# Stats to parse out DM and pH effects

Sasha D. Hafner

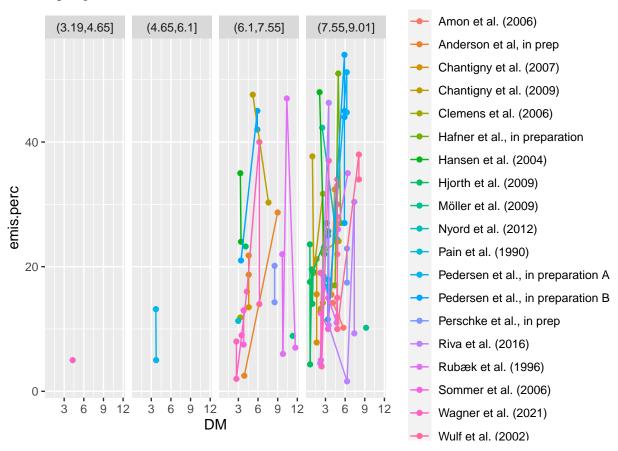
17 January, 2023

## Plots

```
dat$DMgrp <- cut(dat$DM, 4)</pre>
dat$pHgrp <- cut(dat$pH, 4)</pre>
dd <- subset(dat, !is.na(pH) & !is.na(DM))</pre>
ggplot(dd, aes(pH, emis.perc, colour = source)) +
  geom_point() +
  geom_line() +
  facet_wrap(~ DMgrp, ncol = 4)
                                                                              Amon et al. (2006)
        (0.609, 3.39]
                        (3.39, 6.16]
                                        (6.16, 8.93)
                                                        (8.93, 11.7]
                                                                              Anderson et al, in prep
                                                                              Chantigny et al. (2007)
                                                                              Chantigny et al. (2009)
                                                                              Clemens et al. (2006)
                                                                              Hafner et al., in preparation
   40 -
                                                                              Hansen et al. (2004)
                                                                              Hjorth et al. (2009)
emis.perc
                                                                              Möller et al. (2009)
                                                                              Nyord et al. (2012)
                                                                              Pain et al. (1990)
   20 -
                                                                              Pedersen et al., in preparation A
                                                                              Pedersen et al., in preparation B
                                                                              Perschke et al., in prep
                                                                              Riva et al. (2016)
                                                                              Rubæk et al. (1996)
                                                                              Sommer et al. (2006)
                                                                              Wagner et al. (2021)
                                    pН
                                                                              Wulf et al. (2002)
ggplot(dd, aes(DM, emis.perc, colour = source)) +
  geom_point() +
  geom_line() +
```

```
facet_wrap(~ pHgrp, ncol = 4)
```

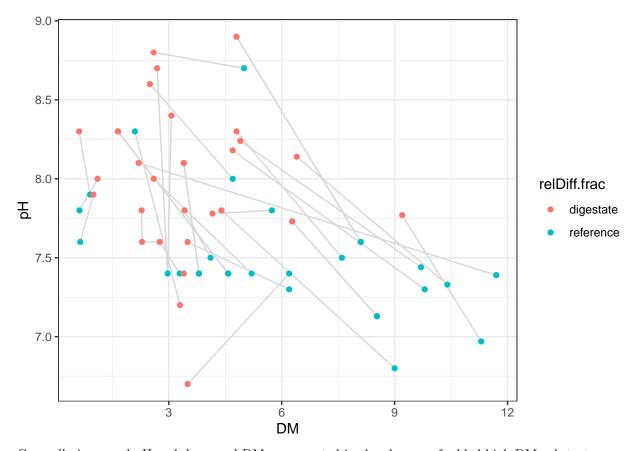
## geom\_path: Each group consists of only one observation. Do you need to adjust
## the group aesthetic?



Not pretty but there do seem to be correlations for both DM and pH.

How did digestion change DM and pH?

```
dd <- subset(dd, !is.na(relDiff.set))
ggplot(dd, aes(DM, pH, colour = relDiff.frac, group = interaction(source, relDiff.set))) +
  geom_line(colour = 'gray85') +
  geom_point() +
  theme_bw()</pre>
```



Generally increased pH and decreased DM, as expected in the absence of added high DM substrates.

