Kinetic Model Coefficient Analysis

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Model Agroscope

$$Y_{rel} \sim A*(1-e^{rate*P_{CO_2}+Env})$$

Wir ersetzen nur rate mit unserer Schätzung k:

$$Y_{rel} \sim A*(1-e^{k*P_{CO_2}+Env})$$

Sind unsere Modelparameter gute Prediktoren??

$$Y_{rel} \sim A * (1 - e^{k*PS + Env})$$

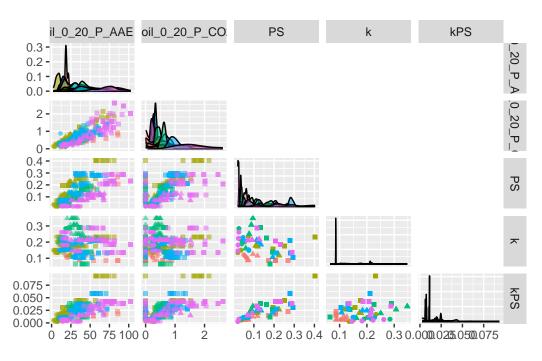
Es gibt noch die Kovariaten Niederschlag pro Jahr, Jahresdurchschnittstemperatur und Temperatur in Jugendphase

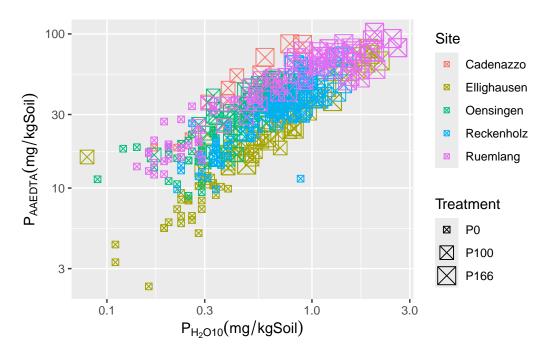
```
#|code-fold: true
#|tidy: true

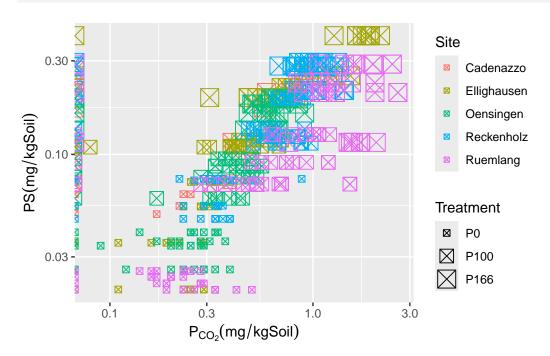
library(GGally)
```

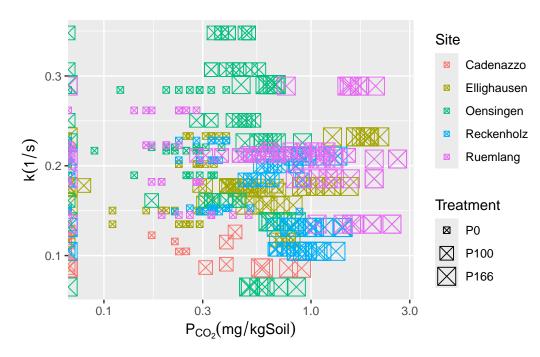
Registered S3 method overwritten by 'GGally':
method from
+.gg ggplot2

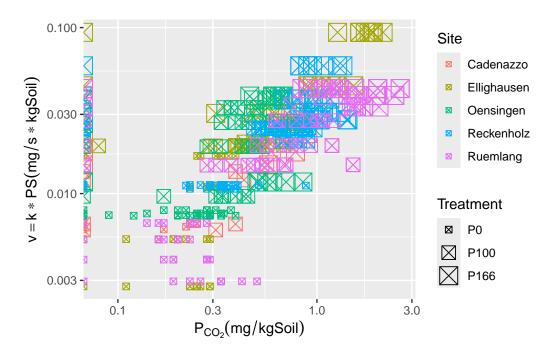
```
ggpairs(D,
   aes(col=Site, shape = Treatment,alpha = 0.6),
   columns = c("soil_0_20_P_AAE10", "soil_0_20_P_C02", "PS", "k", "kPS"),
   lower = list(continuous = wrap("points", size = 1.3)),
   upper = list(continuous = "blank", combo = "blank", discrete = "blank"))  # Adjust size here
```

