

Demo of new simple1 version

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Overview

This demo shows:

1. basic usage,
2. variable substrates,
3. time-variable inputs,
4. speciation (proton-transfer reactions),
5. inhibition,
6. COD balance,

Prep

```
devtools::load_all()
```

```
## i Loading ABM
```

Function arguments

The argument list currently looks like this:

```
abm <- function(  
  days = 365,                # Number of days to run  
  delta_t = 1,               # Time step for output  
  times = NULL,              # Optional vector of times for output  
  mng_pars,  
  man_pars,  
  init_pars = list(conc_init = c(man_pars$comp_fresh, man_pars$VFA_fresh)),  
  grp_pars,  
  mic_pars,  
  sub_pars,  
  chem_pars,  
  inhib_pars = NULL,  
  mt_pars = NULL,  
  ctrl_pars = list(respir = TRUE,  
                    pH_inhib = FALSE,  
                    approx_method = 'early',  
                    par_key = '\\\\.',  
                    rates_calc = 'instant'),  
  var_pars = list(var = NULL),  
  add_pars = NULL,  
  pars = NULL,
```

```

startup = 0,                # Number of times complete simulation should be run before returning result
starting = NULL,           # Output from previous simulation to be starting condition for new one
value = 'ts',              # Type of output
warn = TRUE) {

```

The main changes in arguments are:

- new `sub_pars` for defining substrates
- new `ctrl_pars` for some “control” parameters
- new `var_pars` for *any* parameters that change over time

I have removed the default `*_pars` objects for now.

1. Basic behavior

The simplest usage is with constant slurry production rate and a fixed schedule. We need to set some parameters, first management parameters.

```

mng_pars = list(slurry_prod_rate = 10000,
                slurry_mass = 1000,
                storage_depth = 2,
                resid_depth = 0.1,
                area = 100,
                empty_int = 100,
                temp_C = 20,
                wash_water = 0,
                wash_int = NA,
                rest_d = 0,
                resid_enrich = 1)

```

Next substrate parameters, a new argument. This defines substrates. We could have any number with any names. Note that hydrolysis uses CTM again (like anything here, that could be changed).

```

sub_pars <- list(subs = c('VSd'),
                T_opt_hyd = c(VSd = 60),
                T_min_hyd = c(VSd = 0),
                T_max_hyd = c(VSd = 90),
                hydrol_opt = c(VSd = 0.1),
                sub_fresh = c(VSd = 50),
                sub_init = c(VSd = 50))

```

Microbial parameters are similar to other ABM versions, but inhibition is set separately now.

```

grp_pars <- list(grps = c('m0', 'm1', 'm2', 'sr1'),
                yield = c(default = 0.05, sr1 = 0.065),
                xa_fresh = c(all = 0.05),
                xa_init = c(all = 0.05),
                dd_rate = c(all = 0.02),
                ks = c(default = 1, sr1 = 0.5),
                qhat_opt = c(m0 = 1, m1 = 1, m2 = 2, sr1 = 9),
                T_opt = c(m0 = 18, m1 = 18, m2 = 28, sr1 = 44),
                T_min = c(m0 = 0, m1 = 6.41, m2 = 6.41, sr1 = 0),
                T_max = c(m0 = 25, m1 = 25, m2 = 38, sr1 = 51))

```

The `dd_rate_xa` parameter is for “death and decay”.

```

mic_pars <- list(dd_rate_xa = 0.02)

```

These last two arguments are similar to other versions. VFA is hard-wired and so has its own elements.

```
man_pars <- list(VFA_fresh = c(VFA = 2), pH = 7, dens = 1000)
```

```
chem_pars <- list(COD_conv = c(CH4 = 1/0.2507, xa = 1/0.7069561,
                              VFA = 1/0.9383125, S = 1/0.5015, VS = 1/0.69,
                              CO2_aer = 1/0.436, CO2_sr = 1/1.2,
                              C_xa = 1/0.3753125))
```

```
out1 <- abm(365,
            mng_pars = mng_pars,
            man_pars = man_pars,
            grp_pars = grp_pars,
            mic_pars = mic_pars,
            sub_pars = sub_pars,
            chem_pars = chem_pars)
```

```
## Warning in checkCOD(dat = dat, grps = pars$grps, subs = pars$subs, COD_conv =
## pars$COD_conv, : COD balance is off by 1.7%
```

Output is similar to other versions. (The value argument does not currently work.)

```
head(out1)
```

```
##   time      m0      m1      m2      sr1      VSd      VFA slurry_mass
## 1    0  50.0000  50.0000  50.0000  50.0000  50000.0  2000.00      1000
## 2    1  554.0098  553.8533  558.3748  544.0431  542318.4  29018.66     11000
## 3    2 1066.2767 1065.6732 1083.1940 1028.3035 1022076.9  67371.44     21000
## 4    3 1588.3161 1586.9430 1627.0197 1502.9749 1489597.5 116611.44     31000
## 5    4 2121.2034 2118.7114 2191.8594 1968.2472 1945194.0 176326.70     41000
## 6    5 2665.7726 2661.7877 2779.4361 2424.3064 2389172.2 246127.08     51000
##   CH4_emis_cum CO2_emis_cum slurry_load COD_load CH4_emis_rate temp_C pH m0_eff
## 1      0.0000      0.0000          0          0      25.52844    20  7      0
## 2    163.6272    130.5362      10000    522000    308.65512    20  7      0
## 3    628.8119    501.6449      20000   1044000    626.59326    20  7      0
## 4   1425.4337   1137.1629      30000   1566000    970.52564    20  7      0
## 5   2577.0208   2055.8603      40000   2088000   1335.99741    20  7      0
## 6   4103.8067   3273.8785      50000   2610000   1720.64113    20  7      0
##   m1_eff m2_eff sr1_eff VSd_eff VFA_eff slurry_mass_eff slurry_depth m0_conc
## 1      0      0      0      0      0          0          0.01 0.05000000
## 2      0      0      0      0      0          0          0.11 0.05036453
## 3      0      0      0      0      0          0          0.21 0.05077508
## 4      0      0      0      0      0          0          0.31 0.05123600
## 5      0      0      0      0      0          0          0.41 0.05173667
## 6      0      0      0      0      0          0          0.51 0.05227005
##   m1_conc m2_conc sr1_conc VSd_conc VFA_conc m0_eff_conc m1_eff_conc
## 1 0.05000000 0.05000000 0.05000000 50.00000 2.000000      NaN      NaN
## 2 0.05035030 0.05076135 0.04945846 49.30167 2.638060      NaN      NaN
## 3 0.05074634 0.05158067 0.04896683 48.67033 3.208164      NaN      NaN
## 4 0.05119171 0.05248451 0.04848306 48.05153 3.761660      NaN      NaN
## 5 0.05167589 0.05345999 0.04800603 47.44376 4.300651      NaN      NaN
## 6 0.05219192 0.05449875 0.04753542 46.84651 4.826021      NaN      NaN
##   m2_eff_conc sr1_eff_conc VSd_eff_conc VFA_eff_conc
## 1      NaN      NaN      NaN      NaN
## 2      NaN      NaN      NaN      NaN
## 3      NaN      NaN      NaN      NaN
```

```
## 4      NaN      NaN      NaN      NaN
## 5      NaN      NaN      NaN      NaN
## 6      NaN      NaN      NaN      NaN
```

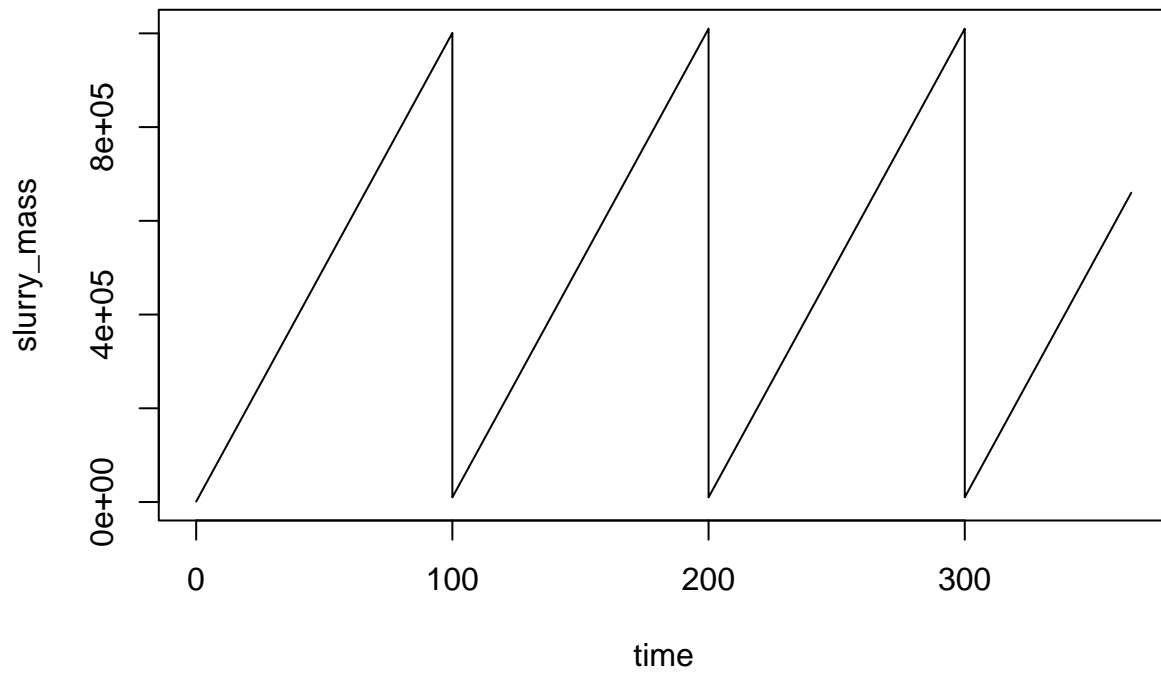
```
tail(out1)
```

```
##      time      m0      m1      m2      sr1      VSd      VFA slurry_mass
## 364  360 74909.98 72497.35 337403.6 17643.06 15468816 4796289      610000
## 365  361 77056.84 74543.26 351549.2 17788.74 15576604 4684393      620000
## 366  362 79234.75 76617.42 366160.3 17931.53 15682002 4557322      630000
## 367  363 81441.36 78717.58 381233.0 18071.50 15785084 4414981      640000
## 368  364 83673.78 80840.93 396758.5 18208.69 15885918 4257395      650000
## 369  365 85928.37 82984.01 412722.1 18343.17 15984571 4084743      660000
##      CH4_emis_cum CO2_emis_cum slurry_load  COD_load CH4_emis_rate temp_C pH
## 364      26846605      21417315      3600000 187920000      125134.1    20  7
## 365      26973866      21518840      3610000 188442000      129394.2    20  7
## 366      27105400      21623774      3620000 188964000      133674.8    20  7
## 367      27241214      21732122      3630000 189486000      137950.5    20  7
## 368      27381289      21843868      3640000 190008000      142189.3    20  7
## 369      27525568      21958969      3650000 190530000      146351.3    20  7
##      m0_eff  m1_eff  m2_eff  sr1_eff  VSd_eff  VFA_eff  slurry_mass_eff
## 364 441740.7 422210.1 2239891 63286.93 53531054 3419880      2991000
## 365 441740.7 422210.1 2239891 63286.93 53531054 3419880      2991000
## 366 441740.7 422210.1 2239891 63286.93 53531054 3419880      2991000
## 367 441740.7 422210.1 2239891 63286.93 53531054 3419880      2991000
## 368 441740.7 422210.1 2239891 63286.93 53531054 3419880      2991000
## 369 441740.7 422210.1 2239891 63286.93 53531054 3419880      2991000
##      slurry_depth  m0_conc  m1_conc  m2_conc  sr1_conc  VSd_conc  VFA_conc
## 364           6.1 0.1228032 0.1188481 0.5531206 0.02892305 25.35872 7.862769
## 365           6.2 0.1242852 0.1202311 0.5670148 0.02869152 25.12355 7.555472
## 366           6.3 0.1257694 0.1216150 0.5812069 0.02846275 24.89207 7.233845
## 367           6.4 0.1272521 0.1229962 0.5956766 0.02823671 24.66419 6.898408
## 368           6.5 0.1287289 0.1243707 0.6103976 0.02801337 24.43987 6.549838
## 369           6.6 0.1301945 0.1257334 0.6253365 0.02779268 24.21905 6.189004
##      m0_eff_conc  m1_eff_conc  m2_eff_conc  sr1_eff_conc  VSd_eff_conc  VFA_eff_conc
## 364      0.14769   0.1411602   0.7488771   0.02115912   17.89738     1.14339
## 365      0.14769   0.1411602   0.7488771   0.02115912   17.89738     1.14339
## 366      0.14769   0.1411602   0.7488771   0.02115912   17.89738     1.14339
## 367      0.14769   0.1411602   0.7488771   0.02115912   17.89738     1.14339
## 368      0.14769   0.1411602   0.7488771   0.02115912   17.89738     1.14339
## 369      0.14769   0.1411602   0.7488771   0.02115912   17.89738     1.14339
```

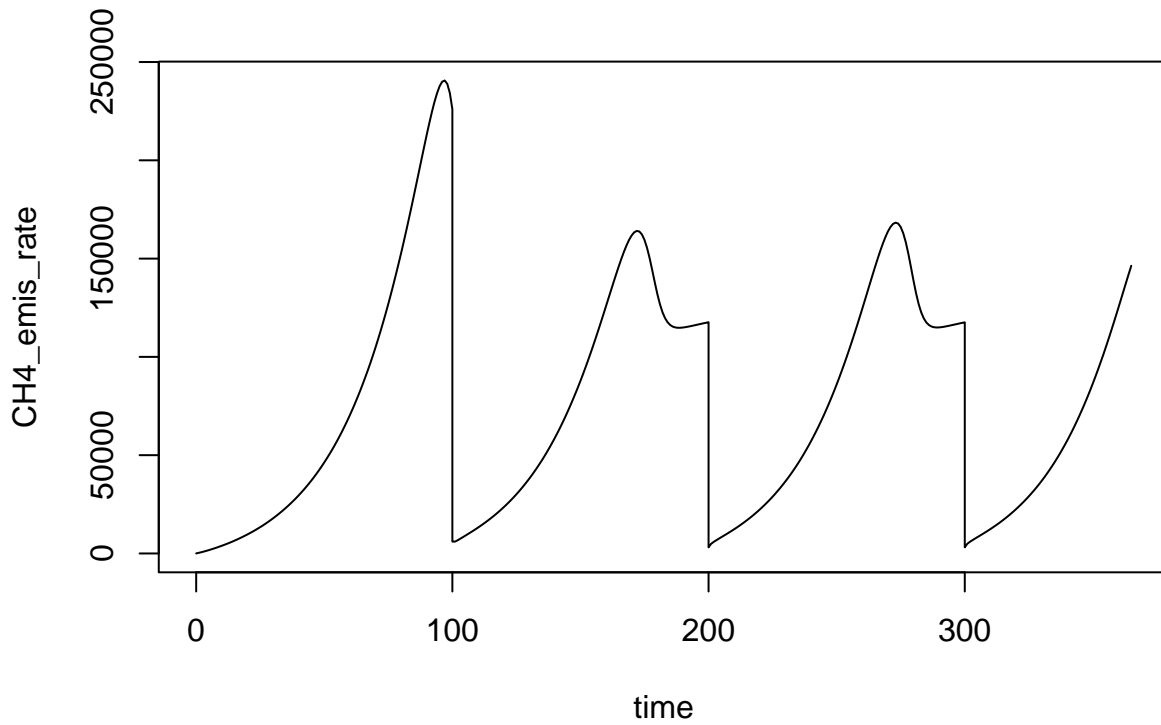
The effluent columns are cumulative. Is this what we had before? I did it for COD balance checking. We will have to discuss what is needed.

Here are some results.