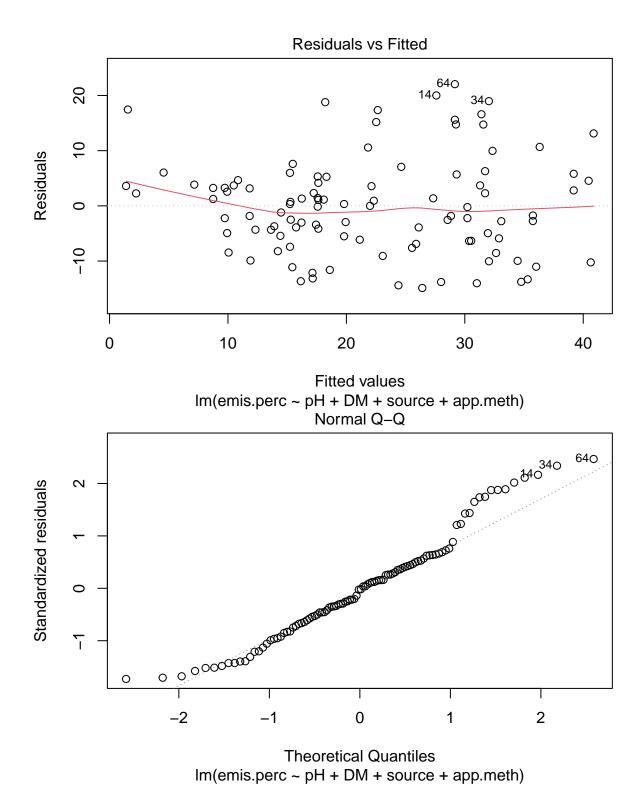
## Models

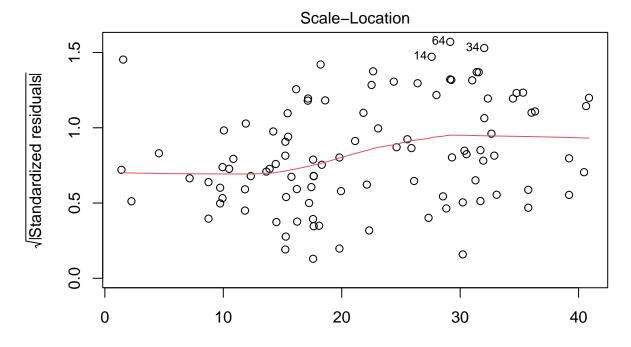
Summary.

```
dfsumm(dat[, c('source', 'app.meth', 'DM', 'pH', 'relDiff.frac', 'emis.perc')])
##
    122 rows and 6 columns
##
##
    122 unique rows
##
                                   source
                                                             app.meth
                                                                           DM
                                                                                    рН
## Class
                                                            character numeric numeric
                                character
## Minimum
                       Amon et al. (2006)
                                                            broadcast
                                                                         0.62
                                                                                   3.2
## Maximum
                       Wulf et al. (2002) trailing shoe + harrowing
                                                                         11.7
                                                                                     9
## Mean
                                      <NA>
                                                                         4.39
                                                                                  7.76
## Unique (excld. NA)
                                                                    6
                                                                           71
                                        21
                                                                                    36
                                                                    7
## Missing values
                                         0
                                                                                    14
## Sorted
                                    FALSE
                                                                FALSE
                                                                        FALSE
                                                                                FALSE
##
##
                       relDiff.frac emis.perc
                                      numeric
## Class
                          character
## Minimum
                          digestate
                                           1.6
## Maximum
                          reference
                                            60
## Mean
                               <NA>
                                          22.7
## Unique (excld. NA)
                                  2
                                            98
## Missing values
                                 46
                                             0
```