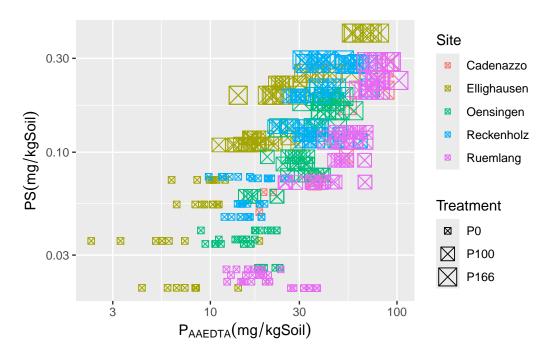


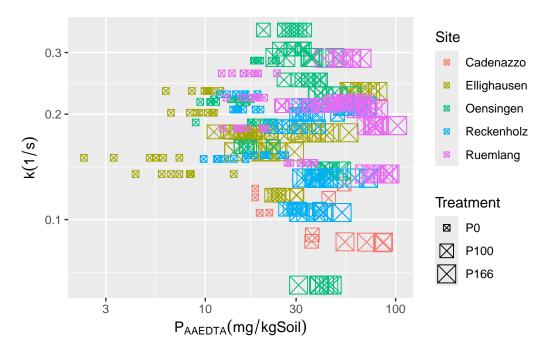


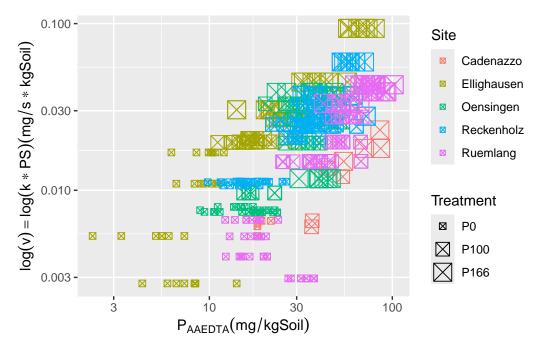












Nun noch die Linearen Regressionen, die ausstehend sind:

Random intercept per year and site, block nested in site. and Treatment nested in site (could also be modelled as a random slope to allow for correlations)

```
#|code-fold: true
#|tidy: true

# Wovon h\u00e4ngen Modelparameter ab?

library(lmerTest)
```

```
Attaching package: 'lmerTest'

The following object is masked from 'package:lme4':

lmer

The following object is masked from 'package:stats':

step
```

```
fit.soil.PS <- lmer(log(PS) ~ soil_0_20_clay+ soil_0_20_pH_H20 + soil_0_20_Corg + soil_0
boundary (singular) fit: see help('isSingular')
                                 ~ soil_0_20_clay+ soil_0_20_pH_H20 + soil_0_20_Corg + soil_0
fit.soil.k <- lmer(k</pre>
boundary (singular) fit: see help('isSingular')
fit.soil.kPS <- lmer(I(log(k*PS))~ soil_0_20_clay+ soil_0_20_pH_H2O + soil_0_20_Corg + soil_0
boundary (singular) fit: see help('isSingular')
fit.soil.CO2 <- lmer(log(soil_0_20_P_CO2)~ soil_0_20_clay+ soil_0_20_pH_H2O + soil_0_20_Corg
boundary (singular) fit: see help('isSingular')
fit.soil.AAE10 <- lmer(log(soil_0_20_P_AAE10)~ soil_0_20_clay+ soil_0_20_pH_H20 + soil_0_20_
fit.kin.Yrel
                 <- lmer(Ymain_rel
                                          ~ k * log(PS) + Treatment + (1|year) + (1|Site)
boundary (singular) fit: see help('isSingular')
fit.kin.Puptake <- lmer(annual_P_uptake ~ k * log(PS) + Treatment + (1|year) + (1|Site)
boundary (singular) fit: see help('isSingular')
fit.kin.Pbalance <- lmer(annual_P_balance ~ k * log(PS) + Treatment + (1|year) + (1|Site)
boundary (singular) fit: see help('isSingular')
anova(fit.soil.PS)
```

```
Type III Analysis of Variance Table with Satterthwaite's method
                 Sum Sq Mean Sq NumDF DenDF F value
                                                        Pr(>F)
soil_0_20_clay
                 0.0719 0.0719
                                   1 70.835
                                              2.3900 0.1265690
soil_0_20_pH_H20 0.0152 0.0152
                                   1 89.035 0.5061 0.4787086
soil 0 20 Corg 0.4704 0.4704
                                  1 65.081 15.6423 0.0001915 ***
soil_0_20_silt
                                   1 70.745
                                              3.5286 0.0644392 .
                 0.1061 0.1061
                10.0459 5.0230
Treatment
                                   2 6.055 167.0386 5.047e-06 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#summary(glht(fit.PS))
# Fazit: PS wird von treatment stark beeinfluss, k eher nicht (dafür von site)
anova(fit.soil.k)
Type III Analysis of Variance Table with Satterthwaite's method
                                           DenDF F value
                   Sum Sq
                            Mean Sq NumDF
                0.0098143 0.0098143
                                       1 69.314 10.0428 0.002277 **
soil_0_20_clay
soil_0_20_pH_H20 0.0091422 0.0091422
                                       1 102.384 9.3551 0.002838 **
soil_0_20_Corg 0.0014112 0.0014112
                                       1 98.359 1.4440 0.232372
                                       1 75.910 4.7792 0.031888 *
soil_0_20_silt
                0.0046704 0.0046704
Treatment
                0.0059043 0.0029521
                                       2 5.405 3.0209 0.131613
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
summary(glht(fit.soil.k))
     Simultaneous Tests for General Linear Hypotheses
Fit: lmer(formula = k ~ soil_0_20_clay + soil_0_20_pH_H20 + soil_0_20_Corg +
    soil_0_20_silt + Treatment + (1 | year) + (1 | Site) + (1 |
    Site:block) + (1 | Site:Treatment), data = D)
Linear Hypotheses:
                      Estimate Std. Error z value Pr(>|z|)
(Intercept) == 0
                      0.074168 0.150771 0.492 0.9965
soil_0_20_clay == 0
                                0.002209 -3.169
                     -0.007001
                                                    <0.01 **
soil_0_20_pH_H20 == 0 0.033720
                                0.011024 3.059
                                                   0.0139 *
soil_0_20_Corg == 0
                     -0.034533
                                0.028737 -1.202
                                                   0.7769
soil_0_20_silt == 0
                      0.005864
                                0.002683
                                          2.186
                                                   0.1662
TreatmentP100 == 0
                                0.015506 0.252
                      0.003910
                                                   0.9999
```

```
TreatmentP166 == 0 -0.031147 0.015685 -1.986
                                                  0.2537
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Adjusted p values reported -- single-step method)
anova(fit.soil.kPS)
Type III Analysis of Variance Table with Satterthwaite's method
                Sum Sq Mean Sq NumDF
                                      DenDF F value
soil_0_20_clay
                0.0055 0.00551
                                  1 77.626 0.1043 0.747639
soil_0_20_pH_H20 0.3773 0.37731
                                  1 101.942 7.1335 0.008807 **
soil_0_20_Corg
                0.0105 0.01052
                                  1 93.639 0.1990 0.656575
soil_0_20_silt
                0.0036 0.00360
                                  1 80.228 0.0681 0.794743
                4.0339 2.01697
                                  2 5.847 38.1329 0.000442 ***
Treatment
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
summary(glht(fit.soil.kPS))
     Simultaneous Tests for General Linear Hypotheses
Fit: lmer(formula = I(log(k * PS)) ~ soil_0_20_clay + soil_0_20_pH_H20 +
    soil_0_20_Corg + soil_0_20_silt + Treatment + (1 | year) +
    (1 | Site) + (1 | Site:block) + (1 | Site:Treatment), data = D)
Linear Hypotheses:
                      Estimate Std. Error z value Pr(>|z|)
(Intercept) == 0
                     -6.657570 1.107392 -6.012
                                                  <0.001 ***
soil_0_20_clay == 0
                                0.016463 -0.323
                                                  0.9997
                     -0.005316
                                           2.671
soil_0_20_pH_H20 == 0 0.216354
                                0.081005
                                                  0.0483 *
soil_0_20_Corg == 0
                      0.094691
                                0.212278
                                           0.446 0.9980
soil_0_20_silt == 0
                      0.005221
                                0.020000
                                           0.261
                                                  0.9999
TreatmentP100 == 0
                      1.064948
                                0.189188
                                           5.629
                                                  <0.001 ***
TreatmentP166 == 0
                      1.634290
                                0.190050
                                           8.599
                                                  <0.001 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Adjusted p values reported -- single-step method)
```

