Demo of new simple1 version

Sasha D. Hafner

02 June, 2025 12:07

Overview

This demo shows:

1. basic usage,
2. variable substrates,
3. time-variable parameters
4. 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 = man_pars$conc_fresh),
  grp_pars,
  mic_pars,
  sub_pars,
  chem_pars,
  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
  starting = NULL,                              # Output from previous simulation to be starting condition
  value = 'ts',                                 # Type of output
  warn = TRUE) {
```

The main changes are:

- `sub_pars` for defining substrates
- `ctrl_pars` for some "control" parameters
- `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 now (like anything here, it could change).

```
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 there is no inhibition for 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(ks_SO4 = 0.00694,
                 km_urea = 0.913,
                 dd_rate_xa = 0.02)
```

These last two are similar to other versions.

```
man_pars <- list(conc_fresh = c(sulfide = 0.01,
                                sulfate = 0.2,
                                TAN = 2.5,
                                VFA = 2,
                                ash = 15),
                 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
```

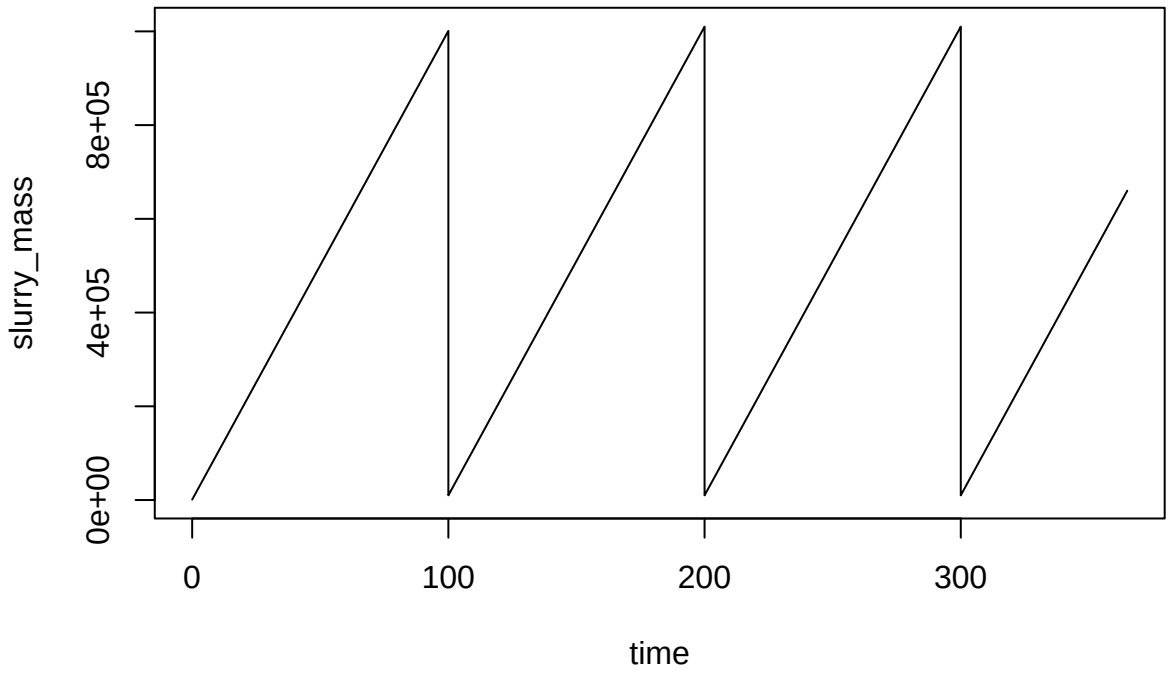
```
tail(out1)
```