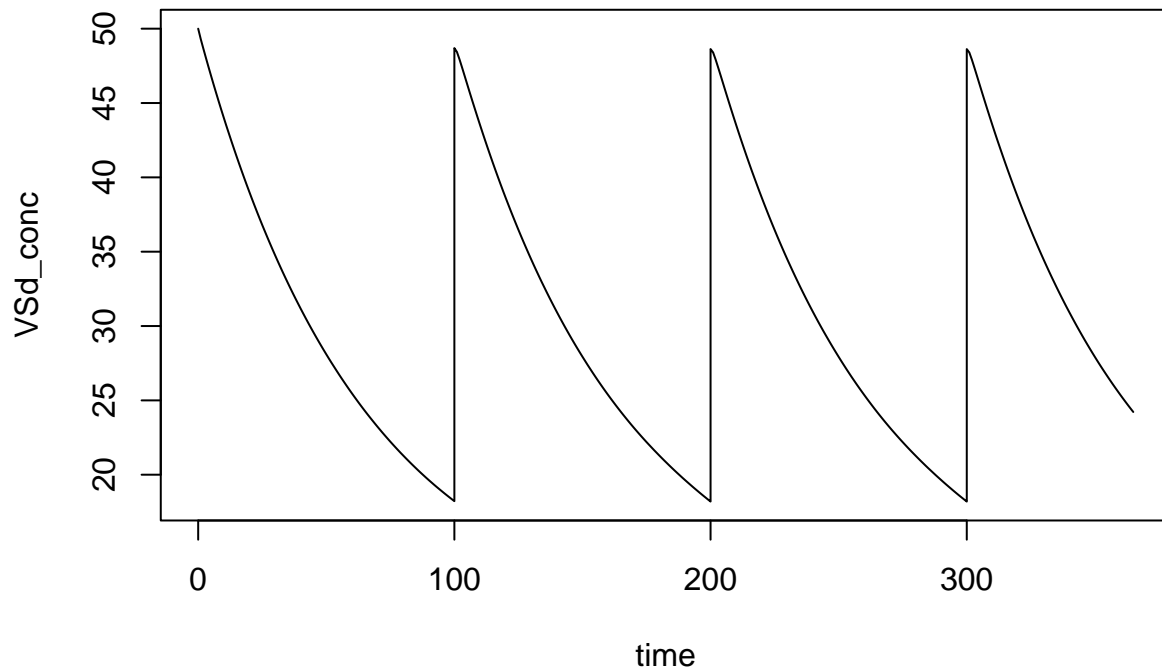
```
plot(slurry_mass ~ time, data = out1, type = 'l')
```



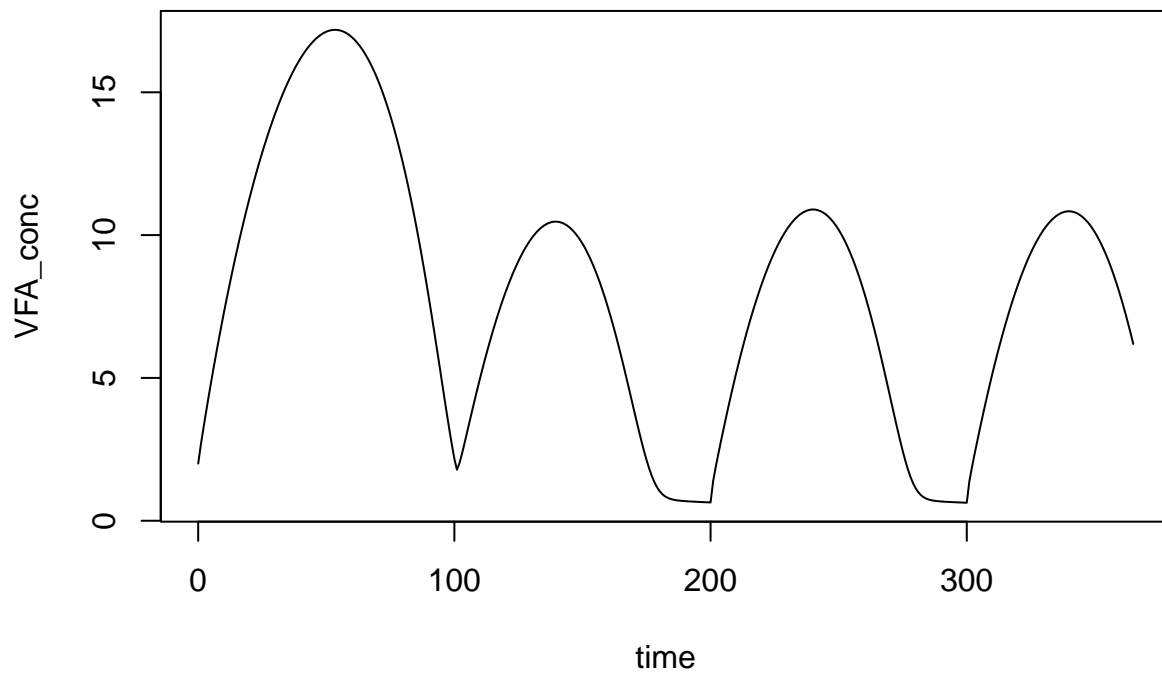
```
plot(CH4_emis_rate ~ time, data = out1, type = 'l')
```



```
plot(VSd_conc ~ time, data = out1, type = 'l')
```

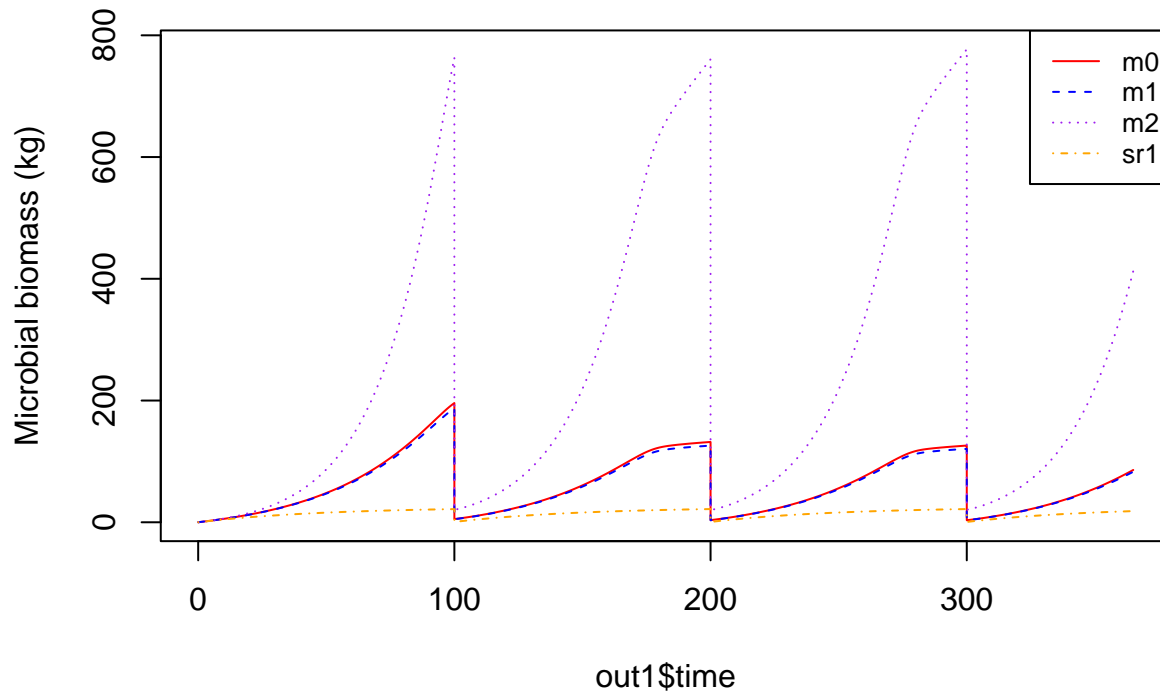


```
plot(VFA_conc ~ time, data = out1, type = 'l')
```



And methanogens.

```
line_colors <- c('red', 'blue', 'purple', 'orange')
matplot(out1$time, out1[, nn <- c('m0', 'm1', 'm2', 'sr1')]/1000,
        type = 'l', lty = c(1:length(nn)), col = line_colors, ylab = 'Microbial biomass (kg)')
legend("topright", legend = nn, lty = c(1:length(nn)), col = line_colors, lwd = 1, cex = 0.8)
```



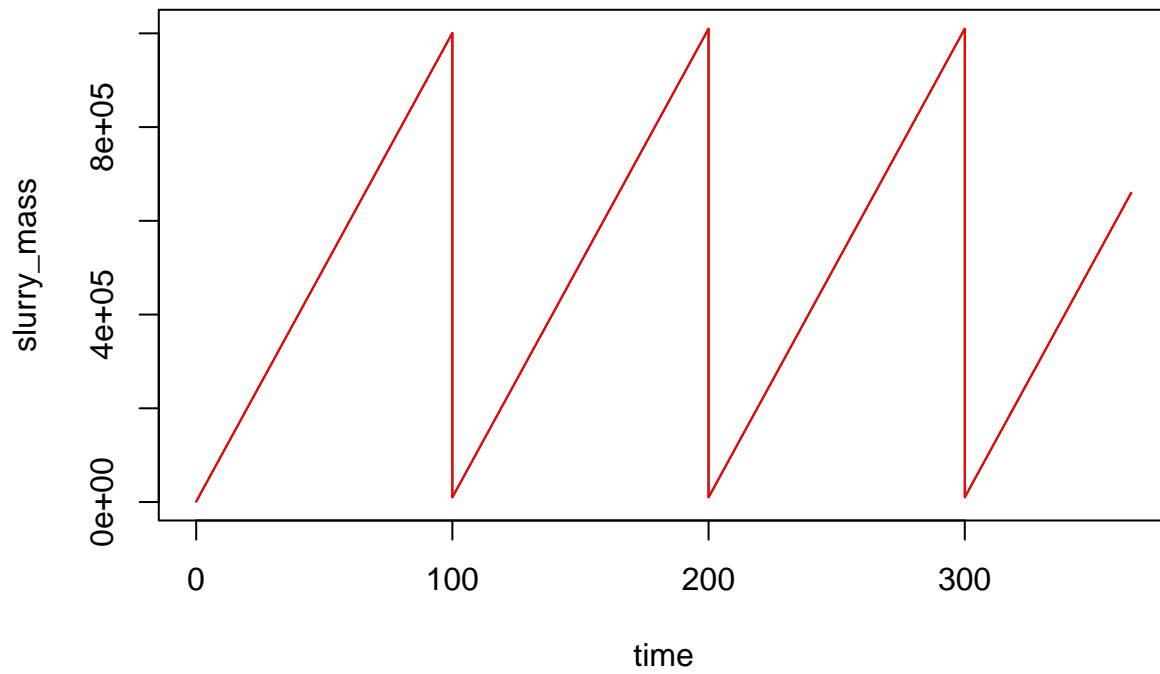
2. Substrate flexibility

Particulate substrates are defined in `sub_pars` now and there are no specific substrates hard-wired in the code. VFA is the only intermediate, and it is hard-wired. Here we will use three substrates. Parameter values have no connection to reality.

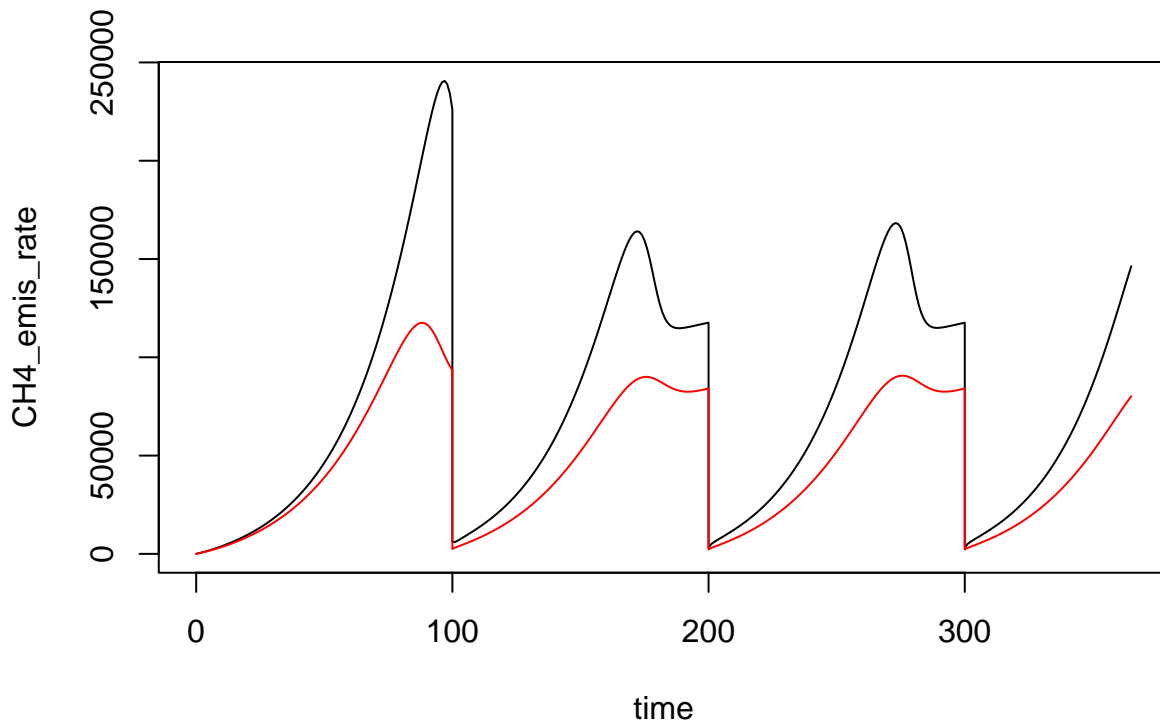
```
sub_pars2 <- list(subs = c('cellulose', 'protein', 'lipids'),
  T_opt_hyd = c(all = 60),
  T_min_hyd = c(all = 0),
  T_max_hyd = c(all = 90),
  hydrol_opt = c(lipids = 0.1, protein = 0.01, cellulose = 0.05),
  sub_fresh = c(lipids = 3, protein = 20, cellulose = 35),
  sub_init = c(lipids = 3, protein = 20, cellulose = 35))
```

```
out2 <- abm(365,
  mng_pars = mng_pars,
  man_pars = man_pars,
  grp_pars = grp_pars,
  mic_pars = mic_pars,
  sub_pars = sub_pars2,
  chem_pars = chem_pars)
```

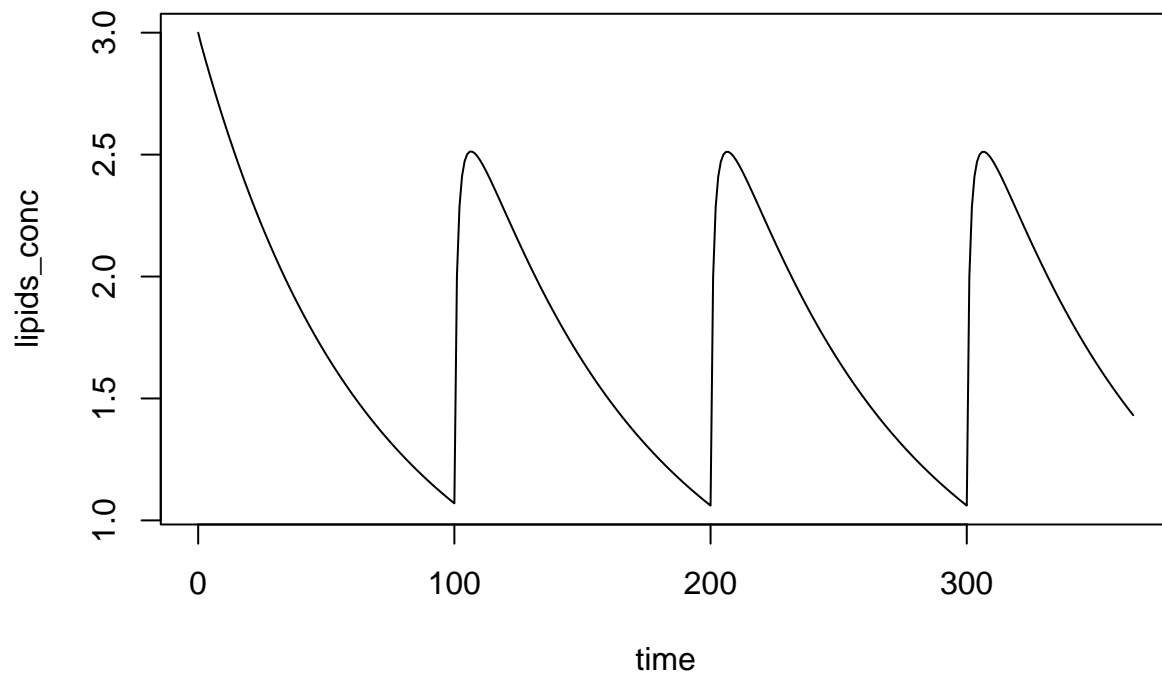
```
plot(slurry_mass ~ time, data = out2, type = 'l')
lines(slurry_mass ~ time, data = out1, col = 'red')
```



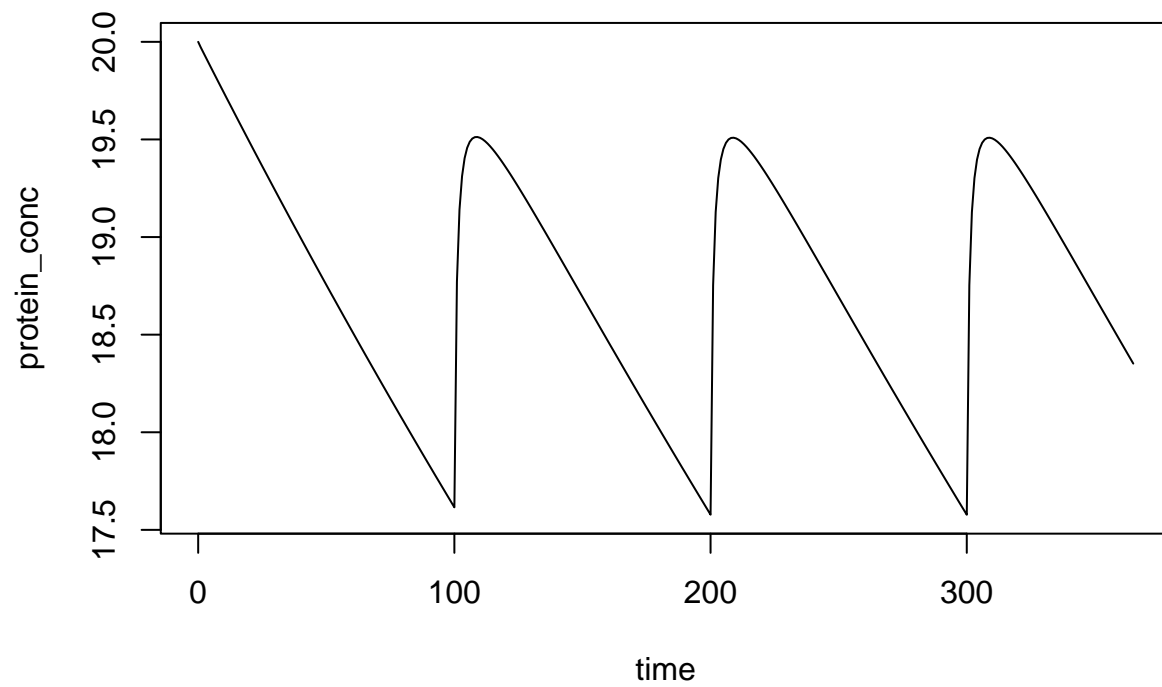
```
plot(CH4_emis_rate ~ time, data = out1, type = 'l')  
lines(CH4_emis_rate ~ time, data = out2, col = 'red')
```



