0422 48 -1.6349736 0.1086  
E.ansum\_prec -0.0863 0.0509 48 -1.6957763 0.0964  
 Correlation:   
 A.(In) A.s\_0\_20\_ A.\_0\_20\_H A.nsm\_s A.nsm\_p k.(In) k.s\_0\_20\_  
A.soil\_0\_20\_clay -0.526   
A.soil\_0\_20\_pH\_H2O -0.768 0.646   
A.ansum\_sun -0.911 0.297 0.539   
A.ansum\_prec -0.566 -0.105 0.077 0.518   
k.(Intercept) 0.250 -0.143 -0.354 -0.165 -0.070   
k.soil\_0\_20\_clay 0.178 -0.103 -0.273 -0.109 -0.039 0.641   
k.soil\_0\_20\_pH\_H2O -0.250 0.146 0.356 0.163 0.068 -1.000 -0.645   
k.ansum\_sun -0.249 0.141 0.351 0.165 0.071 -1.000 -0.629   
k.ansum\_prec -0.252 0.142 0.356 0.165 0.073 -0.998 -0.671   
E.(Intercept) 0.260 -0.151 -0.360 -0.173 -0.076 0.998 0.630   
E.soil\_0\_20\_clay 0.193 -0.061 -0.287 -0.126 -0.073 0.944 0.796   
E.soil\_0\_20\_pH\_H2O -0.262 0.164 0.375 0.169 0.065 -0.996 -0.629   
E.ansum\_sun -0.258 0.146 0.353 0.176 0.077 -0.997 -0.617   
E.ansum\_prec -0.255 0.141 0.352 0.168 0.084 -0.996 -0.665   
 k.\_0\_20\_H k.nsm\_s k.nsm\_p E.(In) E.s\_0\_20\_ E.\_0\_20\_H E.nsm\_s  
A.soil\_0\_20\_clay   
A.soil\_0\_20\_pH\_H2O   
A.ansum\_sun   
A.ansum\_prec   
k.(Intercept)   
k.soil\_0\_20\_clay   
k.soil\_0\_20\_pH\_H2O   
k.ansum\_sun 0.999   
k.ansum\_prec 0.998 0.996   
E.(Intercept) -0.997 -0.998 -0.997   
E.soil\_0\_20\_clay -0.943 -0.941 -0.955 0.940   
E.soil\_0\_20\_pH\_H2O 0.996 0.995 0.993 -0.997 -0.930   
E.ansum\_sun 0.996 0.998 0.994 -0.999 -0.937 0.995   
E.ansum\_prec 0.995 0.995 0.998 -0.997 -0.957 0.992 0.995   
  
Standardized Within-Group Residuals:  
 Min Q1 Med Q3 Max   
-3.52454696 -0.29064469 0.01534025 0.42451197 4.41233128   
  
Number of Observations: 94  
Number of Groups:   
 year Site %in% year block %in% Site %in% year   
 2 8 32

numDF denDF F-value p-value  
A.(Intercept) 1 48 5602.523 <.0001  
A.soil\_0\_20\_clay 1 48 24.781 <.0001  
A.soil\_0\_20\_pH\_H2O 1 48 16.273 0.0002  
A.ansum\_sun 1 48 3.585 0.0644  
A.ansum\_prec 1 48 3.689 0.0607  
k.(Intercept) 1 48 41.991 <.0001  
k.soil\_0\_20\_clay 1 48 7.496 0.0086  
k.soil\_0\_20\_pH\_H2O 1 48 0.758 0.3883  
k.ansum\_sun 1 48 0.424 0.5182  
k.ansum\_prec 1 48 16.020 0.0002  
E.(Intercept) 1 48 25.335 <.0001  
E.soil\_0\_20\_clay 1 48 0.152 0.6987  
E.soil\_0\_20\_pH\_H2O 1 48 0.931 0.3396  
E.ansum\_sun 1 48 0.253 0.6170  
E.ansum\_prec 1 48 2.876 0.0964

# Indices of model performance  
  
AIC | AICc | BIC | RMSE | Sigma  
---------------------------------------------  
796.042 | 806.312 | 844.365 | 10.189 | 10.275

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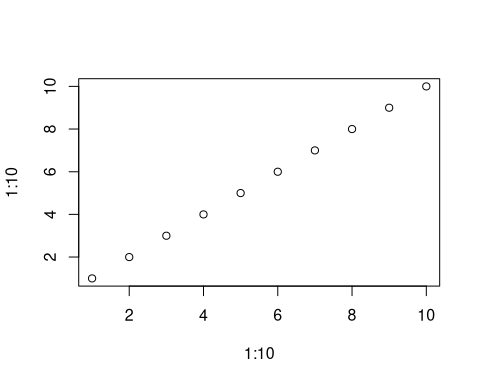
With the covariate and random effect used as by Juliane Hirte we obtain 0.9749806, I don’t know how to interpret that, I fear that the model is overfitting data.

### How do GRUD-measurements of relate to the soil properties -content, clay-content, silt-content and pH?

* Hypothesis II:

# Method

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Source: [Article Notebook](https://Andrapodon.github.io/Master-Thesis-P-kinetics/index.qmd.html)

# Results

# Discussion

# Conclusion

# Acknowledgments

# Legal Disclosure

# References

Knuth, Donald E. 1984. “Literate Programming.” *Comput. J.* 27 (2): 97–111. <https://doi.org/10.1093/comjnl/27.2.97>.

# Appendix

# Supplements