```
##     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
```

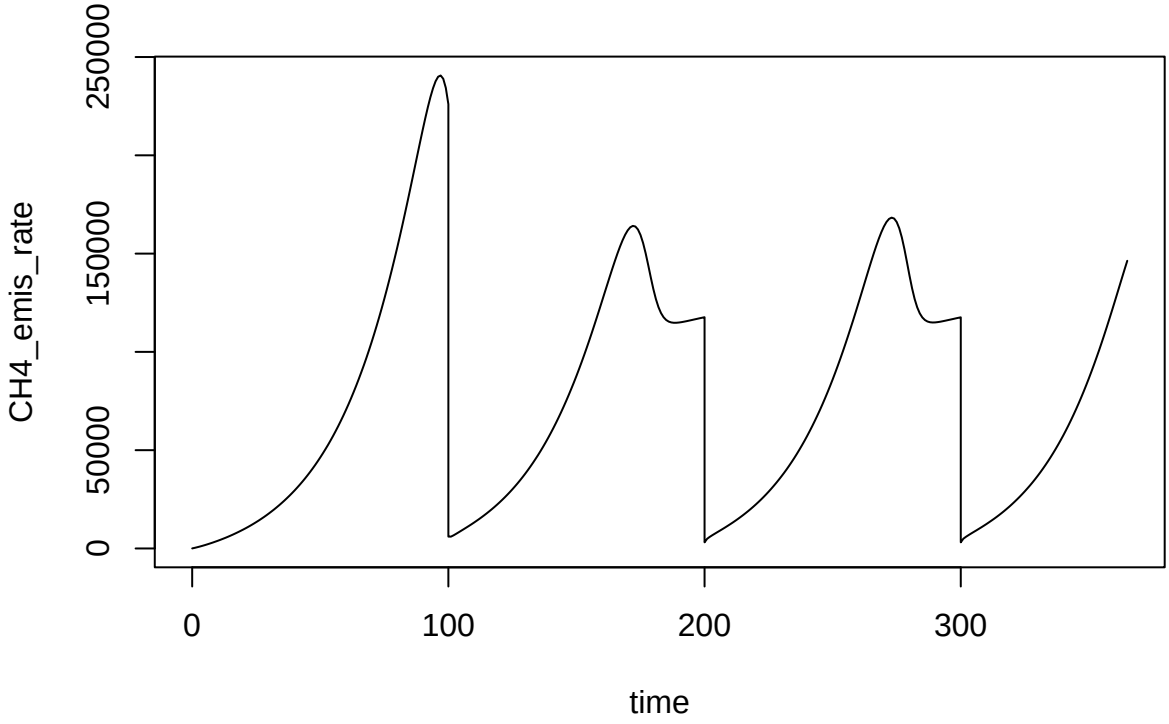
The effluent columns are cumulative. I did this for COD balance checking. We will have to discuss what is needed.

Here are some results.

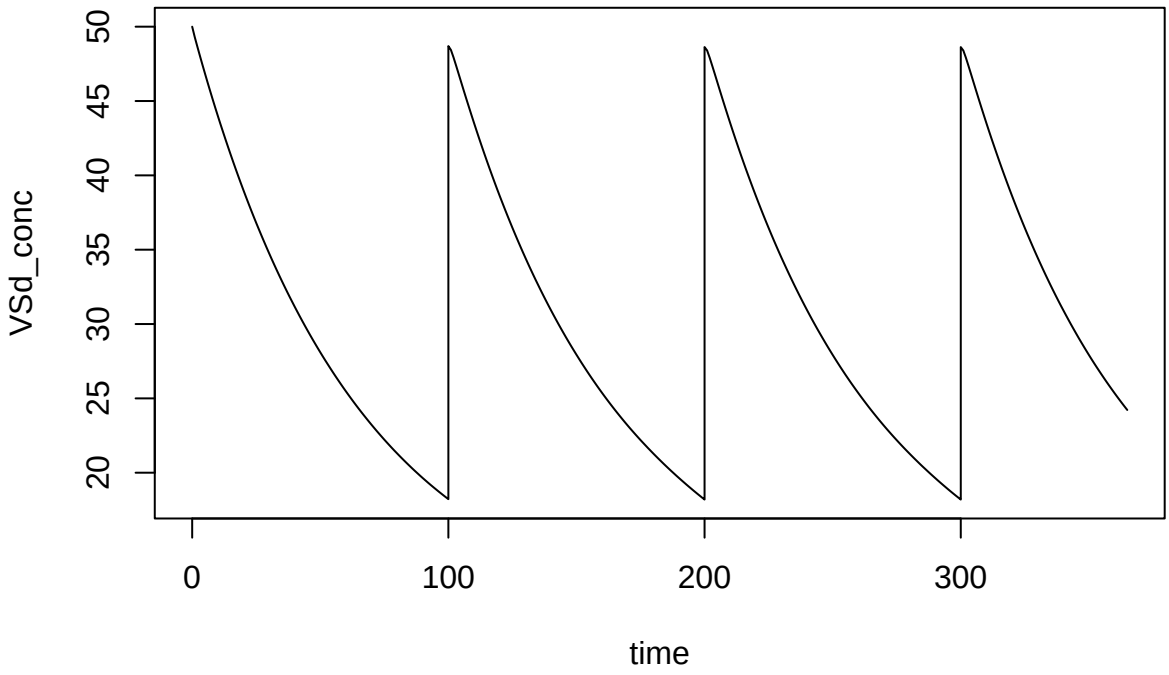
```
plot(slurry_mass ~ time, data = out1, type = 'l')
```



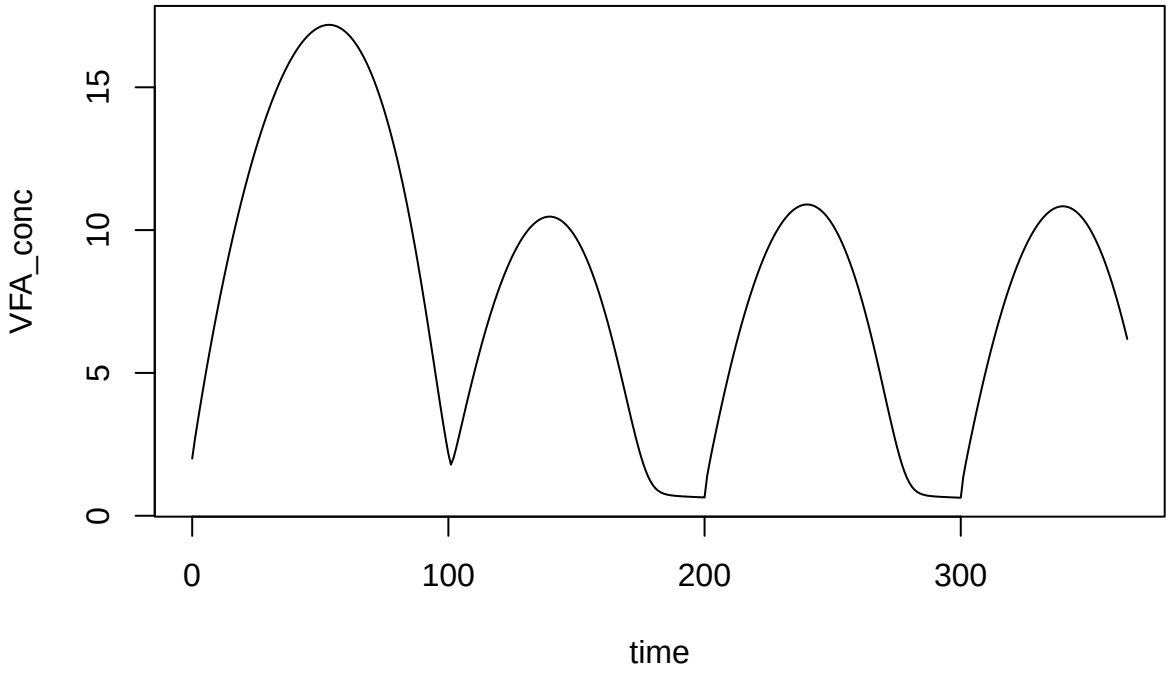