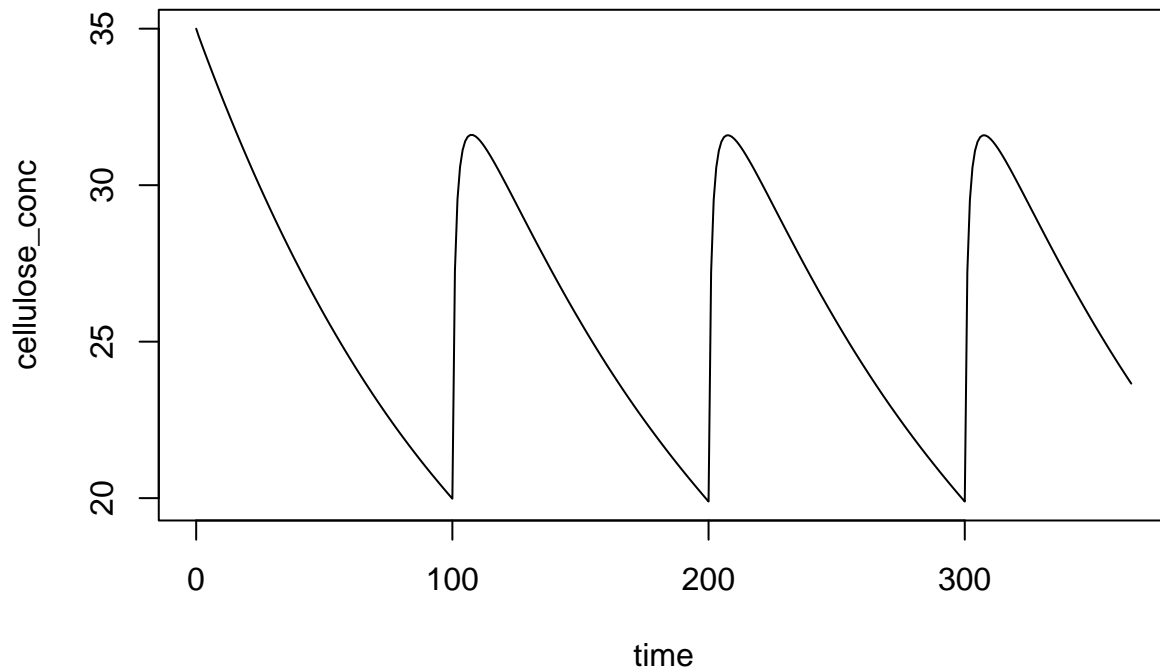
```
plot(lipids_conc ~ time, data = out2, type = 'l')
```

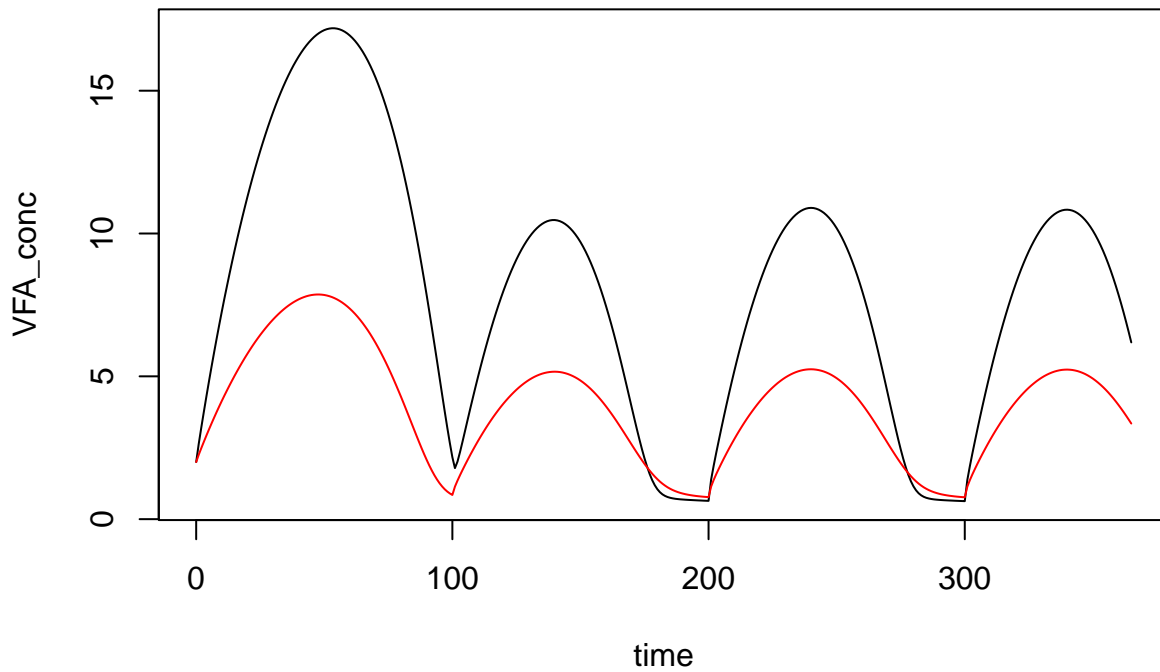
```
plot(protein_conc ~ time, data = out2, type = 'l')
```



```
plot(cellulose_conc ~ time, data = out2, type = 'l')
```



```
plot(VFA_conc ~ time, data = out1, type = 'l')
lines(VFA_conc ~ time, data = out2, col = 'red')
```



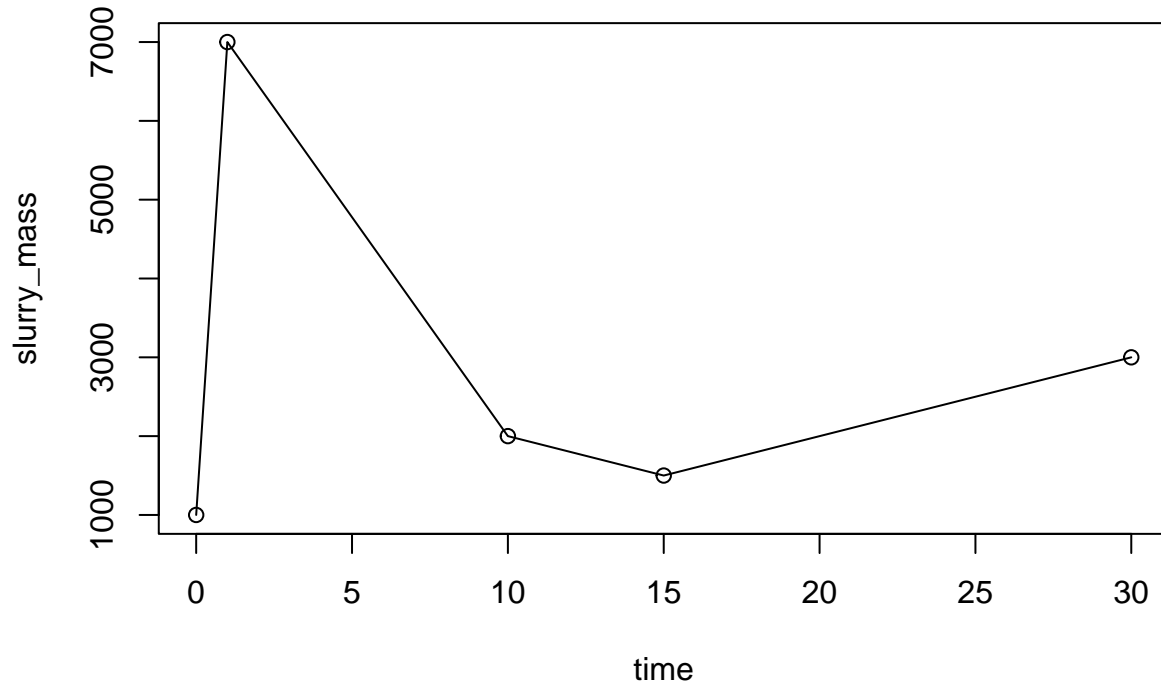
This flexibility comes from an approach similar to what we used for microbial groups.

3. Time-variable inputs part 1

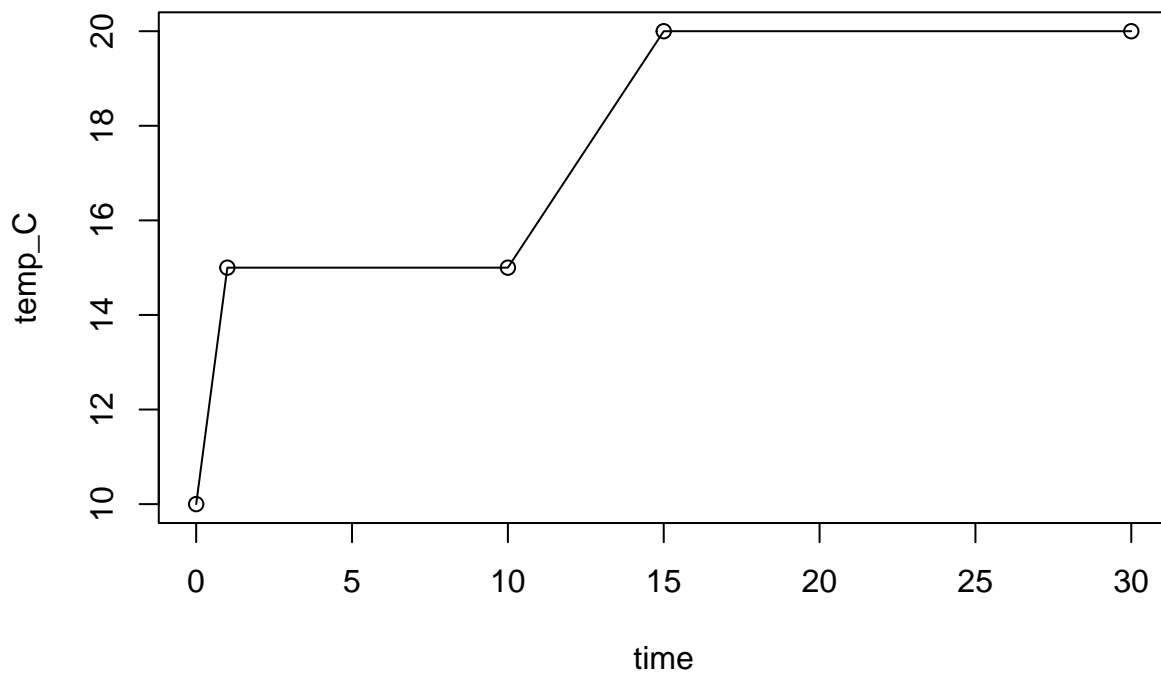
The `abm()` function can handle variability over time in any inputs now. Here slurry mass and temperature will vary.

```
var_dat <- data.frame(time = c(0, 1, 10, 15, 30),
                      slurry_mass = c(1000, 7000, 2000, 1500, 3000),
                      temp_C = c(10, 15, 15, 20, 20))

plot(slurry_mass ~ time, data = var_dat, type = 'o')
```



```
plot(temp_C ~ time, data = var_dat, type = 'o')
```

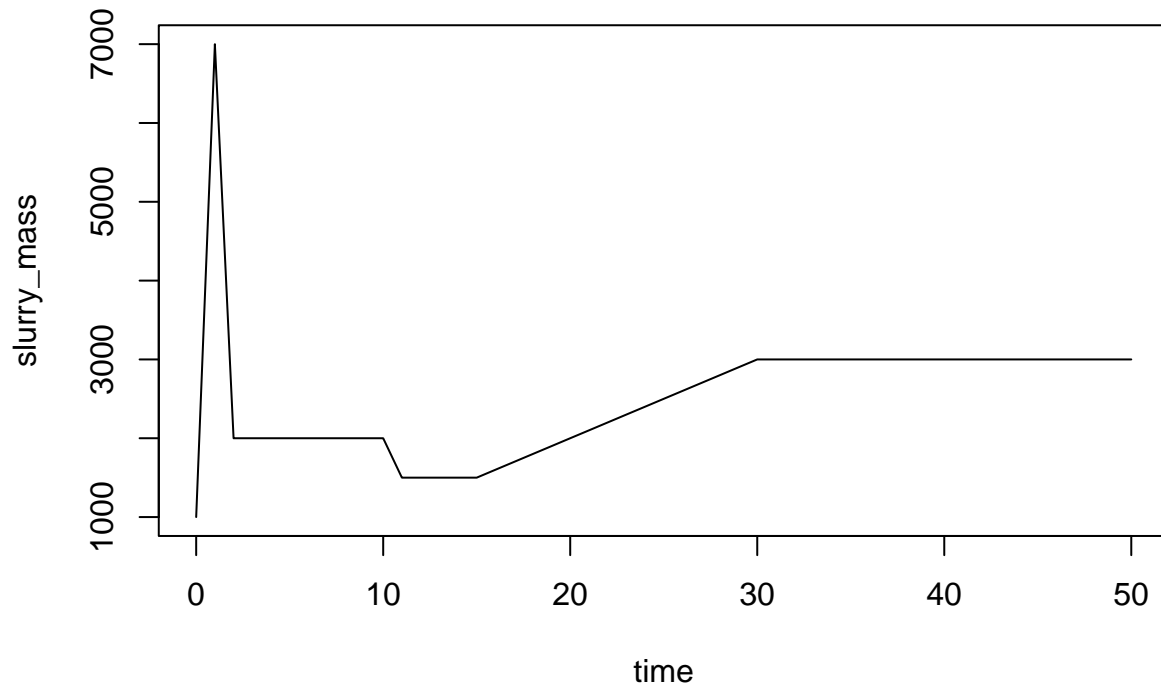


This data frame goes in the `var_pars` argument, which must be a list, even though it might have a single element named `var`. The `var` element is the only required one. The `var` data frame must have a `slurry_mass` column if it is used—it is not possible to use an `abm_regular()`-like approach with variable temperature etc.

```
var_pars <- list(var = var_dat)
```

```
out3a <- abm(50,  
  mng_pars = mng_pars,  
  man_pars = man_pars,  
  grp_pars = grp_pars,  
  mic_pars = mic_pars,  
  sub_pars = sub_pars,  
  chem_pars = chem_pars,  
  var_pars = var_pars)
```

```
plot(slurry_mass ~ time, data = out3a, type = 'l')
```



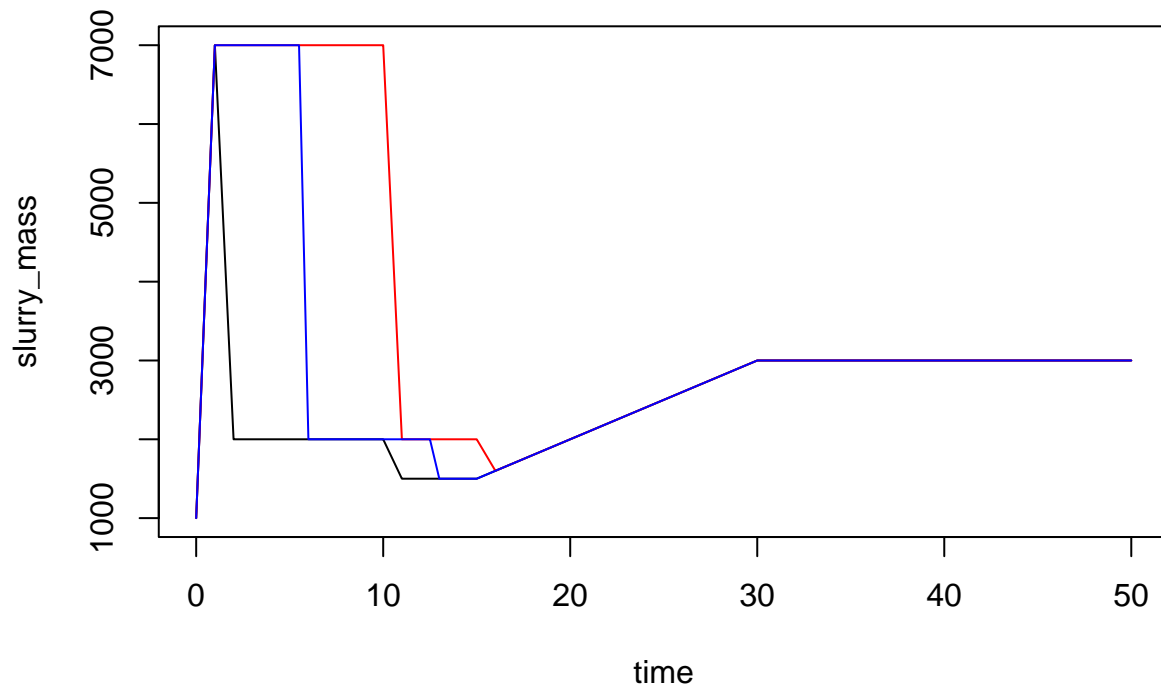
The “late” and “mid” options are still available, but now through `ctrl_pars`. Here we can change the value through `add_pars`

```
out3b <- abm(50,  
  mng_pars = mng_pars,  
  man_pars = man_pars,  
  grp_pars = grp_pars,  
  mic_pars = mic_pars,  
  sub_pars = sub_pars,  
  chem_pars = chem_pars,  
  var_pars = var_pars,  
  add_pars = list(approx_method = 'late'))
```

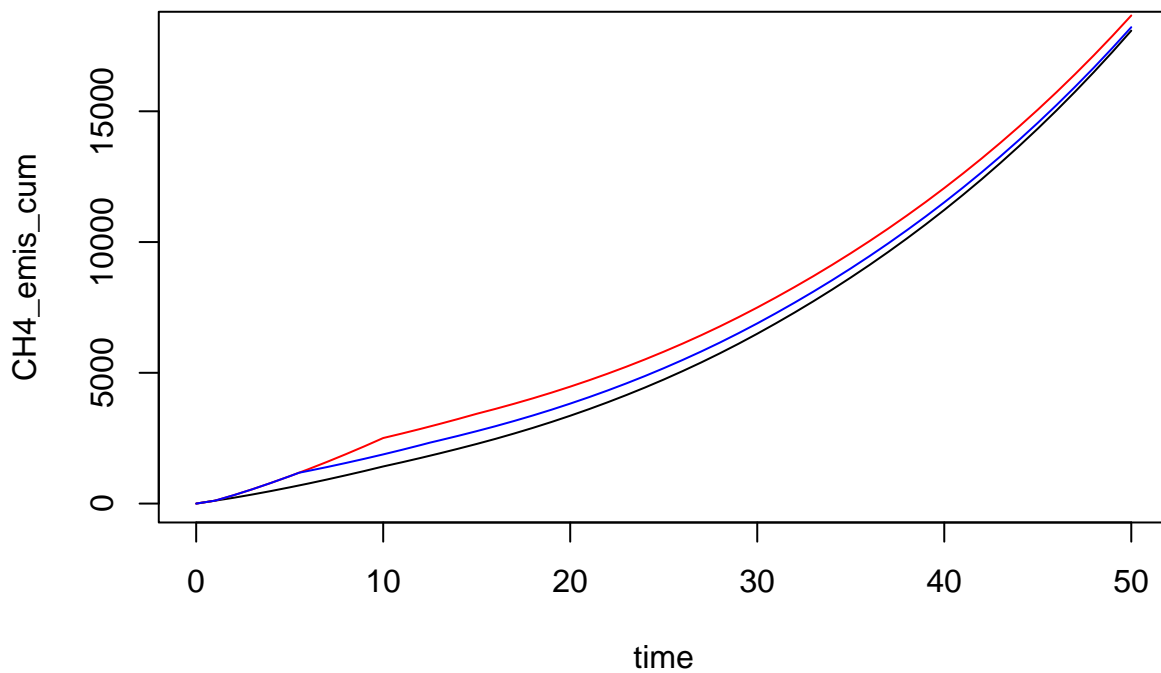
```
out3c <- abm(50,  
  mng_pars = mng_pars,  
  man_pars = man_pars,  
  grp_pars = grp_pars,  
  mic_pars = mic_pars,  
  sub_pars = sub_pars,  
  chem_pars = chem_pars,
```

```
var_pars = var_pars,  
add_pars = list(approx_method = 'mid'))
```

```
plot(slurry_mass ~ time, data = out3a, type = 'l')  
lines(slurry_mass ~ time, data = out3b, col = 'red')  
lines(slurry_mass ~ time, data = out3c, col = 'blue')
```



```
plot(CH4_emis_cum ~ time, data = out3a, type = 'l')  
lines(CH4_emis_cum ~ time, data = out3b, col = 'red')  
lines(CH4_emis_cum ~ time, data = out3c, col = 'blue')
```



4. Time-variable inputs part 2

Here we'll vary fresh substrate concentrations over time.