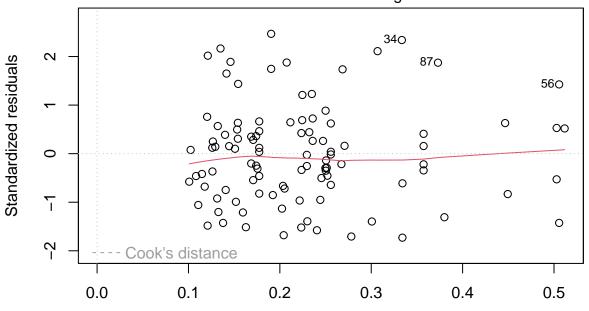
```
## Sorted
                             FALSE
                                       FALSE
##
Overall digestion effect (not expecting much)
m1 <- lm(emis.perc ~ source + app.meth + relDiff.frac, data = dat)
summary.aov(m1)
##
                Df Sum Sq Mean Sq F value
                                            Pr(>F)
## source
                14
                     4828
                            344.9
                                     3.98 0.000137 ***
                            662.1
                                     7.64 0.001252 **
## app.meth
                2
                     1324
                             63.2
                                     0.73 0.397011
## relDiff.frac 1
                       63
## Residuals
                     4420
                             86.7
               51
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## 53 observations deleted due to missingness
tail(coef(m1))
   sourceWagner et al. (2021)
                                  sourceWulf et al. (2002)
##
##
                     12.798830
                                                 20.298830
## app.methopen slot injection
                                     app.methtrailing hose
##
                    -13.750000
                                                  8.000000
##
         app.methtrailing shoe
                                     relDiff.fracreference
##
                            NA
                                                  1.933273
Nothing.
Separate DM and pH effects.
m2 <- lm(emis.perc ~ pH + DM + relDiff.frac + source + app.meth, data = dat)
summary.aov(m2)
##
                Df Sum Sq Mean Sq F value Pr(>F)
## pH
                     67.9
                             67.9
                                    0.914 0.34486
                 1
## DM
                   346.3
                            346.3
                                    4.661 0.03692 *
                 1
## relDiff.frac 1
                      1.8
                             1.8
                                    0.024 0.87754
## source
               12 2495.8
                           208.0
                                    2.799 0.00724 **
                           913.2 12.289 0.00114 **
## app.meth
                1 913.2
## Residuals
                40 2972.6
                            74.3
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## 65 observations deleted due to missingness
drop1(m2, test = 'F')
## Single term deletions
##
## Model:
## emis.perc ~ pH + DM + relDiff.frac + source + app.meth
                Df Sum of Sq
                                       AIC F value Pr(>F)
                               RSS
## <none>
                             2972.6 259.38
                        2.11 2974.7 257.43 0.0284 0.867126
## pH
                 1
                        1.59 2974.2 257.42 0.0213 0.884604
## DM
                1
## relDiff.frac 1
                        2.86 2975.4 257.44 0.0385 0.845358
## source
                10
                   2404.38 5377.0 273.17 3.2354 0.003866 **
                1 913.25 3885.8 272.66 12.2890 0.001139 **
## app.meth
## ---
```

```
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
m3 <- lm(emis.perc ~ pH + DM + source + app.meth, data = dat)
summary.aov(m3)
               Df Sum Sq Mean Sq F value
                                           Pr(>F)
## pH
                1
                     463
                           463.0
                                  4.694 0.033286 *
## DM
                    1312 1312.4 13.305 0.000473 ***
                1
## source
               16
                    4701
                           293.8
                                  2.979 0.000678 ***
               5
                    3023
                           604.6
                                   6.130 7.55e-05 ***
## app.meth
## Residuals
               79
                    7792
                            98.6
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## 19 observations deleted due to missingness
drop1(m3, test = 'F')
## Single term deletions
##
## Model:
## emis.perc ~ pH + DM + source + app.meth
##
            Df Sum of Sq
                             RSS
                                    AIC F value
                                                   Pr(>F)
## <none>
                          7792.1 493.59
## pH
                   529.9 8322.0 498.37 5.3722 0.0230494 *
             1
## DM
             1
                   981.9 8774.1 503.82 9.9554 0.0022695 **
                  4917.5 12709.6 511.98 3.1160 0.0004117 ***
## source
            16
## app.meth 5
                  3023.1 10815.2 517.36 6.1300 7.548e-05 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
cc \leftarrow coef(m3)[1:3]
СС
## (Intercept)
                                    DM
                        рΗ
## -25.475142
                  4.205796
                              2.109639
confint(m3)[1:3, ]
##
                     2.5 %
                              97.5 %
## (Intercept) -63.6388860 12.688603
## pH
                 0.5939860 7.817605
## DM
                 0.7787866 3.440491
cc['pH'] / cc['DM']
##
         рН
## 1.993609
m3 is where it gets interesting. Clear positive effects of DM and pH, although the pH effect seems small
(+4% emission (frac. of TAN) per unit pH change). Effect of pH is about 2x DM effect (1 unit pH change:
1% DM change).
plot(m3, ask = FALSE)
## Warning: not plotting observations with leverage one:
##
     102
```