```
plot(CH4_emis_rate ~ time, data = out1, type = 'l')
```




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

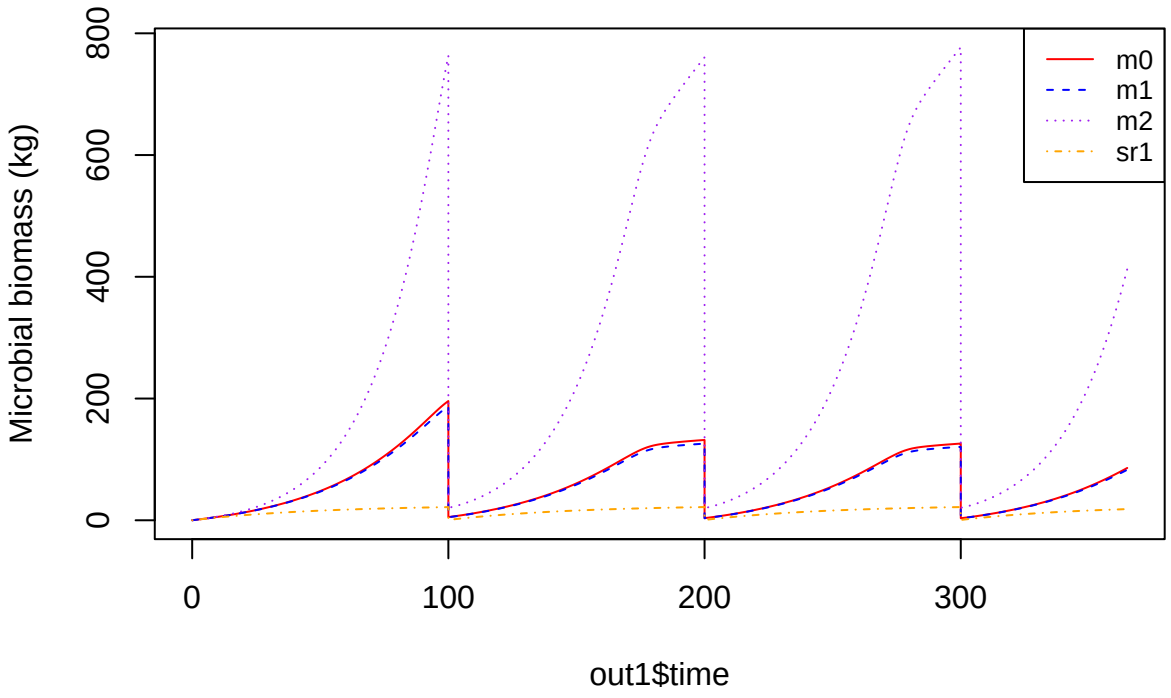