First the data frame with slurry mass.

```
var_dat <- data.frame(time = c(0, 1, 10, 15, 30, 50),  
                      slurry_mass = c(1000, 7000, 2000, 5000, 3000, 10000))
```

```
var_dat
```

```
##   time slurry_mass  
## 1    0         1000  
## 2    1         7000  
## 3   10         2000  
## 4   15         5000  
## 5   30         3000  
## 6   50        10000
```

Then add `sub_fresh` values. Each row needs a list containing a named vector. This is somewhat unusual data frame usage, and there is a user-friendly alternative based on additional data frames in the `var` argument (see next section). But I've kept this demo.

```
var_dat
```

```
##   time slurry_mass  
## 1    0         1000  
## 2    1         7000  
## 3   10         2000  
## 4   15         5000  
## 5   30         3000  
## 6   50        10000
```

```
var_dat$sub_fresh <- rep(list(c(VSd = 50)), nrow(var_dat))  
var_dat$sub_fresh[3] <- list(c(VSd = 100))  
var_dat$sub_fresh[4] <- list(c(VSd = 10))  
var_dat$sub_fresh[5] <- list(c(VSd = 0))  
var_dat$sub_fresh[6] <- list(c(VSd = 200))  
var_dat
```

```
##   time slurry_mass sub_fresh  
## 1    0         1000        50  
## 2    1         7000        50  
## 3   10         2000       100  
## 4   15         5000        10  
## 5   30         3000         0  
## 6   50        10000       200
```

```
var_dat[1, 3]
```

```
## [[1]]  
## VSd  
## 50
```

```
var_dat[5, 3]
```

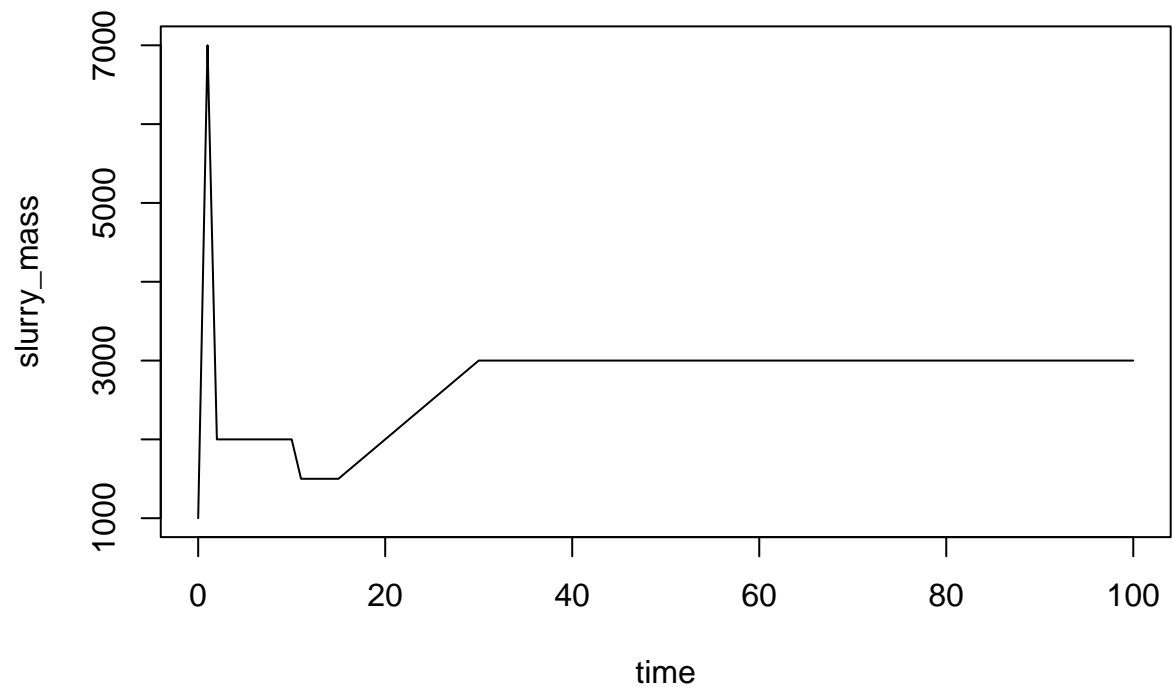
```
## [[1]]  
## VSd  
## 0
```

```
devtools::load_all()
```

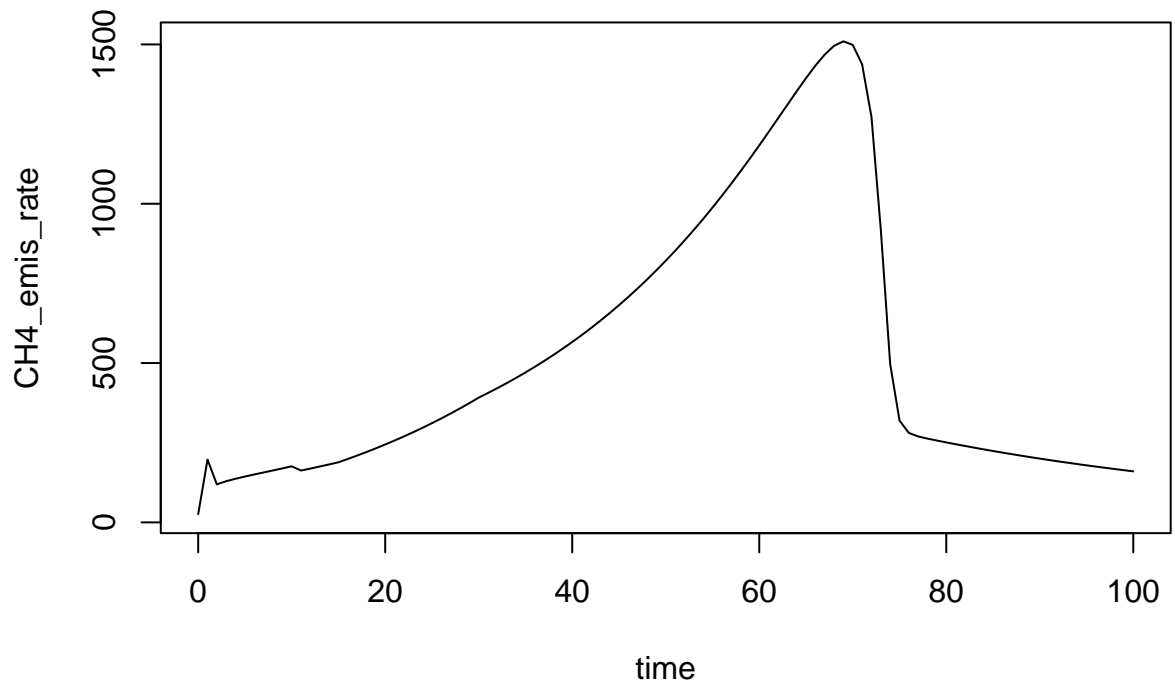
```
## i Loading ABM
```

```
out4a <- abm(100,  
  mng_pars = mng_pars,  
  man_pars = man_pars,  
  grp_pars = grp_pars,  
  mic_pars = mic_pars,  
  sub_pars = sub_pars,  
  chem_pars = chem_pars,  
  var_pars = var_pars)
```

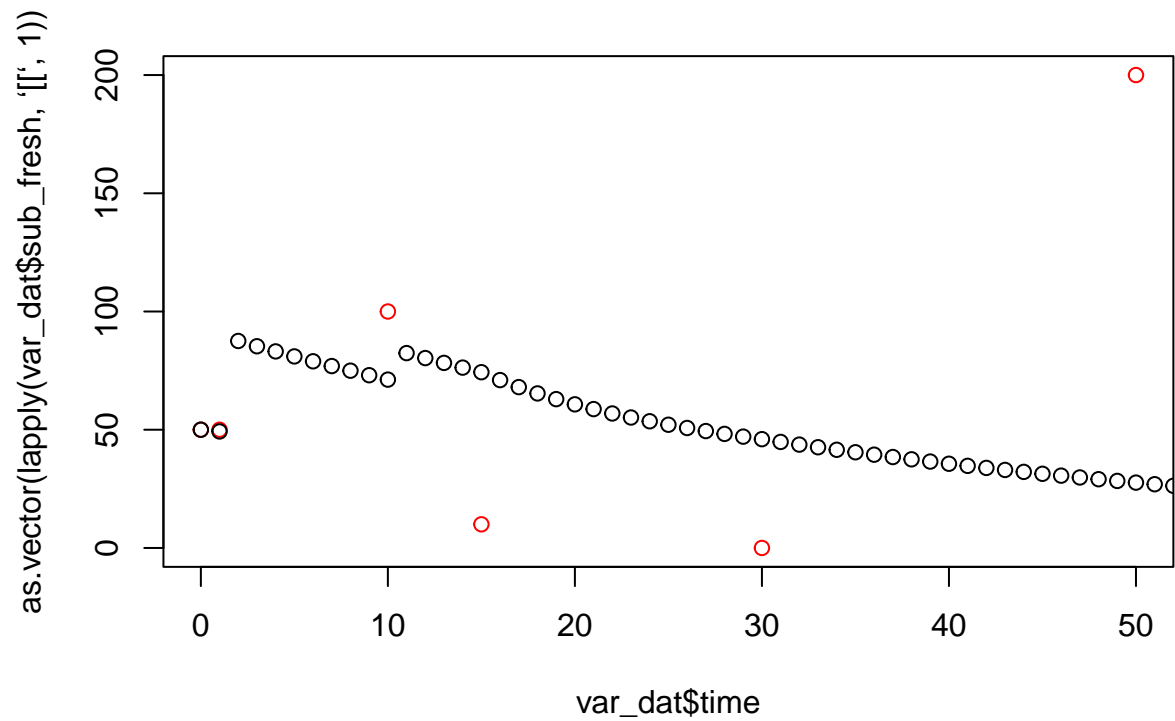
```
plot(slurry_mass ~ time, data = out4a, type = 'l')
```



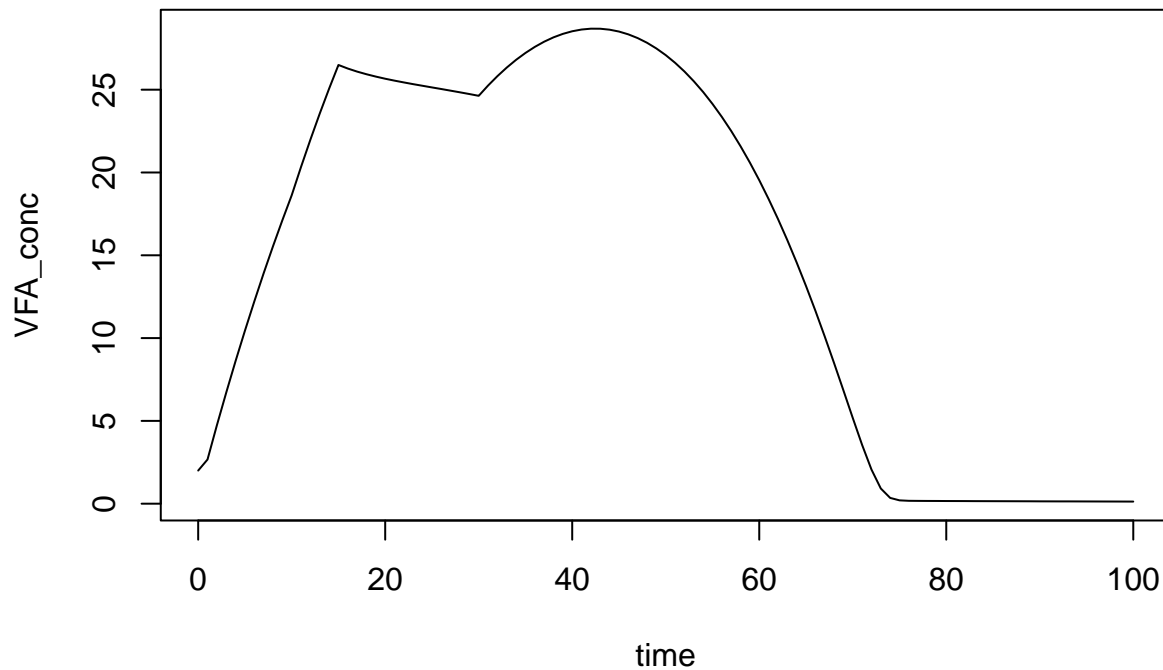
```
plot(CH4_emis_rate ~ time, data = out4a, type = 'l')
```



```
plot(var_dat$time, as.vector(lapply(var_dat$sub_fresh, `[`, 1)), type = 'p', col = 'red')
lines(VSd_conc ~ time, data = out4a, type = 'p')
```



```
plot(VFA_conc ~ time, data = out4a, type = 'l')
```

Let's vary some microbial parameters as well. And pH.

```
var_dat <- data.frame(time = c(0, 1, 10, 15, 30, 50),
                      slurry_mass = c(1000, 7000, 2000, 5000, 3000, 10000),
                      pH = 7 - 0:5/10)
var_dat
```

```
##   time slurry_mass  pH
## 1    0         1000 7.0
## 2    1         7000 6.9
## 3   10         2000 6.8
## 4   15         5000 6.7
## 5   30         3000 6.6
## 6   50        10000 6.5
```

VSd.

```
var_dat$sub_fresh <- rep(list(c(VSd = 50)), nrow(var_dat))
var_dat$sub_fresh[3] <- list(c(VSd = 100))
```

Some microbial parameters for a shift in temperature optima, "adaptation" for example.

```
for (i in 1:nrow(var_dat)) {
  var_dat$T_opt[i] <- list(grp_pars$T_opt + 2 * i)
}
var_dat
```

```
##   time slurry_mass  pH sub_fresh      T_opt
## 1    0         1000 7.0         50 20, 20, 30, 46
## 2    1         7000 6.9         50 22, 22, 32, 48
## 3   10         2000 6.8        100 24, 24, 34, 50
## 4   15         5000 6.7         50 26, 26, 36, 52
## 5   30         3000 6.6         50 28, 28, 38, 54
## 6   50        10000 6.5         50 30, 30, 40, 56
```

```

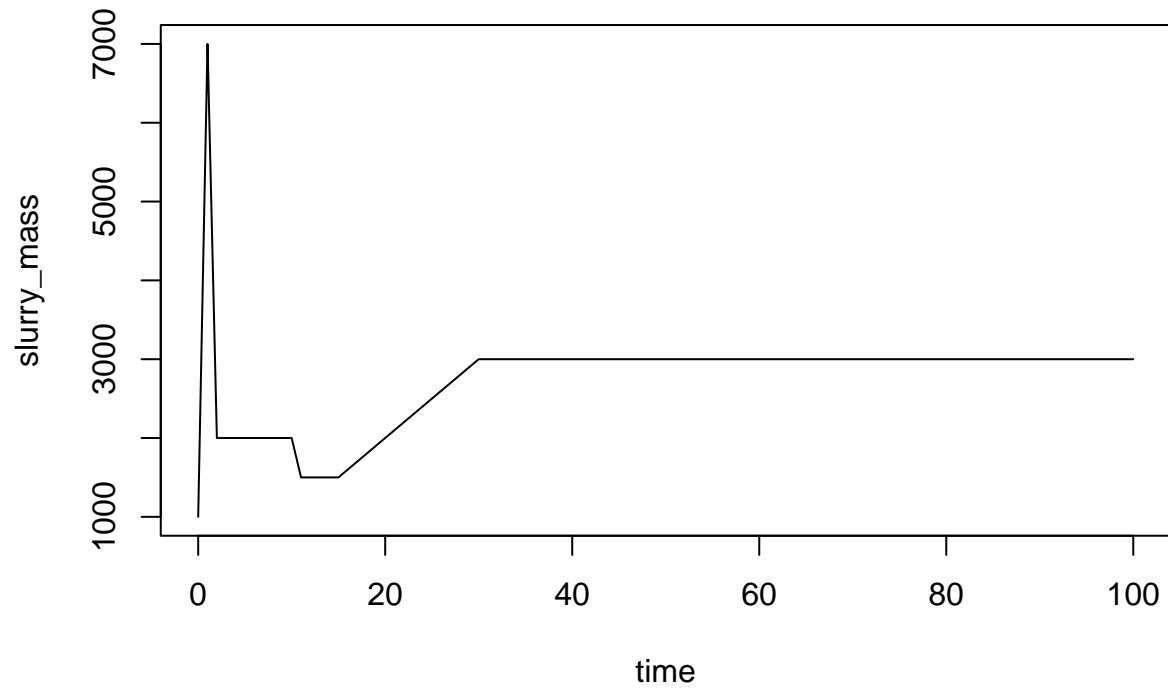
out4b <- abm(100,
  mng_pars = mng_pars,
  man_pars = man_pars,
  grp_pars = grp_pars,
  mic_pars = mic_pars,
  sub_pars = sub_pars,
  chem_pars = chem_pars,
  var_pars = var_pars)