Fitted values
Im(emis.perc ~ pH + DM + source + app.meth)
Residuals vs Leverage



Leverage Im(emis.perc ~ pH + DM + source + app.meth)

We might look at relative effect.

```
m4 <- lm(log10(emis.perc) ~ pH + DM + source + app.meth, data = dat)
summary.aov(m4)</pre>
```

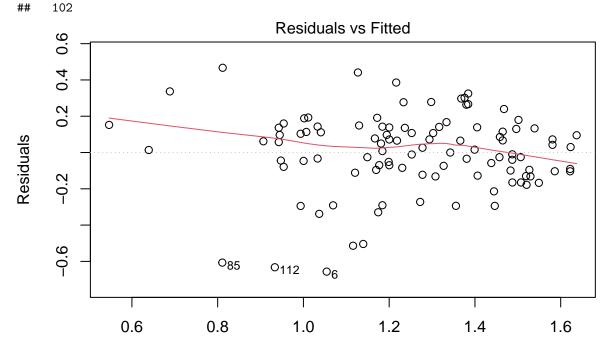
```
## Df Sum Sq Mean Sq F value Pr(>F)
## pH 1 0.726 0.7257 12.252 0.000767 ***
```

```
## DM
                   0.574 0.5744
                                    9.698 0.002570 **
                   2.545
                          0.1591
                                    2.686 0.001971 **
## source
               16
                                    5.702 0.000153 ***
## app.meth
                5
                   1.689
                          0.3377
## Residuals
                   4.679
                          0.0592
               79
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## 19 observations deleted due to missingness
cc <- 100 * (10^ccoef(m4)[1:3] - 1)
СС
  (Intercept)
                                     DM
##
                        рΗ
     -24.47896
                  38.27664
                               11.86561
100 * (10<sup>confint(m4)</sup>[1:3, ] - 1)
                    2.5 %
##
                              97.5 %
## (Intercept) -91.232586 550.52562
## pH
                12.782575
                            69.53354
## DM
                 3.772978
                            20.58934
cc['pH'] / cc['DM']
##
         рН
## 3.225847
```

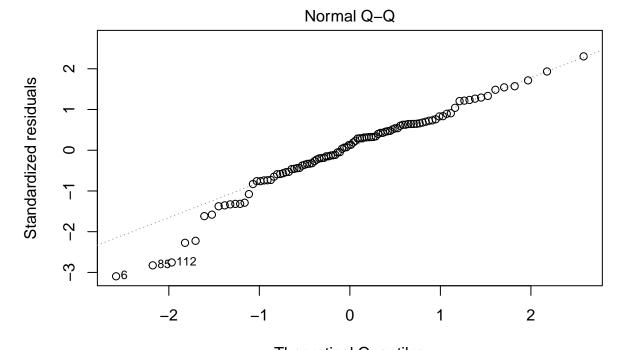
38% increase in emission with a 1 unit increase in pH, seems plausible. Effect of pH here 3x DM effect. Seems more plausible.

```
plot(m4, ask = FALSE)
```

## Warning: not plotting observations with leverage one:

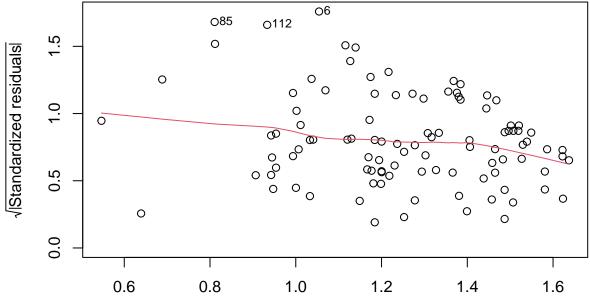


Fitted values Im(log10(emis.perc) ~ pH + DM + source + app.meth)



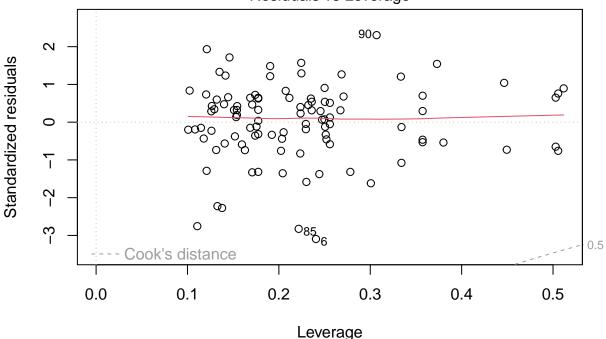
Theoretical Quantiles
Im(log10(emis.perc) ~ pH + DM + source + app.meth)
Scale-Location