```
plot(VFA_conc ~ time, data = out1, type = 'l')
```



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

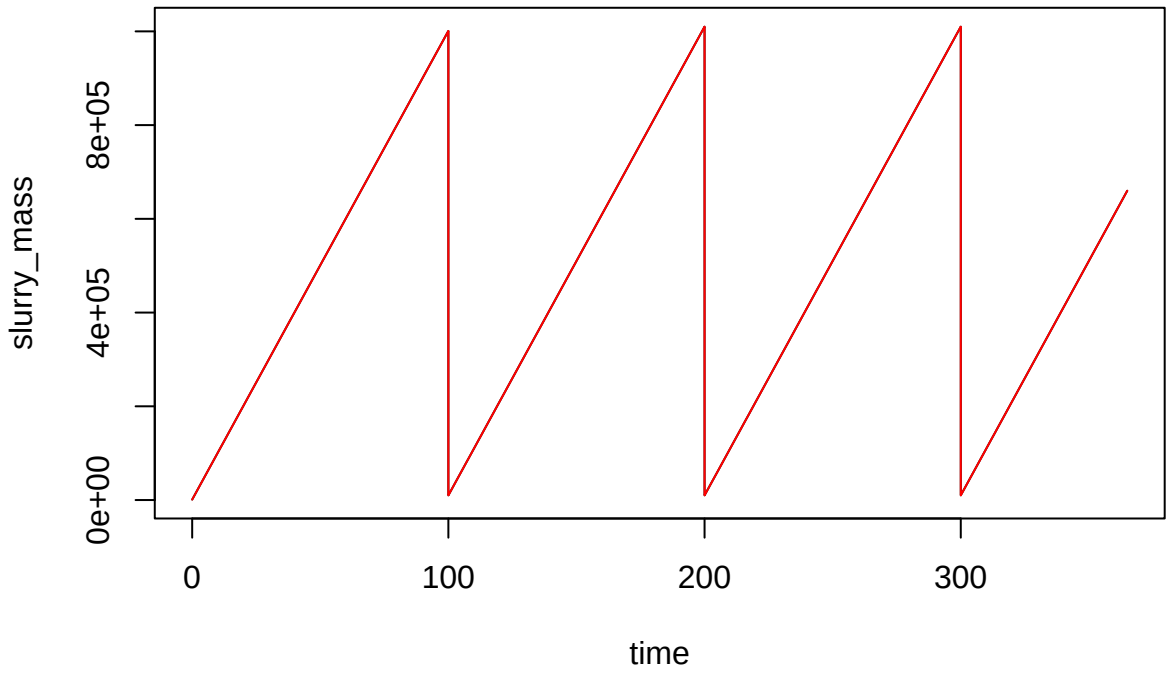
Particulate substrates are defined in `sub_pars` now and there are no particular substrates hard-wired in the code. VFA is the only intermediate, and it is hard-wired. Here we will include two more substrates. The mix of names might not make much sense in this example.