anova(fit.kin.Yrel)

```
Type III Analysis of Variance Table with Satterthwaite's method
         Sum Sq Mean Sq NumDF
                                DenDF F value Pr(>F)
         146.11 146.11
                            1 151.805 0.4824 0.4884
k
log(PS)
          44.91
                 44.91
                            1 226.958 0.1483 0.7005
Treatment 740.92 370.46
                            2
                                4.838 1.2232 0.3716
k:log(PS) 324.35 324.35
                            1 172.913 1.0710 0.3022
anova(fit.kin.Puptake)
Type III Analysis of Variance Table with Satterthwaite's method
           Sum Sq Mean Sq NumDF DenDF F value Pr(>F)
           41.986 41.986
k
                             1 456.19 0.3035 0.5819
log(PS)
           6.315
                   6.315
                             1 457.82 0.0457 0.8309
Treatment 129.470 64.735
                             2 443.37 0.4680 0.6266
k:log(PS) 39.416 39.416
                             1 457.86 0.2850 0.5937
anova(fit.soil.CO2)
Type III Analysis of Variance Table with Satterthwaite's method
                Sum Sq Mean Sq NumDF DenDF F value
                                                      Pr(>F)
                0.0118 0.01181
                                   1 48.798 0.1428 0.7071250
soil_0_20_clay
soil_0_20_pH_H20 0.0686 0.06858
                                   1 65.341 0.8297 0.3657041
soil_0_20_Corg
                0.2993 0.29934
                                   1 37.017 3.6216 0.0648334 .
soil_0_20_silt
                0.0665 0.06645
                                   1 22.514 0.8040 0.3793909
                4.8977 2.44886
                                   2 5.827 29.6281 0.0008839 ***
Treatment
```

anova(fit.soil.AAE10)

```
Type III Analysis of Variance Table with Satterthwaite's method
                Sum Sq Mean Sq NumDF DenDF F value
soil_0_20_clay
                0.0491 0.0491
                                  1 58.650 1.1361 0.2908517
soil_0_20_pH_H20 0.2473 0.2473
                                  1 75.287 5.7214 0.0192552 *
                0.2830 0.2830
                                  1 45.764 6.5490 0.0138669 *
soil_0_20_Corg
                0.0572 0.0572
                                  1 87.560 1.3231 0.2531704
soil_0_20_silt
Treatment
              7.5352 3.7676
                                  2 4.841 87.1720 0.0001598 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

anova(fit.kin.Pbalance)