```

```

plot(slurry_mass ~ time, data = out4b, type = 'l')

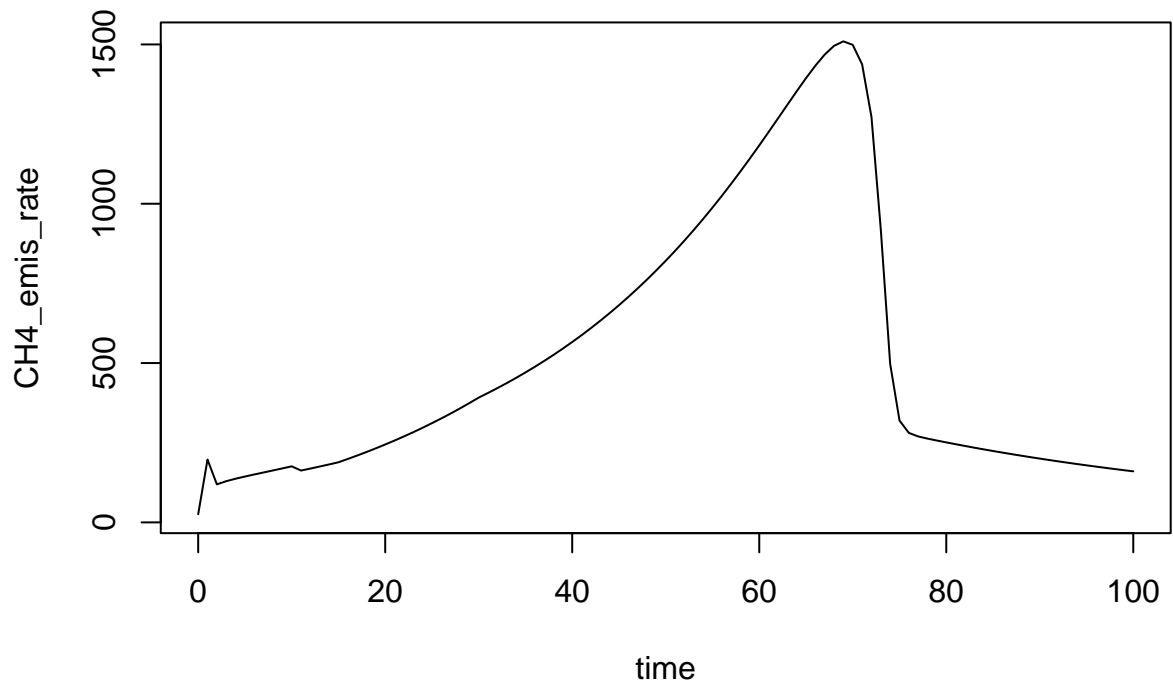
```



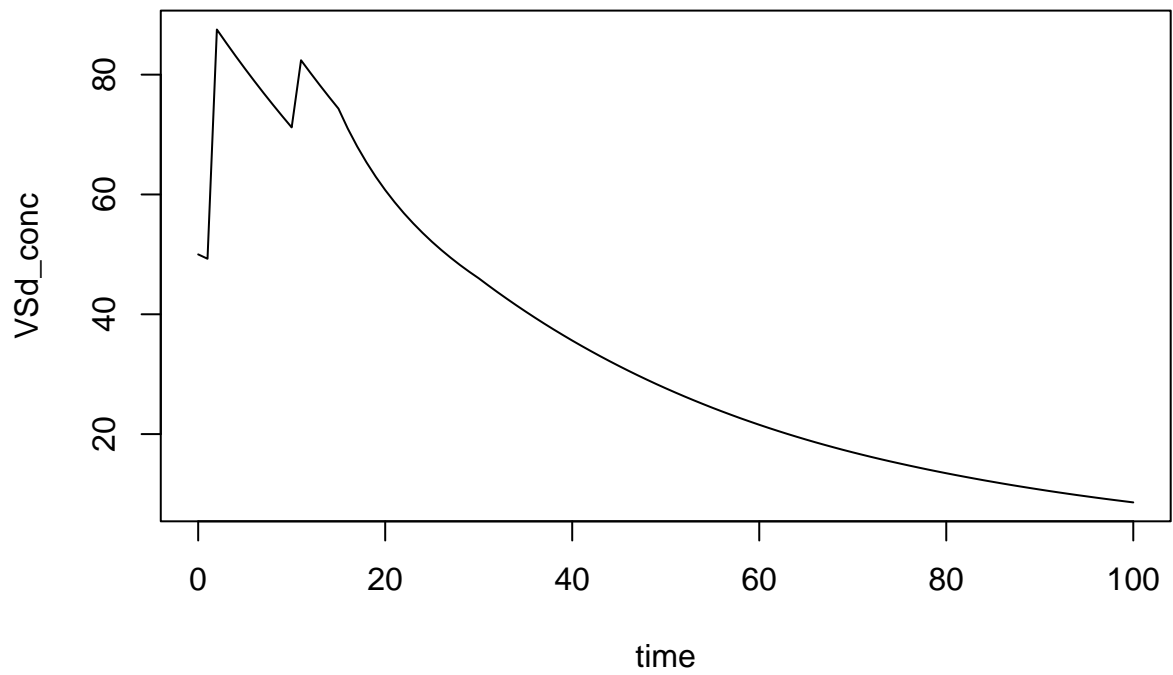
```

plot(CH4_emis_rate ~ time, data = out4b, type = 'l')

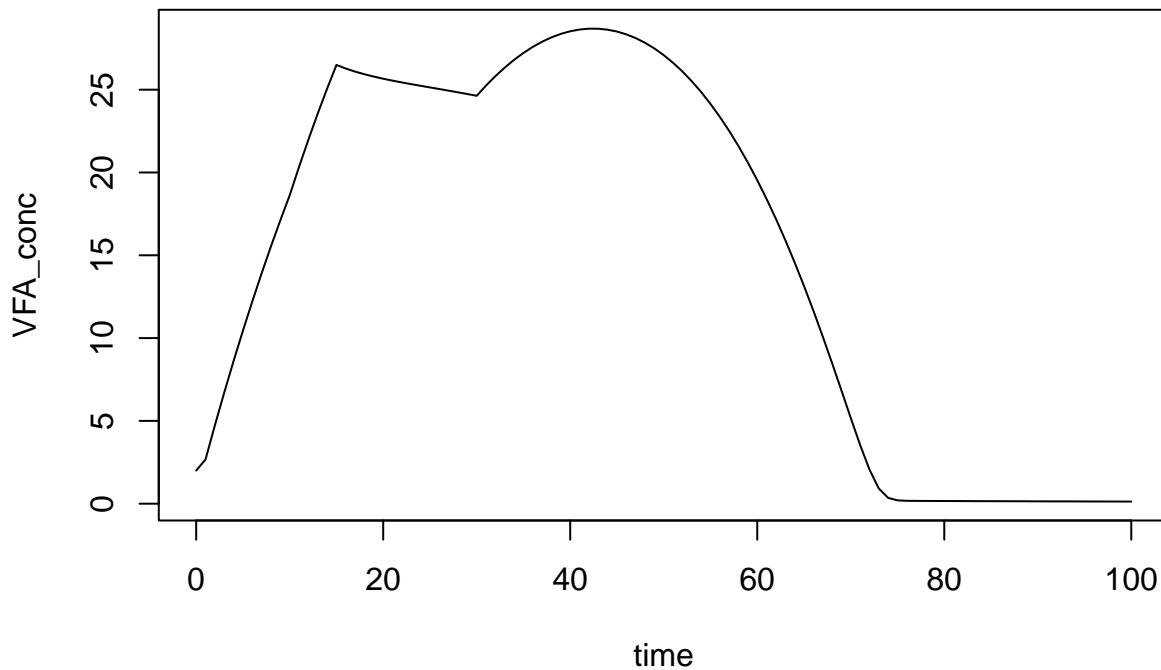
```



```
plot(VSd_conc ~ time, data = out4b, type = 'l')
```



```
plot(VFA_conc ~ time, data = out4b, type = 'l')
```



5. Time-variable inputs part 3

The list-in-data frame approach is clunky. Here is an alternative.

```
var_dat <- data.frame(time = c(0, 1, 10, 15, 30, 50),
                      slurry_mass = c(1000, 7000, 2000, 5000, 3000, 10000))
var_dat
```

```
##   time slurry_mass
## 1    0         1000
## 2    1         7000
## 3   10         2000
## 4   15         5000
## 5   30         3000
## 6   50        10000
```

Make a separate data frame for each other argument (any name, but note column names!).

```
sub_fresh_dat = data.frame(time = c(0, 1, 10, 15, 30, 50),
                           VSd = c(50, 100, 0, 0, 200, 50))
```

```
T_opt_dat = data.frame(time = c(0, 1, 10, 15, 30, 50),
                        m1 = 20 + 0:5 * 2,
                        m2 = 20 + 0:5 * 2,
                        m3 = 30 + 0:5 * 2,
                        sr1 = 46 + 0:5 * 2)
```

and combine them in a list, using the parameter element names for element names (e.g., `sub_fresh` is the name of an element in `sub_pars`).

```
var_pars <- list(var = var_dat, sub_fresh = sub_fresh_dat, T_opt = T_opt_dat)
```

```
devtools::load_all()
```

```
## i Loading ABM
```

```

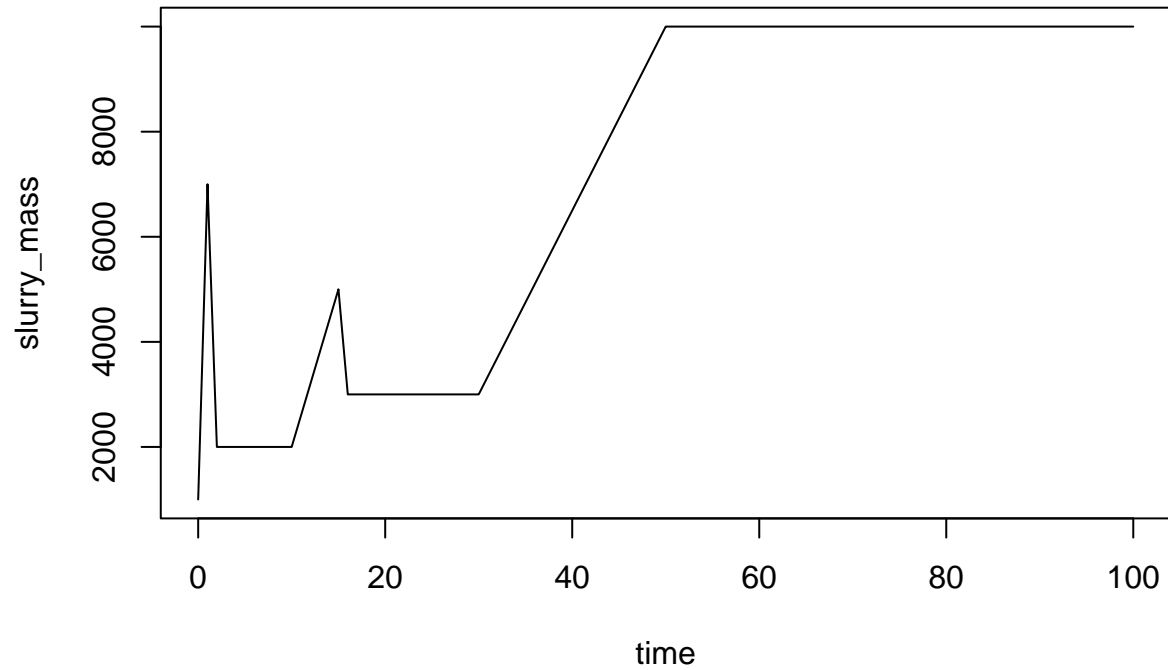
out5 <- abm(100,
  mng_pars = mng_pars,
  man_pars = man_pars,
  grp_pars = grp_pars,
  mic_pars = mic_pars,
  sub_pars = sub_pars,
  chem_pars = chem_pars,
  var_pars = var_pars)

```

```

plot(slurry_mass ~ time, data = out5, type = 'l')

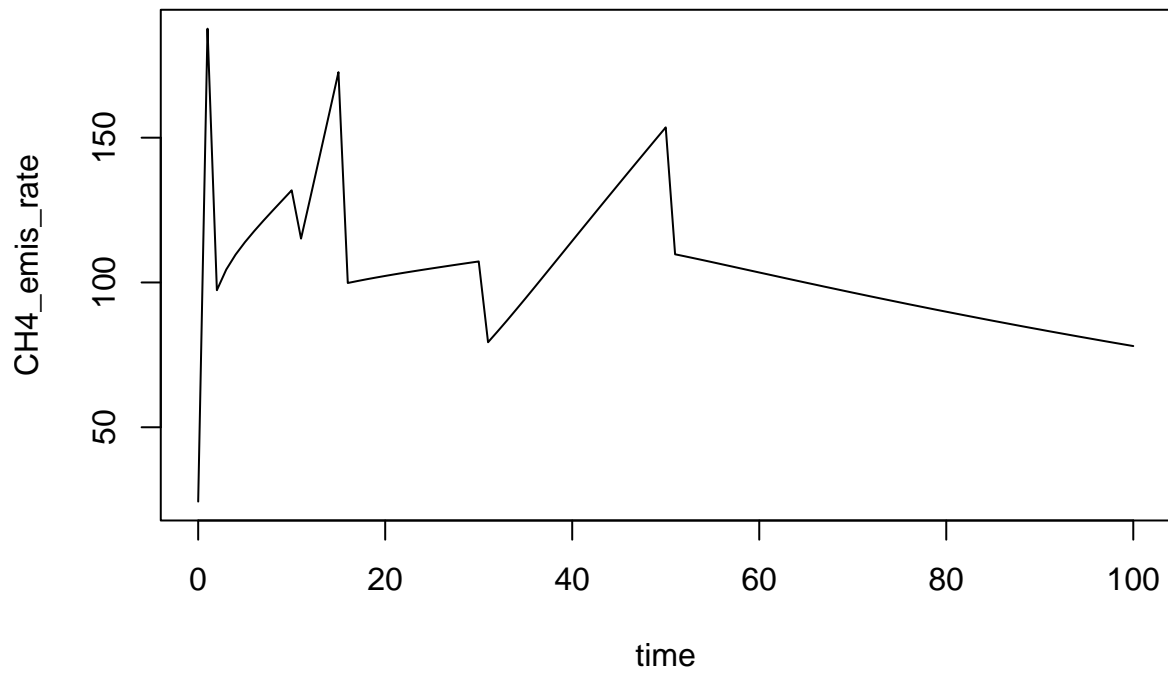
```



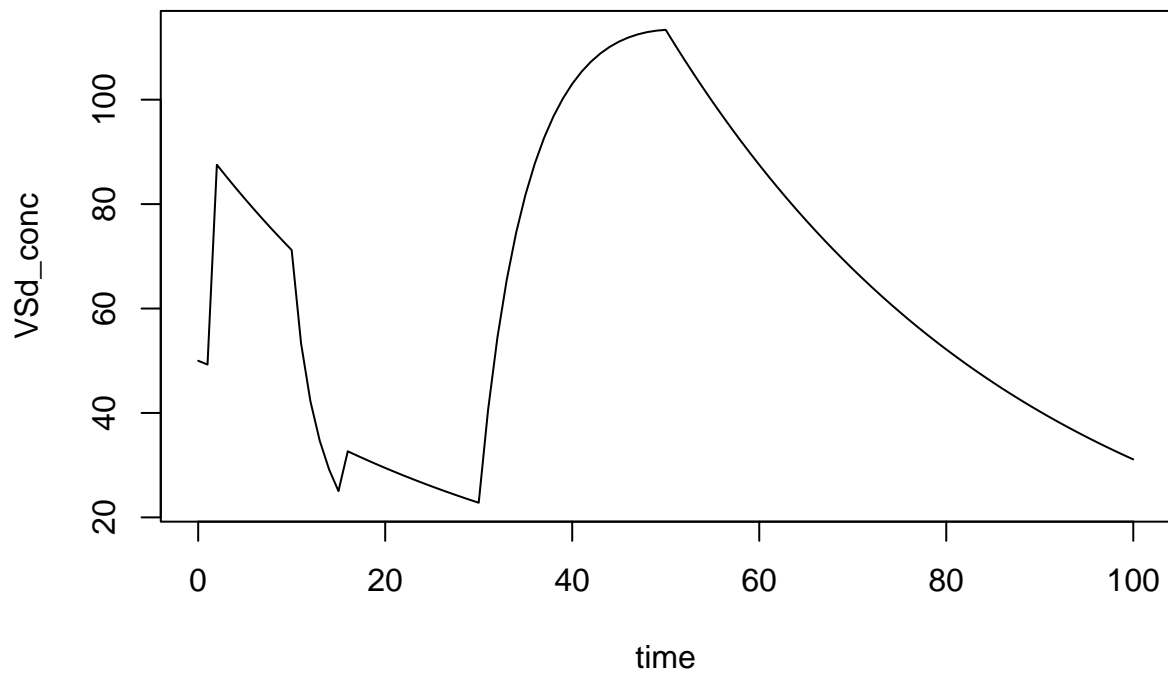
```

plot(CH4_emis_rate ~ time, data = out5, type = 'l')

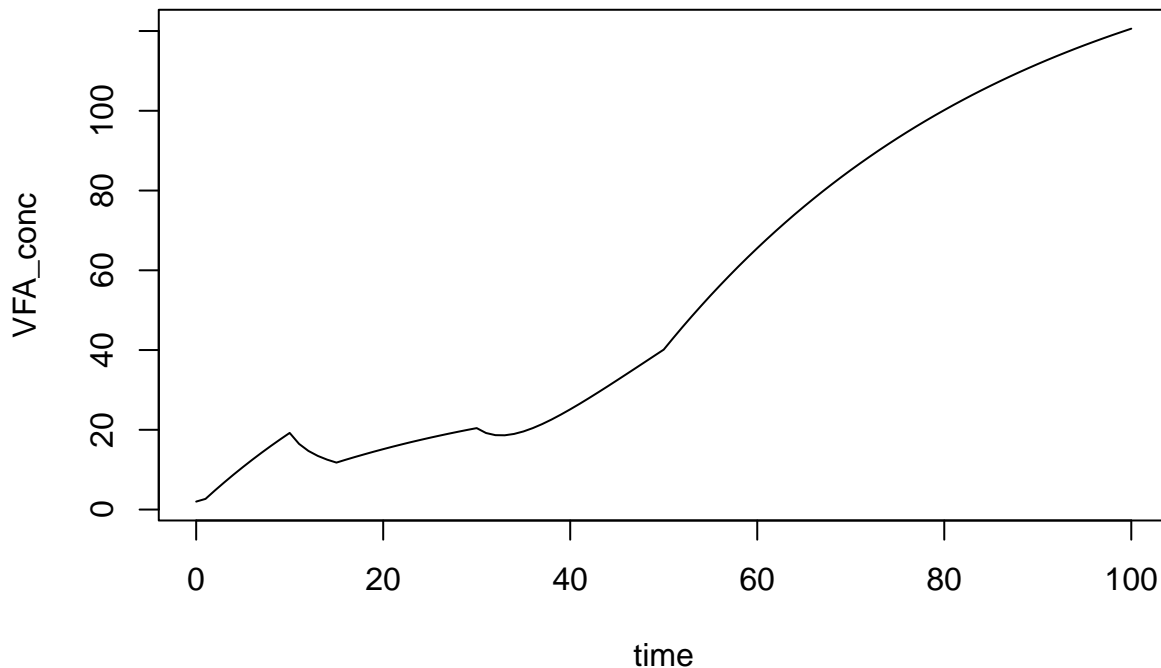
```



```
plot(VSd_conc ~ time, data = out5, type = 'l')
```



```
plot(VFA_conc ~ time, data = out5, type = 'l')
```