```
sub_pars2 <- list(subs = c('VSd', 'protein', 'cellulose'),
                  T_opt_hyd = c(all = 60),
                  T_min_hyd = c(all = 0),
                  T_max_hyd = c(all = 90),
                  hydrol_opt = c(VSd = 0.1, protein = 0.01, cellulose = 0.05),
                  sub_fresh = c(VSd = 50, protein = 20, cellulose = 35),
                  sub_init = c(VSd = 50, protein = 20, cellulose = 35))
```

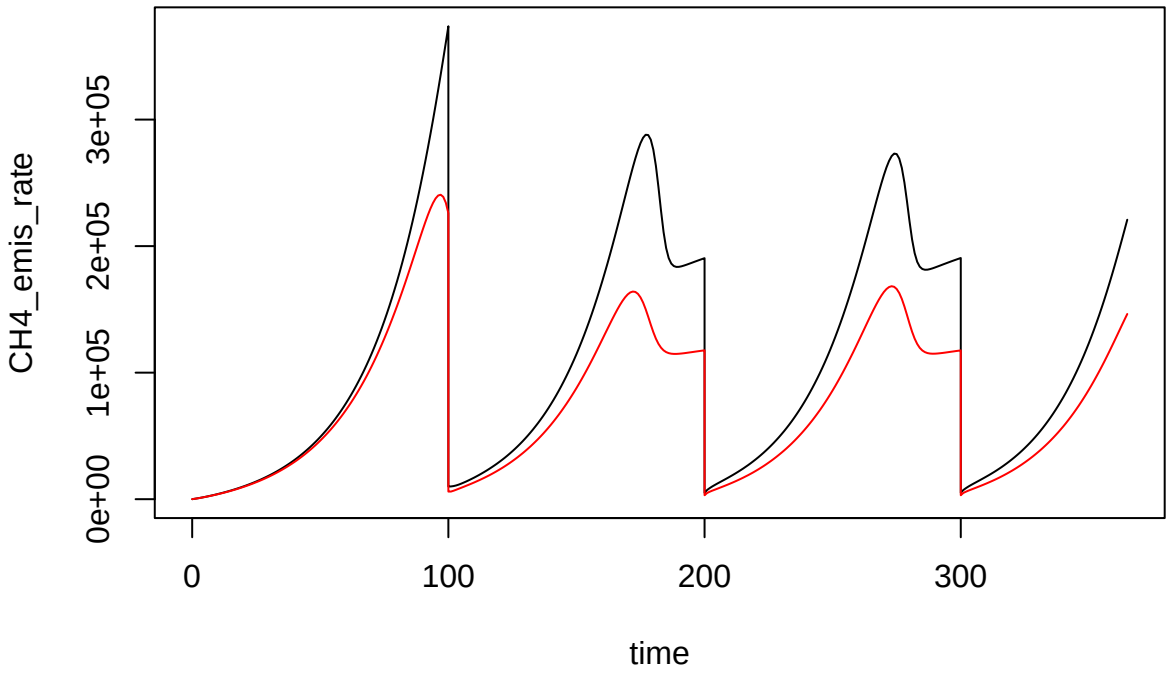
```
out2 <- abm(365,
            mng_pars = mng_pars,
            man_pars = man_pars,
            grp_pars = grp_pars,
            mic_pars = mic_pars,
            sub_pars = sub_pars2,
            chem_pars = chem_pars)
```