```
Type III Analysis of Variance Table with Satterthwaite's method
           Sum Sq Mean Sq NumDF DenDF F value
                                                  Pr(>F)
             20.3
                     20.3
                              1 457.51 0.0960
                                                  0.7568
log(PS)
             12.9
                     12.9
                              1 455.60 0.0613
                                                  0.8046
Treatment 15488.3 7744.1
                              2 379.27 36.7144 2.658e-15 ***
                              1 455.83 0.0477
k:log(PS)
             10.1
                     10.1
                                                  0.8272
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
summary(fit.kin.Pbalance)
Linear mixed model fit by REML. t-tests use Satterthwaite's method [
lmerModLmerTest]
Formula: annual_P_balance ~ k * log(PS) + Treatment + (1 | year) + (1 |
    Site) + (1 | Site:block) + (1 | Site:Treatment)
   Data: D
REML criterion at convergence: 3854.5
Scaled residuals:
             1Q Median
    Min
                             3Q
                                    Max
-3.8654 -0.5354 -0.0249 0.5914 3.3879
Random effects:
 Groups
                Name
                            Variance Std.Dev.
 Site:block
                (Intercept)
                              0.00
                                      0.000
 Site:Treatment (Intercept)
                              0.00
                                      0.000
 year
                (Intercept) 51.80
                                      7.197
 Site
                (Intercept) 21.44
                                      4.631
 Residual
                            210.93
                                     14.523
Number of obs: 471, groups:
Site:block, 20; Site:Treatment, 15; year, 8; Site, 5
Fixed effects:
              Estimate Std. Error
                                       df t value Pr(>|t|)
(Intercept)
               -16.980
                           10.354 231.810 -1.640
                                                     0.102
k
               -12.679
                           40.918 457.507 -0.310
                                                     0.757
log(PS)
                -0.916
                            3.701 455.596 -0.248
                                                     0.805
TreatmentP100
                21.950
                            2.907 382.869
                                          7.552 3.18e-13 ***
```

```
TreatmentP166 37.991
                        4.435 317.155 8.566 4.74e-16 ***
k:log(PS) -3.788
                         17.345 455.832 -0.218
                                                   0.827
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Correlation of Fixed Effects:
           (Intr) k
                         lg(PS) TrP100 TrP166
           -0.590
k
log(PS)
            0.888 - 0.713
TretmntP100 -0.542 -0.165 -0.407
TretmntP166 -0.627 -0.126 -0.481 0.868
k:log(PS)
          -0.565 0.944 -0.776 -0.140 -0.126
optimizer (nloptwrap) convergence code: 0 (OK)
boundary (singular) fit: see help('isSingular')
```

fit.kin.Pbalance |> r.squaredGLMM()

R2m R2c [1,] 0.4228263 0.5715903

fit.kin.Puptake |> r.squaredGLMM()

R2m R2c [1,] 0.01723874 0.6121275

```
fit.kin.Yrel |> r.squaredGLMM()
```

R2m R2c [1,] 0.03304352 0.8042098

Verhalten der Modelparameter und Ertragsdaten auf P-CO2 und P-AAE10

Since we now model two measurement methods, we do not expect correlations by Site/year/etc

```
~ log(soil_0_20_P_CO2) + log(soil_0_20_P_AAE10), D)
fit.grud.k
                 <-lim(k)
fit.grud.kPS
                 <- lm(I(log(k*PS))
                                     ~ log(soil_0_20_P_CO2) + log(soil_0_20_P_AAE10), D)
                                       ~ log(soil_0_20_P_CO2) + log(soil_0_20_P_AAE10) + '
fit.grud.Yrel
               <- lmer(Ymain_rel
# this is hopeless, since cannot log becaus of 0's
fit.grud.Puptake <- lmer(annual_P_uptake ~ log(soil_0_20_P_CO2) + log(soil_0_20_P_AA
boundary (singular) fit: see help('isSingular')
                                              ~ log(soil_0_20_P_CO2) + log(soil_0_20_1
fit.grud.Pbalance
                  <- lmer(annual_P_balance
boundary (singular) fit: see help('isSingular')
#summary(glht(fit.PS))
# Fazit: PS wird von treatment stark beeinfluss, k eher nicht (dafür von site)
summary(glht(fit.grud.PS))
    Simultaneous Tests for General Linear Hypotheses
Fit: lm(formula = log(PS) ~ log(soil_0_20_P_CO2) + log(soil_0_20_P_AAE10),
   data = D)
Linear Hypotheses:
                          Estimate Std. Error t value Pr(>|t|)
(Intercept) == 0
                         log(soil_0_20_P_C02) == 0 1.02613 0.06084 16.866 <1e-04 ***
log(soil_0_20_P_AAE10) == 0 -0.02995 0.06127 -0.489 0.793
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Adjusted p values reported -- single-step method)
summary(glht(fit.grud.k))
```

Simultaneous Tests for General Linear Hypotheses

Fit: lm(formula = k ~ log(soil_0_20_P_CO2) + log(soil_0_20_P_AAE10),