6. Flexible solutes

Any conservative solute can be added in `man_pars`, using any names. I am moving toward using a “master species” approach, so it makes sense to use the chemical formula of the primary species, with `p` or `m` for a charge symbol. The `comp` part of the name below is for “component”.

```
man_pars6 <- list(comps = c('H2S', 'SO4m2', 'NH4p'),
                  comp_fresh = c(H2S = 0.01, SO4m2 = 0.2, NH4p = 2.5),
                  VFA_fresh = c(VFA = 2),
                  pH = 7, dens = 1000)
```

Note that VFA is still special—it has a fixed name in the code and is not conservative.

```
devtools::load_all()
```

```
## i Loading ABM
```

```
out6a <- abm(365,
             mng_pars = mng_pars,
             man_pars = man_pars6,
             grp_pars = grp_pars,
             mic_pars = mic_pars,
             sub_pars = sub_pars,
             chem_pars = chem_pars)
```

```
## Warning in checkCOD(dat = dat, grps = pars$grps, subs = pars$subs, COD_conv =
## pars$COD_conv, : COD balance is off by 1.7%
```

```
tail(out6a)
```

```
##      time      m0      m1      m2      sr1      VSd H2S SO4m2  NH4p
## 364  360 74909.98 72497.35 337403.6 17643.06 15468816 6100 122000 1525000
## 365  361 77056.84 74543.26 351549.2 17788.74 15576604 6200 124000 1550000
## 366  362 79234.75 76617.42 366160.3 17931.53 15682002 6300 126000 1575000
## 367  363 81441.36 78717.58 381233.0 18071.50 15785084 6400 128000 1600000
```

```

## 368 364 83673.78 80840.93 396758.5 18208.69 15885918 6500 130000 1625000
## 369 365 85928.37 82984.01 412722.1 18343.17 15984571 6600 132000 1650000
##      VFA slurry_mass CH4_emis_cum CO2_emis_cum slurry_load COD_load
## 364 4796289      610000      26846605      21417315      3600000 187920000
## 365 4684393      620000      26973866      21518840      3610000 188442000
## 366 4557322      630000      27105400      21623774      3620000 188964000
## 367 4414981      640000      27241214      21732122      3630000 189486000
## 368 4257395      650000      27381289      21843868      3640000 190008000
## 369 4084743      660000      27525568      21958969      3650000 190530000
##      CH4_emis_rate temp_C pH      m0_eff      m1_eff      m2_eff      sr1_eff      VSd_eff      H2S_eff
## 364      125134.1      20 7 441740.7 422210.1 2239891 63286.93 53531054 29910
## 365      129394.2      20 7 441740.7 422210.1 2239891 63286.93 53531054 29910
## 366      133674.8      20 7 441740.7 422210.1 2239891 63286.93 53531054 29910
## 367      137950.5      20 7 441740.7 422210.1 2239891 63286.93 53531054 29910
## 368      142189.3      20 7 441740.7 422210.1 2239891 63286.93 53531054 29910
## 369      146351.3      20 7 441740.7 422210.1 2239891 63286.93 53531054 29910
##      S04m2_eff NH4p_eff VFA_eff slurry_mass_eff slurry_depth      m0_conc      m1_conc
## 364      598200 7477500 3419880      2991000      6.1 0.1228032 0.1188481
## 365      598200 7477500 3419880      2991000      6.2 0.1242852 0.1202311
## 366      598200 7477500 3419880      2991000      6.3 0.1257694 0.1216150
## 367      598200 7477500 3419880      2991000      6.4 0.1272521 0.1229962
## 368      598200 7477500 3419880      2991000      6.5 0.1287289 0.1243707
## 369      598200 7477500 3419880      2991000      6.6 0.1301945 0.1257334
##      m2_conc      sr1_conc VSd_conc H2S_conc S04m2_conc NH4p_conc VFA_conc
## 364 0.5531206 0.02892305 25.35872      0.01      0.2      2.5 7.862769
## 365 0.5670148 0.02869152 25.12355      0.01      0.2      2.5 7.555472
## 366 0.5812069 0.02846275 24.89207      0.01      0.2      2.5 7.233845
## 367 0.5956766 0.02823671 24.66419      0.01      0.2      2.5 6.898408
## 368 0.6103976 0.02801337 24.43987      0.01      0.2      2.5 6.549838
## 369 0.6253365 0.02779268 24.21905      0.01      0.2      2.5 6.189004
##      m0_eff_conc m1_eff_conc m2_eff_conc sr1_eff_conc VSd_eff_conc H2S_eff_conc
## 364      0.14769      0.1411602      0.7488771      0.02115912      17.89738      0.01
## 365      0.14769      0.1411602      0.7488771      0.02115912      17.89738      0.01
## 366      0.14769      0.1411602      0.7488771      0.02115912      17.89738      0.01
## 367      0.14769      0.1411602      0.7488771      0.02115912      17.89738      0.01
## 368      0.14769      0.1411602      0.7488771      0.02115912      17.89738      0.01
## 369      0.14769      0.1411602      0.7488771      0.02115912      17.89738      0.01
##      S04m2_eff_conc NH4p_eff_conc VFA_eff_conc
## 364      0.2      2.5      1.14339
## 365      0.2      2.5      1.14339
## 366      0.2      2.5      1.14339
## 367      0.2      2.5      1.14339
## 368      0.2      2.5      1.14339
## 369      0.2      2.5      1.14339

```

```
head(out6a)
```

```

##      time      m0      m1      m2      sr1      VSd H2S S04m2      NH4p
## 1      0 50.0000 50.0000 50.0000 50.0000 50000.0 10 200 2500
## 2      1 554.0098 553.8533 558.3748 544.0431 542318.4 110 2200 27500
## 3      2 1066.2767 1065.6732 1083.1940 1028.3035 1022076.9 210 4200 52500
## 4      3 1588.3161 1586.9430 1627.0197 1502.9749 1489597.5 310 6200 77500
## 5      4 2121.2034 2118.7114 2191.8594 1968.2472 1945194.0 410 8200 102500
## 6      5 2665.7726 2661.7877 2779.4361 2424.3064 2389172.2 510 10200 127500
##      VFA slurry_mass CH4_emis_cum CO2_emis_cum slurry_load COD_load

```



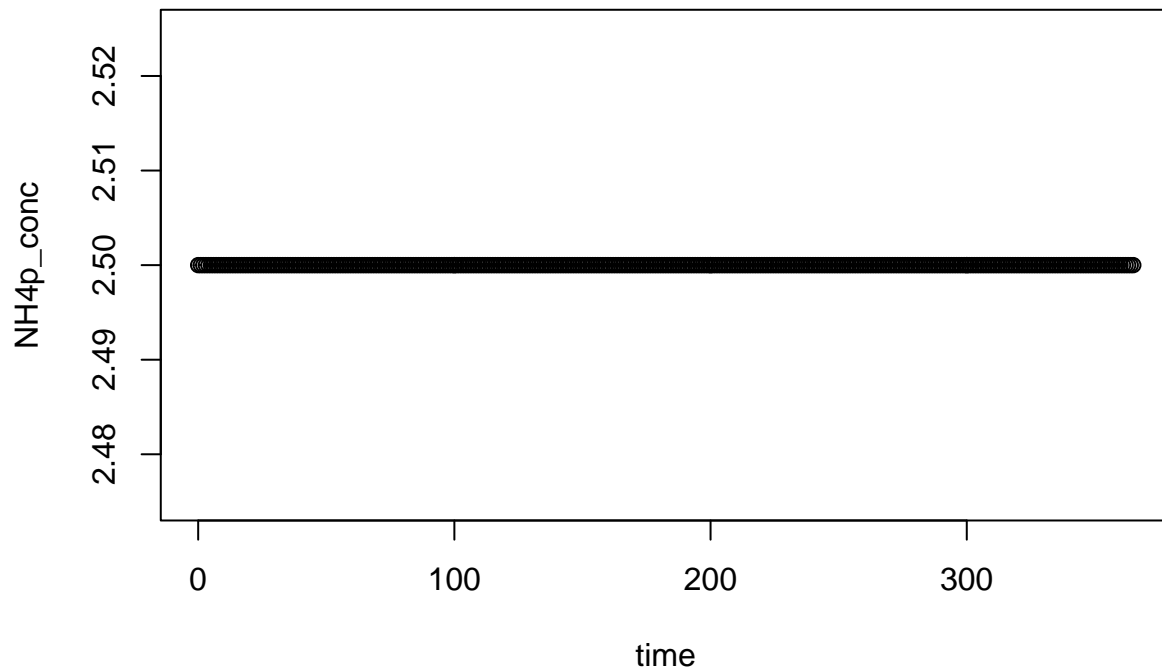
```

## 1 2000.00 1000 0.0000 0.0000 0 0
## 2 29018.66 11000 163.6272 130.5362 10000 522000
## 3 67371.44 21000 628.8119 501.6449 20000 1044000
## 4 116611.44 31000 1425.4337 1137.1629 30000 1566000
## 5 176326.70 41000 2577.0208 2055.8603 40000 2088000
## 6 246127.08 51000 4103.8067 3273.8785 50000 2610000
## CH4_emis_rate temp_C pH m0_eff m1_eff m2_eff sr1_eff VSd_eff H2S_eff
## 1 25.52844 20 7 0 0 0 0 0 0
## 2 308.65512 20 7 0 0 0 0 0 0
## 3 626.59326 20 7 0 0 0 0 0 0
## 4 970.52564 20 7 0 0 0 0 0 0
## 5 1335.99741 20 7 0 0 0 0 0 0
## 6 1720.64113 20 7 0 0 0 0 0 0
## S04m2_eff NH4p_eff VFA_eff slurry_mass_eff slurry_depth m0_conc m1_conc
## 1 0 0 0 0 0.01 0.05000000 0.05000000
## 2 0 0 0 0 0.11 0.05036453 0.05035030
## 3 0 0 0 0 0.21 0.05077508 0.05074634
## 4 0 0 0 0 0.31 0.05123600 0.05119171
## 5 0 0 0 0 0.41 0.05173667 0.05167589
## 6 0 0 0 0 0.51 0.05227005 0.05219192
## m2_conc sr1_conc VSd_conc H2S_conc S04m2_conc NH4p_conc VFA_conc
## 1 0.05000000 0.05000000 50.00000 0.01 0.2 2.5 2.000000
## 2 0.05076135 0.04945846 49.30167 0.01 0.2 2.5 2.638060
## 3 0.05158067 0.04896683 48.67033 0.01 0.2 2.5 3.208164
## 4 0.05248451 0.04848306 48.05153 0.01 0.2 2.5 3.761660
## 5 0.05345999 0.04800603 47.44376 0.01 0.2 2.5 4.300651
## 6 0.05449875 0.04753542 46.84651 0.01 0.2 2.5 4.826021
## m0_eff_conc m1_eff_conc m2_eff_conc sr1_eff_conc VSd_eff_conc H2S_eff_conc
## 1 NaN NaN NaN NaN NaN NaN NaN
## 2 NaN NaN NaN NaN NaN NaN NaN
## 3 NaN NaN NaN NaN NaN NaN NaN
## 4 NaN NaN NaN NaN NaN NaN NaN
## 5 NaN NaN NaN NaN NaN NaN NaN
## 6 NaN NaN NaN NaN NaN NaN NaN
## S04m2_eff_conc NH4p_eff_conc VFA_eff_conc
## 1 NaN NaN NaN
## 2 NaN NaN NaN
## 3 NaN NaN NaN
## 4 NaN NaN NaN
## 5 NaN NaN NaN
## 6 NaN NaN NaN

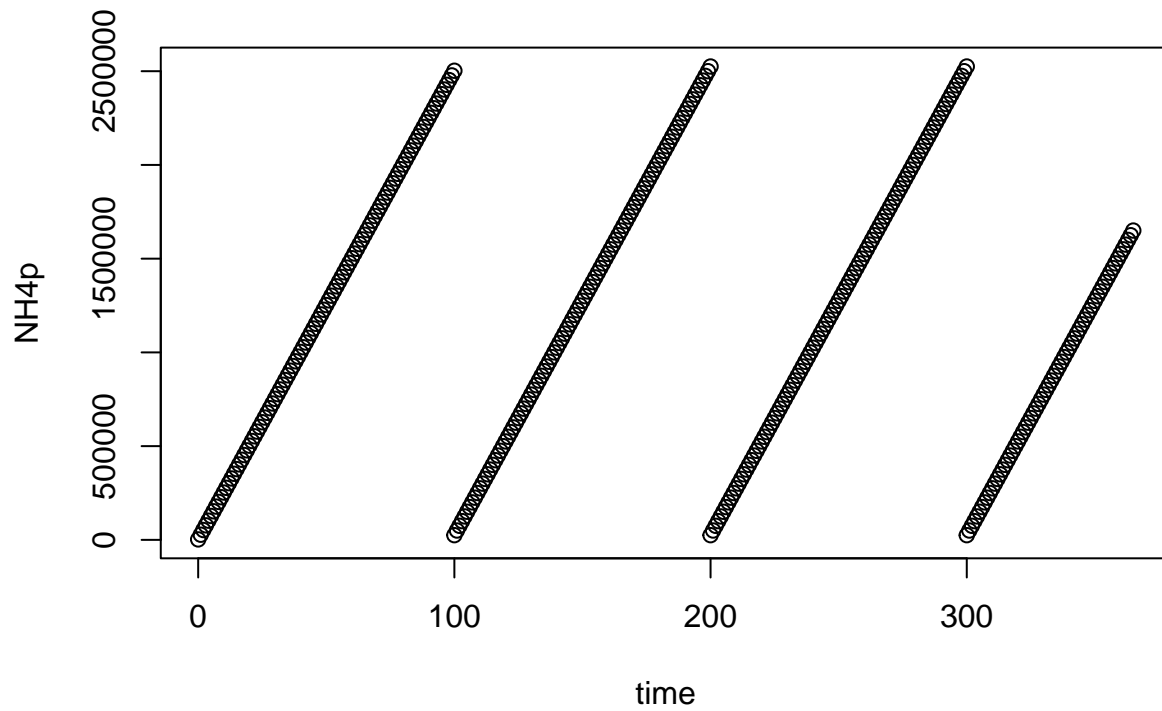
```

Conservative components are boring in output (without inhibition or volatilization).

```
plot(NH4p_conc ~ time, data = out6a)
```



```
plot(NH4p ~ time, data = out6a)
```



We can see dilution effects at least if some washing water is added.

```
mng_pars6 = list(slurry_prod_rate = 10000,
                  slurry_mass = 1000,
                  storage_depth = 2,
                  resid_depth = 0.1,
                  area = 100,
                  empty_int = 100,
                  temp_C = 20,
```

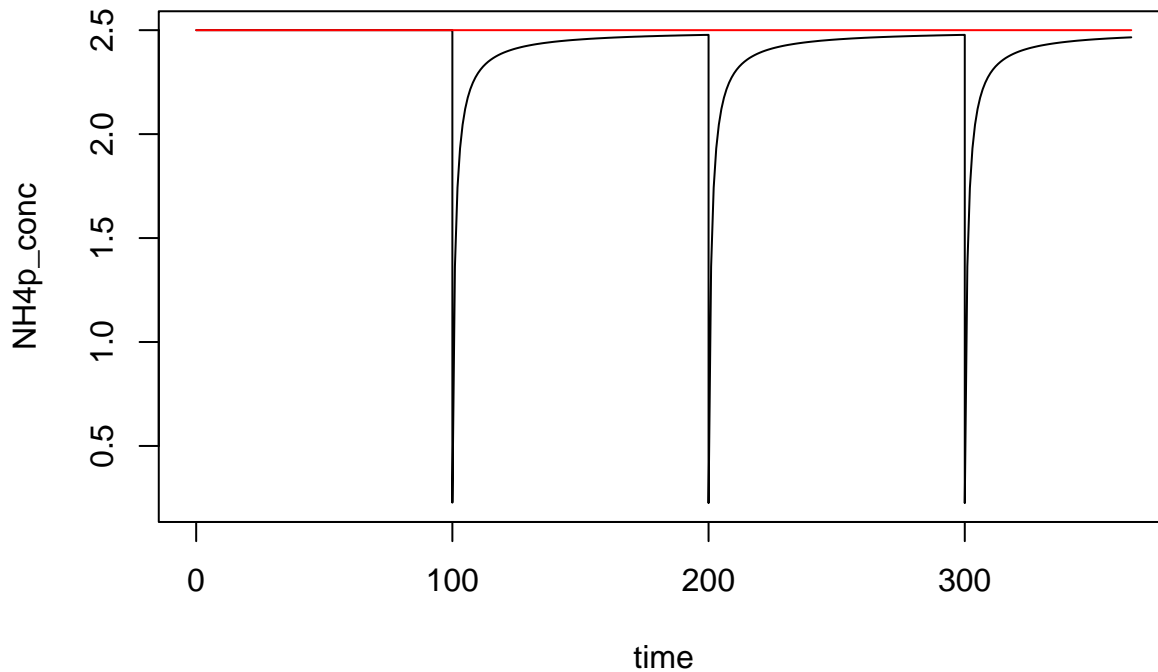
```

        wash_water = 100000,
        wash_int = 100,
        rest_d = 0,
        resid_enrich = 1)

out6b <- abm(365,
  mng_pars = mng_pars6,
  man_pars = man_pars6,
  grp_pars = grp_pars,
  mic_pars = mic_pars,
  sub_pars = sub_pars,
  chem_pars = chem_pars)

## Warning in checkCOD(dat = dat, grps = pars$grps, subs = pars$subs, COD_conv =
## pars$COD_conv, : COD balance is off by 32%
plot(NH4p_conc ~ time, data = out6b, type = 'l')
lines(NH4p_conc ~ time, data = out6a, col = 'red')