O6



Fitted values Im(log10(emis.perc) ~ pH + DM + source + app.meth)

#### Residuals vs Leverage



Im(log10(emis.perc) ~ pH + DM + source + app.meth)

#### Mixed-effects model

As Johanna pointed out, source is really a random effect.

```
dfsumm(dd[, c('pH', 'DM', 'app.meth', 'source')])
##
    62 rows and 4 columns
##
##
    52 unique rows
##
                                    DM
                                             app.meth
                                                                   source
                            рΗ
## Class
                       numeric numeric
                                            character
                                                                character
## Minimum
                           6.7
                                  0.62
                                            broadcast Amon et al. (2006)
## Maximum
                           8.9
                                  11.7 trailing shoe Wulf et al. (2002)
## Mean
                          7.79
                                  4.63
                                                 <NA>
                                                                     <NA>
## Unique (excld. NA)
                            28
                                    46
                                                    4
                                                                       15
                                                    5
## Missing values
                             0
                                      0
                                                                        0
## Sorted
                         FALSE
                                 FALSE
                                                FALSE
                                                                     TRUE
##
dsub <- subset(dat, !is.na(pH) & !is.na(DM) & !is.na(app.meth))</pre>
m5 <- lmer(log10(emis.perc) ~ pH + DM + app.meth + (1|source), data = dsub)
summary(m5)
## Linear mixed model fit by REML ['lmerMod']
## Formula: log10(emis.perc) ~ pH + DM + app.meth + (1 | source)
      Data: dsub
##
##
## REML criterion at convergence: 35.5
##
```

```
## Scaled residuals:
##
       Min 1Q
                     Median
                                    30
                                            Max
## -2.69602 -0.37275 0.00472 0.58206 1.67428
##
## Random effects:
                         Variance Std.Dev.
## Groups Name
          (Intercept) 0.01438 0.1199
## source
                         0.05913 0.2432
## Residual
## Number of obs: 103, groups: source, 17
##
## Fixed effects:
##
                                     Estimate Std. Error t value
## (Intercept)
                                     -0.02950
                                                 0.35422 - 0.083
## pH
                                      0.15097
                                                 0.03999
                                                          3.775
## DM
                                                 0.01355
                                                          3.575
                                      0.04846
## app.methclosed slot injection
                                     -0.63499
                                                 0.13515 -4.699
## app.methopen slot injection
                                     -0.35685
                                                 0.14158 -2.520
## app.methtrailing hose
                                     -0.06463
                                                 0.09715
                                                          -0.665
## app.methtrailing shoe
                                     -0.05203
                                                 0.12593 -0.413
## app.methtrailing shoe + harrowing -0.20991
                                                 0.26252 -0.800
## Correlation of Fixed Effects:
                                    app.mthcsi app.mthpsi app.mh app.ms
##
               (Intr) pH
                             DM
## pH
               -0.961
              -0.405 0.281
## DM
## app.mthclsi -0.089 -0.017 -0.034
## app.mthpnsi -0.210 0.088 -0.079
                                     0.280
## app.mthtrlh -0.375 0.194 -0.040 0.412
                                                0.575
## app.mthtrls -0.281 0.134 0.018 0.317
                                                0.539
                                                           0.608
## app.mthts+h -0.024 -0.038 -0.015 0.184
                                                0.160
                                                           0.240 0.187
ccm <- 100 * (10^fixef(m5)[1:3] - 1)
ccm
## (Intercept)
                                    DM
                        рΗ
    -6.566185
                 41.569348
                             11.805280
100 * (10<sup>confint(m5)[4:5,] - 1)</sup>
## Computing profile confidence intervals \dots
          2.5 % 97.5 %
## pH 19.334246 69.27394
## DM 5.430987 18.50035
ccm['pH'] / ccm['DM']
         рΗ
## 3.521251
Large t statistics and similar coefficients as classical linear model m4. Compare:
СС
## (Intercept)
                                    DM
                        рΗ
     -24.47896
                  38.27664
                              11.86561
##
ccm
## (Intercept)
                        рΗ
                                    DM
```

```
-6.566185
                41.569348
                            11.805280
But, let's try likelihood ratio test (I think that's what anova() is doing here).
m0 <- lmer(log10(emis.perc) ~ app.meth + (1|source), data = dsub)
mOpH <- lmer(log10(emis.perc) ~ DM + app.meth + (1|source), data = dsub)
mODM <- lmer(log10(emis.perc) ~ pH + app.meth + (1|source), data = dsub)
anova(m5, m0pH)
## refitting model(s) with ML (instead of REML)
## Data: dsub
## Models:
## mOpH: log10(emis.perc) ~ DM + app.meth + (1 | source)
## m5: log10(emis.perc) ~ pH + DM + app.meth + (1 | source)
               AIC
                    BIC logLik deviance Chisq Df Pr(>Chisq)
       npar
          9 39.919 63.631 -10.9594 21.9189
## mOpH
## m5
         10 27.293 53.641 -3.6466
                                   7.2932 14.626 1 0.0001311 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
anova (m5, mODM)
## refitting model(s) with ML (instead of REML)
## Data: dsub
## Models:
## mODM: log10(emis.perc) ~ pH + app.meth + (1 | source)
## m5: log10(emis.perc) ~ pH + DM + app.meth + (1 | source)
       npar
               AIC
                    BIC logLik deviance Chisq Df Pr(>Chisq)
          9 38.512 62.225 -10.2561 20.5123
## m5
         10 27.293 53.641 -3.6466 7.2932 13.219 1 0.0002771 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
anova(m5, m0)
## refitting model(s) with ML (instead of REML)
## Data: dsub
## Models:
## m0: log10(emis.perc) ~ app.meth + (1 | source)
## m5: log10(emis.perc) ~ pH + DM + app.meth + (1 | source)
                    BIC logLik deviance Chisq Df Pr(>Chisq)
             AIC
        8 44.082 65.160 -14.0409 28.0817
## mO
## m5
       10 27.293 53.641 -3.6466
                                  7.2932 20.788 2 3.061e-05 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
Predictions
```