```
data = D)
Linear Hypotheses:
                           Estimate Std. Error t value Pr(>|t|)
                           (Intercept) == 0
log(soil_0_20_P_C02) == 0 -0.026427 0.007388 -3.577 < 0.001 ***
log(soil_0_20_P_AAE10) == 0 0.021027 0.007440
                                              2.826 0.00847 **
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
(Adjusted p values reported -- single-step method)
summary(glht(fit.grud.kPS))
    Simultaneous Tests for General Linear Hypotheses
Fit: lm(formula = I(log(k * PS)) ~ log(soil_0_20_P_CO2) + log(soil_0_20_P_AAE10),
   data = D)
Linear Hypotheses:
                          Estimate Std. Error t value Pr(>|t|)
(Intercept) == 0
                          -3.63331
                                     0.24159 -15.039
                                                      <0.001 ***
                                     0.06160 14.690
log(soil_0_20_P_C02) == 0 0.90485
                                                     <0.001 ***
log(soil_0_20_P_AAE10) == 0 0.04814
                                     0.06203
                                               0.776
                                                     0.587
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Adjusted p values reported -- single-step method)
summary(fit.grud.Yrel)
Linear mixed model fit by REML. t-tests use Satterthwaite's method [
lmerModLmerTest]
Formula:
Ymain_rel ~ log(soil_0_20_P_CO2) + log(soil_0_20_P_AAE10) + Treatment +
    (1 | year) + (1 | Site) + (1 | Site:block) + (1 | Site:Treatment)
  Data: D
```

Scaled residuals:

REML criterion at convergence: 1726.8

Min 1Q Median 3Q Max

-2.98805 -0.62531 -0.03449 0.57660 3.15994 Random effects: Groups Variance Std.Dev. Name Site:block (Intercept) 1.815 1.347 Site:Treatment (Intercept) 26.585 5.156 (Intercept) 175.180 13.236 Site (Intercept) 22.431 4.736 Residual 194.780 13.956 Number of obs: 212, groups: Site:block, 16; Site:Treatment, 12; year, 5; Site, 4 Fixed effects: df t value Pr(>|t|) Estimate Std. Error (Intercept) 70.659 16.451 69.722 4.295 5.54e-05 *** log(soil_0_20_P_CO2) 1.155 3.967 152.164 0.291 0.7713 log(soil_0_20_P_AAE10) 8.099 4.176 78.407 1.939 0.0561 . TreatmentP100 4.062 5.052 9.299 0.804 0.4414 TreatmentP166 1.599 6.208 18.950 0.258 0.7996 Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1 Correlation of Fixed Effects: (Intr) 1(_0_20_P_C 1(_0_20_P_A TrP100 1(_0_20_P_C 0.722 1(_0_20_P_A -0.867 -0.602 TretmntP100 0.019 -0.179 -0.278TretmntP166 0.013 -0.329 -0.307 0.663 summary(fit.grud.Puptake) Linear mixed model fit by REML. t-tests use Satterthwaite's method [lmerModLmerTest] Formula: annual_P_uptake ~ log(soil_0_20_P_C02) + log(soil_0_20_P_AAE10) + Treatment + (1 | year) + (1 | Site) + (1 | Site:block) + (1 | Site:Treatment) Data: D REML criterion at convergence: 3112.7

Max

3Q

Scaled residuals:

1Q Median

Min

-2.5656 -0.4852 0.0615 0.5877 4.0429

Random effects:

Groups Variance Std.Dev. Name 0.000 0.000 Site:block (Intercept) Site:Treatment (Intercept) 0.000 0.000 (Intercept) 144.870 12.036 Site (Intercept) 8.992 2.999 Residual 107.132 10.350

Number of obs: 412, groups:

Site:block, 20; Site:Treatment, 15; year, 7; Site, 5

Fixed effects:

	Estimate	${\tt Std.} \ {\tt Error}$	df	t value	Pr(> t)
(Intercept)	14.2487	8.9343	57.6545	1.595	0.116
log(soil_0_20_P_C02)	2.0836	1.9505	283.2590	1.068	0.286
log(soil_0_20_P_AAE10)	0.8228	2.0797	128.3639	0.396	0.693
TreatmentP100	1.5242	1.8127	372.9659	0.841	0.401
TreatmentP166	1.1812	2.5495	364.9432	0.463	0.643

Correlation of Fixed Effects:

(Intr) 1(_0_20_P_C 1(_0_20_P_A TrP100 1(_0_20_P_C 0.679 1(_0_20_P_A -0.808 -0.613 TretmntP100 0.109 -0.267 -0.374 TretmntP166 0.071 -0.408 -0.357 0.797 optimizer (nloptwrap) convergence code: 0 (OK) boundary (singular) fit: see help('isSingular')

summary(fit.grud.Pbalance)