```



7. Speciation

Acid-base reactions are needed for inhibition. They can be added for any component. The `chem_pars` argument can accept temperature-dependent log K_a expressions.

```

man_pars7 <- list(comps = c('H2S', 'NH4p'),
  comp_fresh = c(H2S = 0.01, NH4p = 2.5),
  VFA_fresh = c(VFA = 2),
  pH = 7, dens = 1000)

chem_pars7 <- list(COD_conv = c(CH4 = 1/0.2507, xa = 1/0.7069561,
  VFA = 1/0.9383125, S = 1/0.5015, VS = 1/0.69,
  CO2_aer = 1/0.436, CO2_sr = 1/1.2,
  C_xa = 1/0.3753125),

```

```

specs = c('NH3', 'HSm', 'VFAm'),
mspec = c(NH3 = 'NH4p', HSm = 'H2S', VFAm = 'VFA'),
lka = c(NH3 = '- 0.09046 - 2729.31/temp_K',
        HSm = '- 3448.7/temp_K + 47.479 - 7.5227 * log(temp_K)',
        VFAm = '- 4.8288 + 21.42/temp_K')
)

```

Here **comps** are the chemical “components”, or “master species”, as described a bit above. All are automatically included as chemical species in **packPars()**. In the **chem_pars** argument, **specs** are the other (non-master) species that the master species are in equilibrium with. And **mspec** are the associated master species. So the NH3 species comes from NH4+. When there is speciation, the master species are always taken as the protonated ones. So the species in **specs** always have one less proton than their associated master species. Only 2 species are supported for any component.

```
devtools::load_all()
```

```
## i Loading ABM
```

```

out7 <- abm(365,
  mng_pars = mng_pars,
  man_pars = man_pars6,
  grp_pars = grp_pars,
  mic_pars = mic_pars,
  sub_pars = sub_pars,
  chem_pars = chem_pars7)

```

```

## Warning in checkCOD(dat = dat, grps = pars$grps, subs = pars$subs, COD_conv =
## pars$COD_conv, : COD balance is off by 1.7%

```

```
head(out7)
```

```

##      time      m0      m1      m2      sr1      VSd H2S S04m2  NH4p
## 1      0  50.0000  50.0000  50.0000  50.0000  50000.0  10   200   2500
## 2      1  554.0098  553.8533  558.3748  544.0431  542318.4 110  2200  27500
## 3      2 1066.2767 1065.6732 1083.1940 1028.3035 1022076.9 210  4200  52500
## 4      3 1588.3161 1586.9430 1627.0197 1502.9749 1489597.5 310  6200  77500
## 5      4 2121.2034 2118.7114 2191.8594 1968.2472 1945194.0 410  8200 102500
## 6      5 2665.7726 2661.7877 2779.4361 2424.3064 2389172.2 510 10200 127500
##      VFA slurry_mass CH4_emis_cum CO2_emis_cum slurry_load COD_load
## 1      2000.00      1000      0.0000      0.0000      0      0
## 2     29018.66     11000     163.6272     130.5362     10000  522000
## 3     67371.44     21000     628.8119     501.6449     20000 1044000
## 4    116611.44     31000    1425.4337    1137.1629     30000 1566000
## 5    176326.70     41000    2577.0208    2055.8603     40000 2088000
## 6    246127.08     51000    4103.8067    3273.8785     50000 2610000
##      CH4_emis_rate temp_C pH m0_eff m1_eff m2_eff sr1_eff VSd_eff H2S_eff
## 1      25.52844      20  7      0      0      0      0      0      0
## 2      308.65512      20  7      0      0      0      0      0      0
## 3      626.59326      20  7      0      0      0      0      0      0
## 4      970.52564      20  7      0      0      0      0      0      0
## 5     1335.99741      20  7      0      0      0      0      0      0
## 6     1720.64113      20  7      0      0      0      0      0      0
##      S04m2_eff NH4p_eff VFA_eff slurry_mass_eff slurry_depth  m0_conc  m1_conc
## 1           0         0         0              0         0.01 0.05000000 0.05000000
## 2           0         0         0              0         0.11 0.05036453 0.05035030
## 3           0         0         0              0         0.21 0.05077508 0.05074634

```

```

## 4      0      0      0      0      0.31 0.05123600 0.05119171
## 5      0      0      0      0      0.41 0.05173667 0.05167589
## 6      0      0      0      0      0.51 0.05227005 0.05219192
##      m2_conc   sr1_conc VSd_conc H2S_conc SO4m2_conc NH4p_conc VFA_conc
## 1 0.05000000 0.05000000 50.00000      0.01      0.2      2.5 2.000000
## 2 0.05076135 0.04945846 49.30167      0.01      0.2      2.5 2.638060
## 3 0.05158067 0.04896683 48.67033      0.01      0.2      2.5 3.208164
## 4 0.05248451 0.04848306 48.05153      0.01      0.2      2.5 3.761660
## 5 0.05345999 0.04800603 47.44376      0.01      0.2      2.5 4.300651
## 6 0.05449875 0.04753542 46.84651      0.01      0.2      2.5 4.826021
##      m0_eff_conc m1_eff_conc m2_eff_conc sr1_eff_conc VSd_eff_conc H2S_eff_conc
## 1      NaN      NaN      NaN      NaN      NaN      NaN
## 2      NaN      NaN      NaN      NaN      NaN      NaN
## 3      NaN      NaN      NaN      NaN      NaN      NaN
## 4      NaN      NaN      NaN      NaN      NaN      NaN
## 5      NaN      NaN      NaN      NaN      NaN      NaN
## 6      NaN      NaN      NaN      NaN      NaN      NaN
##      SO4m2_eff_conc NH4p_eff_conc VFA_eff_conc
## 1      NaN      NaN      NaN
## 2      NaN      NaN      NaN
## 3      NaN      NaN      NaN
## 4      NaN      NaN      NaN
## 5      NaN      NaN      NaN
## 6      NaN      NaN      NaN

```

But chemical species are actually ignored unless they are used in inhibition.

8. Inhibition

Any chemical species can inhibit any microbial group. Inhibition parameters (currently initial and complete concentrations, with linear response, why not?) are entered in a matrix.

```

ilwr <- matrix(
  c(5, 0.2, 10, 0.5,
    5, 0.2, 10, 0.5,
    5, 0.2, 10, 0.5,
    5, 0.2, 10, 0.5),
  nrow = 4,
  byrow = TRUE,
  dimnames = list(
    c('m0', 'm1', 'm2', 'sr1'),
    c('NH4p', 'NH3', 'VFAm', 'VFA')
  )
)

iupr <- matrix(
  c(9, 0.9, 30, 1,
    9, 0.9, 30, 1,
    9, 0.9, 30, 1,
    9, 0.9, 30, 1),
  nrow = 4,
  byrow = TRUE,
  dimnames = list(
    c('m0', 'm1', 'm2', 'sr1'),

```

```

    c('NH4p', 'NH3', 'VFAm', 'VFA')
  )
)

inhib_pars <- list(
  ilwr = ilwr,
  iupr = iupr
)

inhib_pars

## $ilwr
##      NH4p NH3 VFAm VFA
## m0      5 0.2  10 0.5
## m1      5 0.2  10 0.5
## m2      5 0.2  10 0.5
## sr1     5 0.2  10 0.5
##
## $iupr
##      NH4p NH3 VFAm VFA
## m0      9 0.9  30  1
## m1      9 0.9  30  1
## m2      9 0.9  30  1
## sr1     9 0.9  30  1

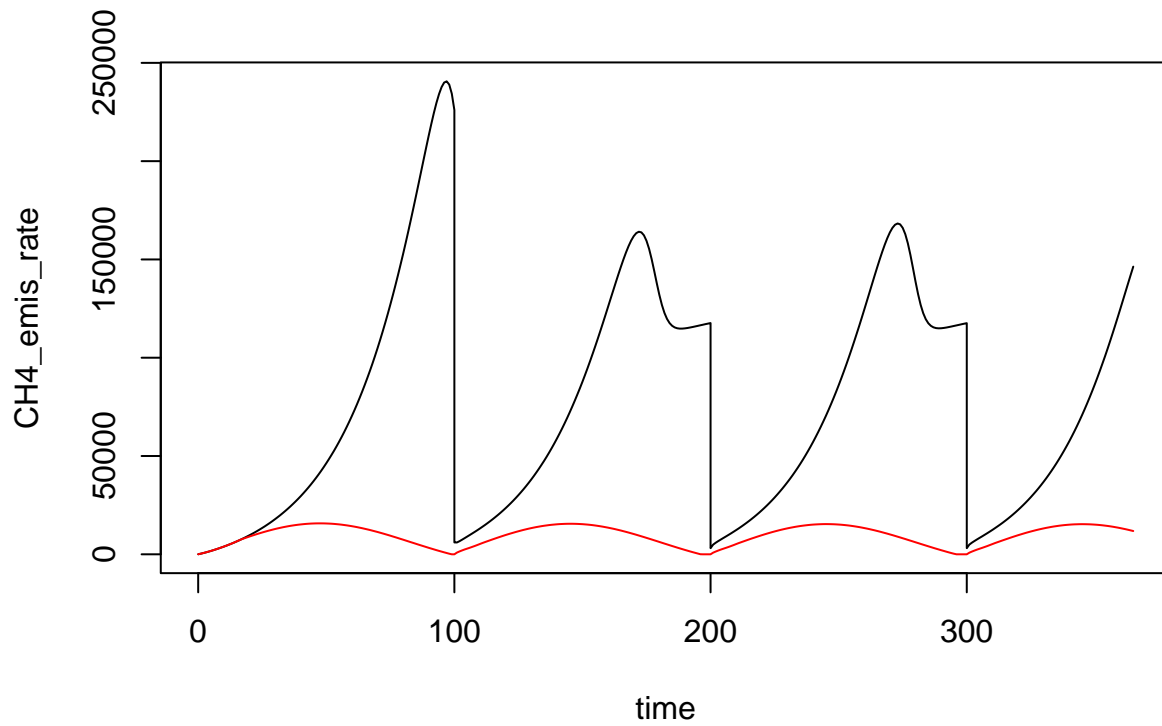
man_pars8 <- list(comps = c('H2S', 'NH4p'),
  comp_fresh = c(H2S = 0.01,
    NH4p = 2.5),
  VFA_fresh = c(VFA = 2),
  pH = 7, dens = 1000)

chem_pars8 <- list(COD_conv = c(CH4 = 1/0.2507, xa = 1/0.7069561,
  VFA = 1/0.9383125, S = 1/0.5015, VS = 1/0.69,
  CO2_aer = 1/0.436, CO2_sr = 1/1.2,
  C_xa = 1/0.3753125),
  specs = c('NH3', 'HSm', 'VFAm'),
  mspec = c(NH3 = 'NH4p', HSm = 'H2S', VFAm = 'VFA'),
  lka = c(NH3 = '- 0.09046 - 2729.31/temp_K',
    HSm = '- 3448.7/temp_K + 47.479 - 7.5227* log(temp_K)',
    VFAm = '-4.8288 + 21.42/temp_K')
)

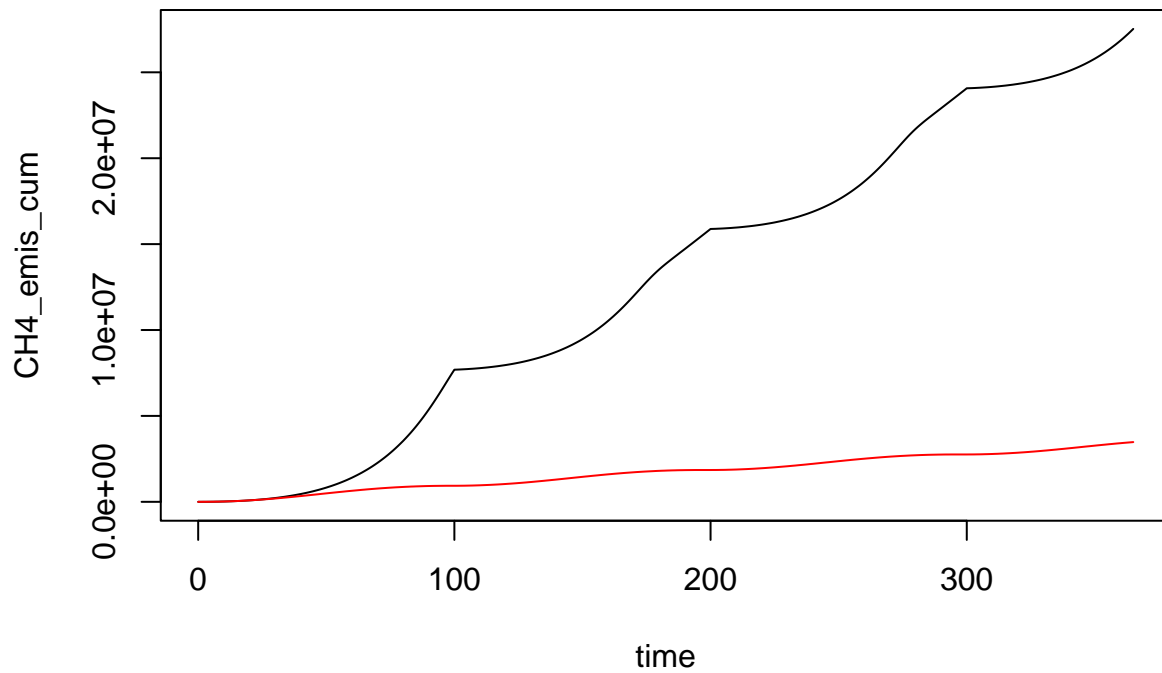
out8 <- abm(365,
  mng_pars = mng_pars,
  man_pars = man_pars7,
  grp_pars = grp_pars,
  mic_pars = mic_pars,
  sub_pars = sub_pars,
  chem_pars = chem_pars7,
  inhib_pars = inhib_pars
)

plot(CH4_emis_rate ~ time, data = out7, type = 'l')
lines(CH4_emis_rate ~ time, data = out8, col = 'red')

```



```
plot(CH4_emis_cum ~ time, data = out7, type = 'l')
lines(CH4_emis_cum ~ time, data = out8, col = 'red')
```



9. Volatilization

Any chemical species can volatilize.

```
man_pars9 <- list(comps = c('H2S', 'NH4p'),
                  comp_fresh = c(H2S = 0.01, NH4p = 2.5),
```

```
VFA_fresh = c(VFA = 2),
pH = 7, dens = 1000)
```

We need to set mass transfer coefficient values (m/d) for any species that volatilizes.

```
chem_pars9 <- list(COD_conv = c(CH4 = 1/0.2507, xa = 1/0.7069561,
                                VFA = 1/0.9383125, S = 1/0.5015, VS = 1/0.69,
                                CO2_aer = 1/0.436, CO2_sr = 1/1.2,
                                C_xa = 1/0.3753125),
  specs = c('NH3', 'HSm', 'VFAm'),
  mspec = c(NH3 = 'NH4p', HSm = 'H2S', VFAm = 'VFA'),
  lka = c(NH3 = '- 0.09046 - 2729.31/temp_K',
          HSm = '- 3448.7/temp_K + 47.479 - 7.5227 * log(temp_K)',
          VFAm = '-4.8288 + 21.42/temp_K'),
  kla = c(NH3 = 0.01, H2S = 0.01, VFA = 0.01) * 86400)
```

```
devtools::load_all()
```

```
## i Loading ABM
```

```
out9 <- abm(365,
  mng_pars = mng_pars,
  man_pars = man_pars9,
  grp_pars = grp_pars,
  mic_pars = mic_pars,
  sub_pars = sub_pars,
  chem_pars = chem_pars9,
  inhib_pars = inhib_pars
)
```

```
## Warning in checkCOD(dat = dat, grps = pars$grps, subs = pars$subs, COD_conv =
## pars$COD_conv, : COD balance is off by 2%
```