Might be interesting to see how predictions here stack up against current DK EFs (based on ALFAM2).

```
dat$si <- factor(as.integer(factor(dat$source)))
m6 <- lm(log10(emis.perc) ~ pH + DM + si + app.meth, data = dat)
coef(m6)</pre>
```

```
## (Intercept) pH
## -0.12193204 0.14074882
```

```
##
                                     DM
                                                                          si2
##
                            0.04869660
                                                                  0.17827981
##
                                    si3
                                                                          si4
##
                            0.05756898
                                                                  0.20300552
##
                                    si5
                                                                          si6
                            0.40397579
                                                                  0.37177705
##
##
                                                                         si8
                            0.48801250
##
                                                                  0.29512484
##
                                   si11
                                                                        si14
##
                            0.42117908
                                                                  0.26718720
##
                                   si15
                                                                        si16
##
                            0.70218532
                                                                  0.11573208
##
                                   si17
                                                                        si18
                            0.20769066
##
                                                                  0.25782185
##
                                   si19
                                                                        si20
                           -0.01567678
                                                                  0.14392388
##
                                            app.methclosed slot injection
##
                                   si21
                            0.25760194
                                                                 -0.67956909
##
##
         app.methopen slot injection
                                                      app.methtrailing hose
##
                           -0.57136678
                                                                 -0.13501678
##
                app.methtrailing shoe app.methtrailing shoe + harrowing
##
                           -0.31414078
                                                                 -0.27965539
preddat <- data.frame(scenario = c('ref', 'dig', 'dig+'), si = factor(19),</pre>
                        app.meth = 'trailing hose',
DM = c(6.5, 5.1, 6.5), pH = c(7, 7.9, 7.9))
preddat$emis <- 10^predict(m6, newdata = preddat)</pre>
knitr::kable(preddat)
```

| scenario             | si | app.meth      | DM  | рН  | emis     |
|----------------------|----|---------------|-----|-----|----------|
| ref                  | 19 | trailing hose | 6.5 | 7.0 | 10.69409 |
| $\operatorname{dig}$ | 19 | trailing hose | 5.1 | 7.9 | 12.23609 |
| dig+                 | 19 | trailing hose | 6.5 | 7.9 | 14.31588 |