```
Linear mixed model fit by REML. t-tests use Satterthwaite's method [
lmerModLmerTest]
Formula: annual_P_balance ~ log(soil_0_20_P_CO2) + log(soil_0_20_P_AAE10) +
    Treatment + (1 | year) + (1 | Site) + (1 | Site:block) +
    (1 | Site:Treatment)
    Data: D
```

REML criterion at convergence: 3269.3

Scaled residuals:

Min 1Q Median 3Q Max

-4.3875 -0.5837 -0.1052 0.6817 2.9298

Random effects:

Groups Variance Std.Dev. Name 0.00 0.000 Site:block (Intercept) Site:Treatment (Intercept) 0.00 0.000 (Intercept) 61.91 7.868 Site (Intercept) 10.76 3.280 Residual 160.52 12.670

Number of obs: 412, groups:

Site:block, 20; Site:Treatment, 15; year, 7; Site, 5

Fixed effects:

Estimate Std. Error df t value Pr(>|t|) 9.699 84.718 -1.716 (Intercept) -16.6400.0899 . log(soil_0_20_P_CO2) -5.004 2.365 257.039 -2.116 0.0353 * log(soil_0_20_P_AAE10) -1.1202.504 104.202 -0.447 0.6556 TreatmentP100 22.377 2.210 361.468 10.127 <2e-16 *** TreatmentP166 38.888 3.105 349.644 12.523 <2e-16 ***

Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1

Correlation of Fixed Effects:

(Intr) 1(_0_20_P_C 1(_0_20_P_A TrP100

1(_0_20_P_C 0.751

1(_0_20_P_A -0.895 -0.609

TretmntP100 0.114 -0.273 -0.369

TretmntP166 0.072 -0.414 -0.354 0.796

optimizer (nloptwrap) convergence code: 0 (OK)
boundary (singular) fit: see help('isSingular')

fit.grud.Pbalance |> r.squaredGLMM()

R2m R2c [1,] 0.4145326 0.5969757

fit.grud.Puptake |> r.squaredGLMM()

R2m R2c

[1,] 0.02058153 0.5979709

```
fit.grud.Yrel |> r.squaredGLMM()
```

R2m R2c [1,] 0.09773311 0.5823498

save.image(file = "~/Documents/Master Thesis/Master-Thesis-P-kinetics/data/results_coefficient