The state variable vector and output data frame automatically expand for the new values.

```
head(out9)
```

```
##      time      m0      m1      m2      sr1      VSd      H2S      NH4p
## 1      0  50.0000  50.0000  50.0000  50.0000  50000.0  10.00000  2500.00
## 2      1  553.9008  553.7459  558.2172  544.0431  542318.4  20.30920  26666.73
## 3      2 1065.8886 1065.2914 1082.6272 1028.3035 1022076.9  38.77174  50838.30
## 4      3 1587.5229 1586.1630 1625.8481 1502.9749 1489597.4  57.23445  75010.55
## 5      4 2119.9030 2117.4331 2189.9160 1968.2472 1945193.9  75.69717  99183.09
## 6      5 2663.8768 2659.9251 2776.5686 2424.3064 2389172.0  94.15990 123355.78
##      VFA slurry_mass CH4_emis_cum CO2_emis_cum NH3_emis_cum H2S_emis_cum
## 1  2000.00      1000      0.0000      0.0000      0.000      0.0000
## 2 27920.12     11000     161.8334     129.1053     833.273     89.6908
## 3 64914.06     21000     622.3551     496.4939    1661.702    171.2283
## 4 112537.32     31000    1412.0784    1126.5085    2489.451    252.7655
## 5 170383.30     41000    2554.8558    2038.1778    3316.914    334.3028
## 6 238067.72     51000    4071.0922    3247.7800    4144.219    415.8401
##      VFA_emis_cum slurry_load COD_load CH4_emis_rate temp_C pH m0_eff m1_eff
## 1      0.000      0      0      25.52844     20 7      0      0
## 2    1106.072     10000    522000     305.28189     20 7      0      0
## 3    2484.484     20000   1044000     620.73997     20 7      0      0
## 4    4130.203     30000   1566000     962.63333     20 7      0      0
## 5    6036.464     40000   2088000    1326.29785     20 7      0      0
```



```

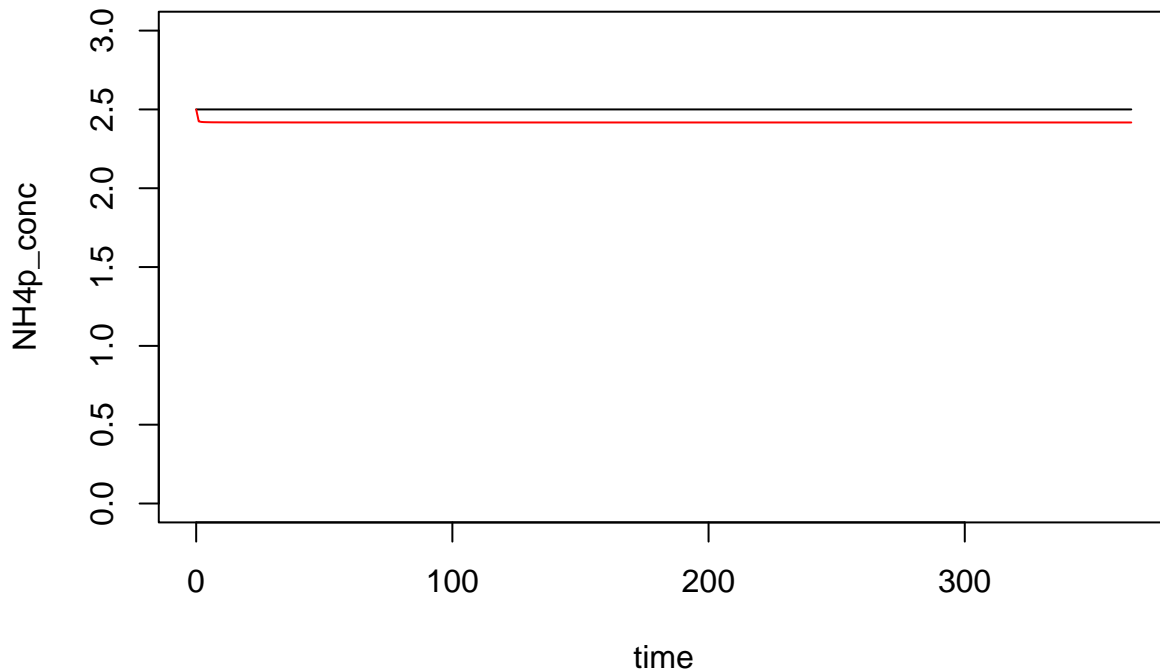
## 6      8196.713      50000 2610000      1709.25431      20 7      0      0
##  m2_eff sr1_eff VSd_eff H2S_eff NH4p_eff VFA_eff slurry_mass_eff slurry_depth
## 1      0      0      0      0      0      0      0      0.01
## 2      0      0      0      0      0      0      0      0.11
## 3      0      0      0      0      0      0      0      0.21
## 4      0      0      0      0      0      0      0      0.31
## 5      0      0      0      0      0      0      0      0.41
## 6      0      0      0      0      0      0      0      0.51
##      m0_conc      m1_conc      m2_conc      sr1_conc VSd_conc      H2S_conc NH4p_conc
## 1 0.05000000 0.05000000 0.05000000 0.05000000 50.00000 0.01000000 2.500000
## 2 0.05035462 0.05034054 0.05074702 0.04945846 49.30167 0.001846291 2.424248
## 3 0.05075660 0.05072816 0.05155368 0.04896683 48.67033 0.001846273 2.420871
## 4 0.05121041 0.05116655 0.05244671 0.04848306 48.05153 0.001846273 2.419695
## 5 0.05170495 0.05164471 0.05341259 0.04800603 47.44375 0.001846273 2.419100
## 6 0.05223288 0.05215539 0.05444252 0.04753542 46.84651 0.001846273 2.418741
##  VFA_conc m0_eff_conc m1_eff_conc m2_eff_conc sr1_eff_conc VSd_eff_conc
## 1 2.000000      NaN      NaN      NaN      NaN      NaN      NaN
## 2 2.538192      NaN      NaN      NaN      NaN      NaN      NaN
## 3 3.091146      NaN      NaN      NaN      NaN      NaN      NaN
## 4 3.630236      NaN      NaN      NaN      NaN      NaN      NaN
## 5 4.155690      NaN      NaN      NaN      NaN      NaN      NaN
## 6 4.667995      NaN      NaN      NaN      NaN      NaN      NaN
##  H2S_eff_conc NH4p_eff_conc VFA_eff_conc
## 1      NaN      NaN      NaN
## 2      NaN      NaN      NaN
## 3      NaN      NaN      NaN
## 4      NaN      NaN      NaN
## 5      NaN      NaN      NaN
## 6      NaN      NaN      NaN

```

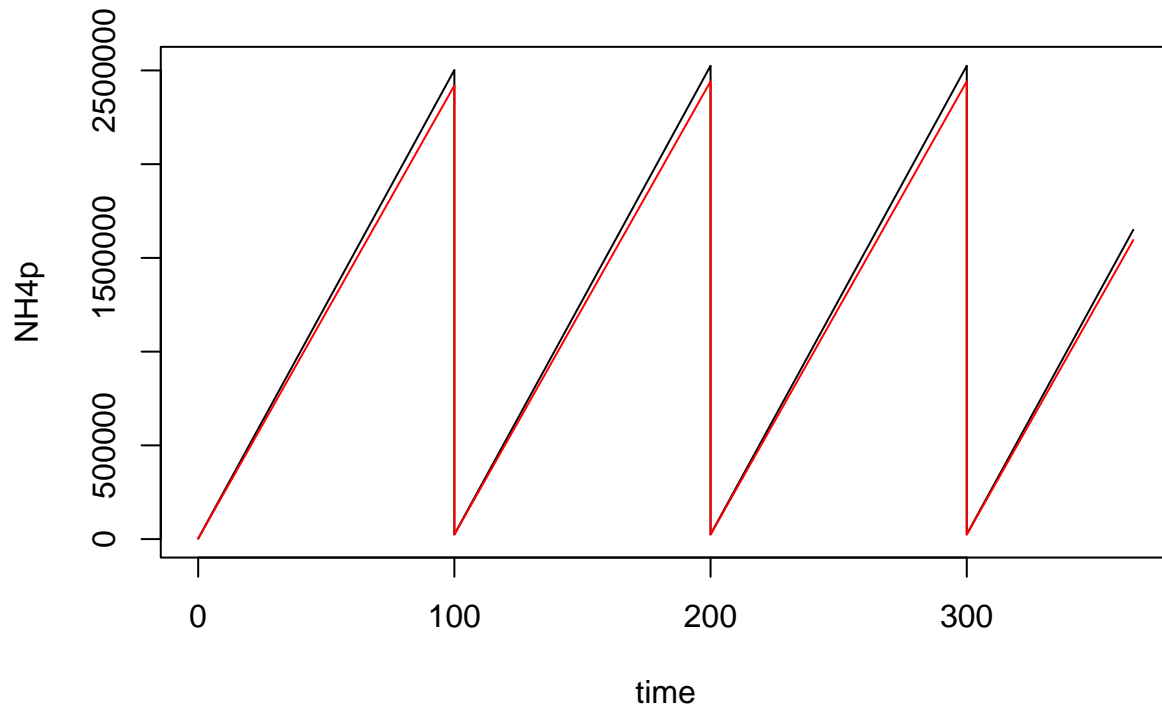
```

plot(NH4p_conc ~ time, data = out8, type = 'l', ylim = c(0, 3))
lines(NH4p_conc ~ time, data = out9, col = 'red')

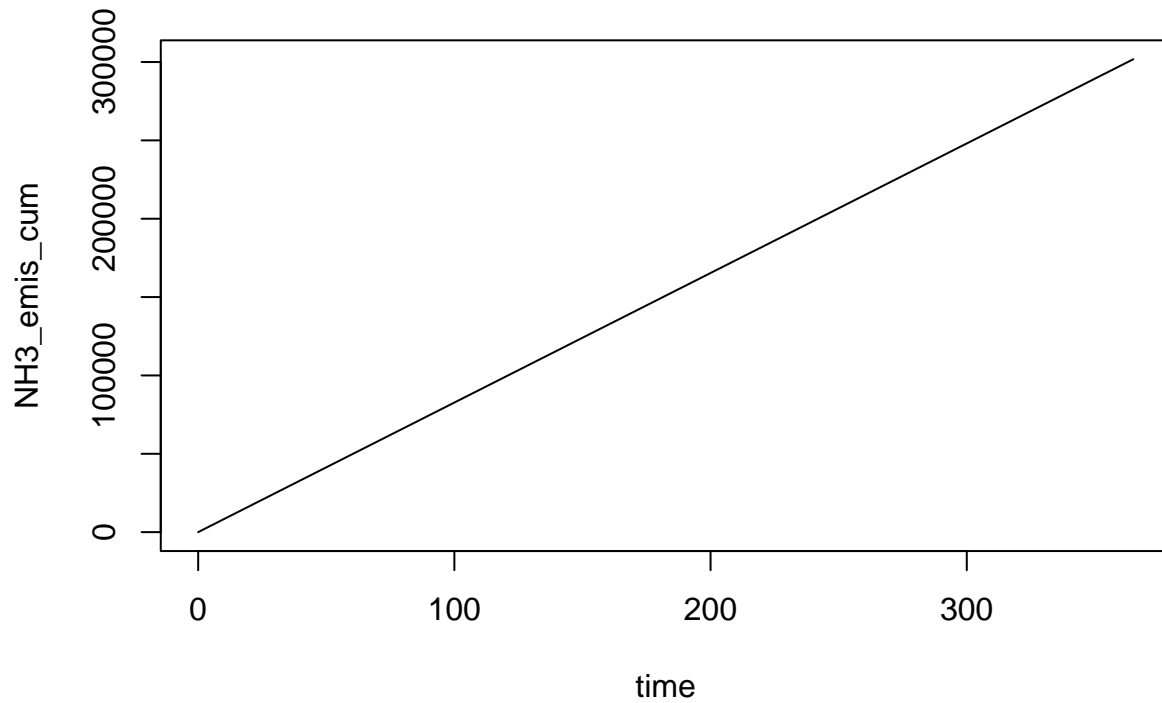
```



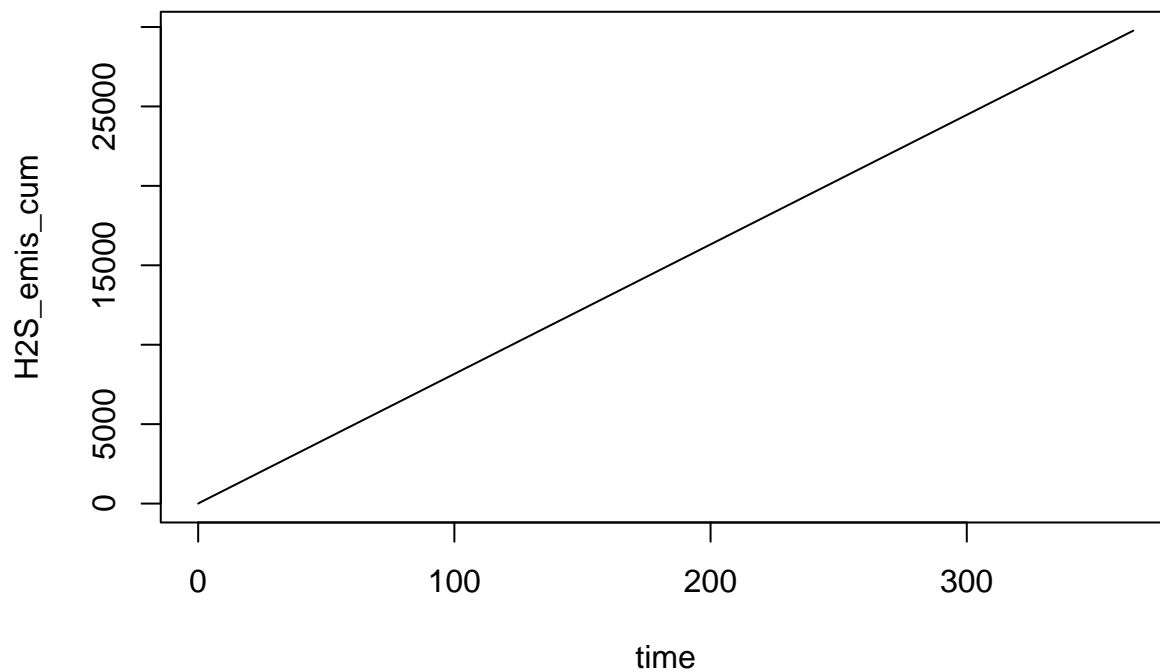
```
plot(NH4p ~ time, data = out8, type = 'l')
lines(NH4p ~ time, data = out9, col = 'red')
```



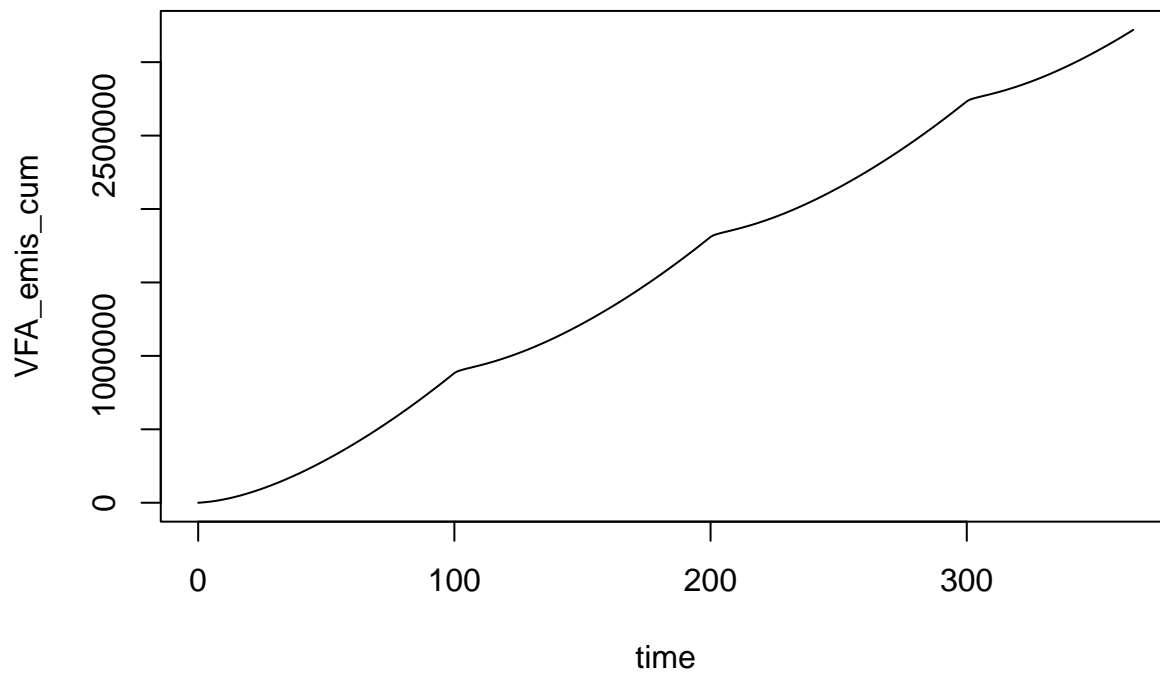
```
plot(NH3_emis_cum ~ time, data = out9, type = 'l')
```



```
plot(H2S_emis_cum ~ time, data = out9, type = 'l')
```



```
plot(VFA_emis_cum ~ time, data = out9, type = 'l')
```



9. COD balance

There is now a `checkCOD()` function that runs on `abm()` results before returning them. For now the tolerance is fixed at 1%. Some of the examples above do not meet that criterion for some reason. At least one shows a real problem that needs to be identified. For the emission example above, the problem is that VFA is emitted but that loss is not included in the balance check. We can make it worse by pretending the the charged form can volatilize (VFA changed to VFAm below).

```

chem_pars10 <- list(COD_conv = c(CH4 = 1/0.2507, xa = 1/0.7069561,
                                VFA = 1/0.9383125, S = 1/0.5015, VS = 1/0.69,
                                CO2_aer = 1/0.436, CO2_sr = 1/1.2,
                                C_xa = 1/0.3753125),
                  specs = c('NH3', 'HSm', 'VFAm'),
                  mspec = c(NH3 = 'NH4p', HSm = 'H2S', VFAm = 'VFA'),
                  lka = c(NH3 = '- 0.09046 - 2729.31/temp_K',
                          HSm = '- 3448.7/temp_K + 47.479 - 7.5227 * log(temp_K)',
                          VFAm = '-4.8288 + 21.42/temp_K'),
                  kla = c(NH3 = 0.01, H2S = 0.01, VFAm = 0.01) * 86400)

out10 <- abm(365,
             mng_pars = mng_pars,
             man_pars = man_pars9,
             grp_pars = grp_pars,
             mic_pars = mic_pars,
             sub_pars = sub_pars,
             chem_pars = chem_pars10,
             inhib_pars = inhib_pars
            )

```

```

## Warning in checkCOD(dat = dat, grps = pars$grps, subs = pars$subs, COD_conv =
## pars$COD_conv, : COD balance is off by 36%

```