```
## Warning in checkCOD(dat = dat, grps = pars$grps, subs = pars$subs, COD_conv =
## pars$COD_conv, : COD balance is off by 1.1%
```

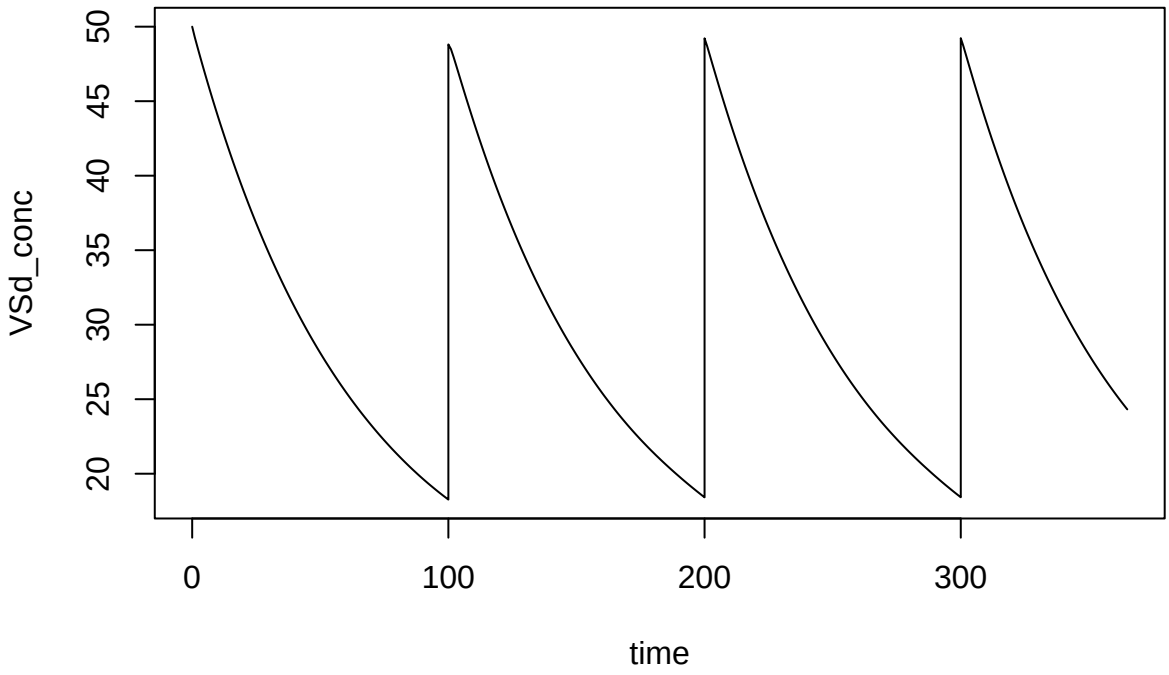
```
plot(slurry_mass ~ time, data = out2, type = 'l')
lines(slurry_mass ~ time, data = out1, col = 'red')
```



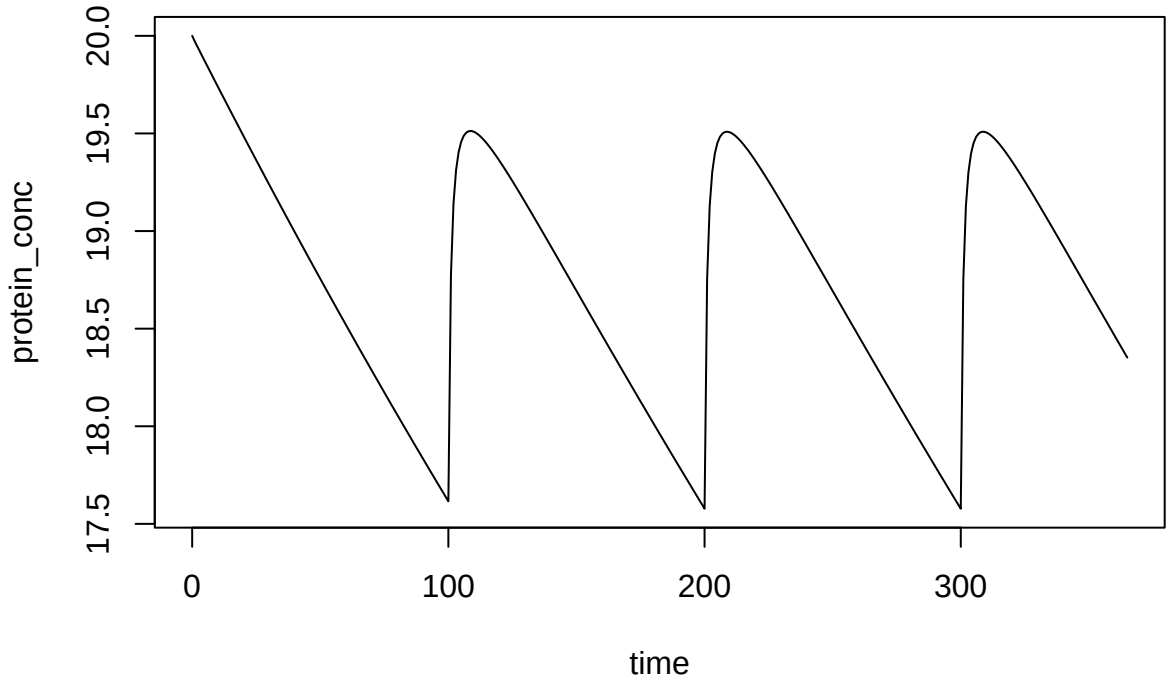

```
plot(CH4_emis_rate ~ time, data = out2, type = 'l')
lines(CH4_emis_rate ~ time, data = out1, col = 'red')
```



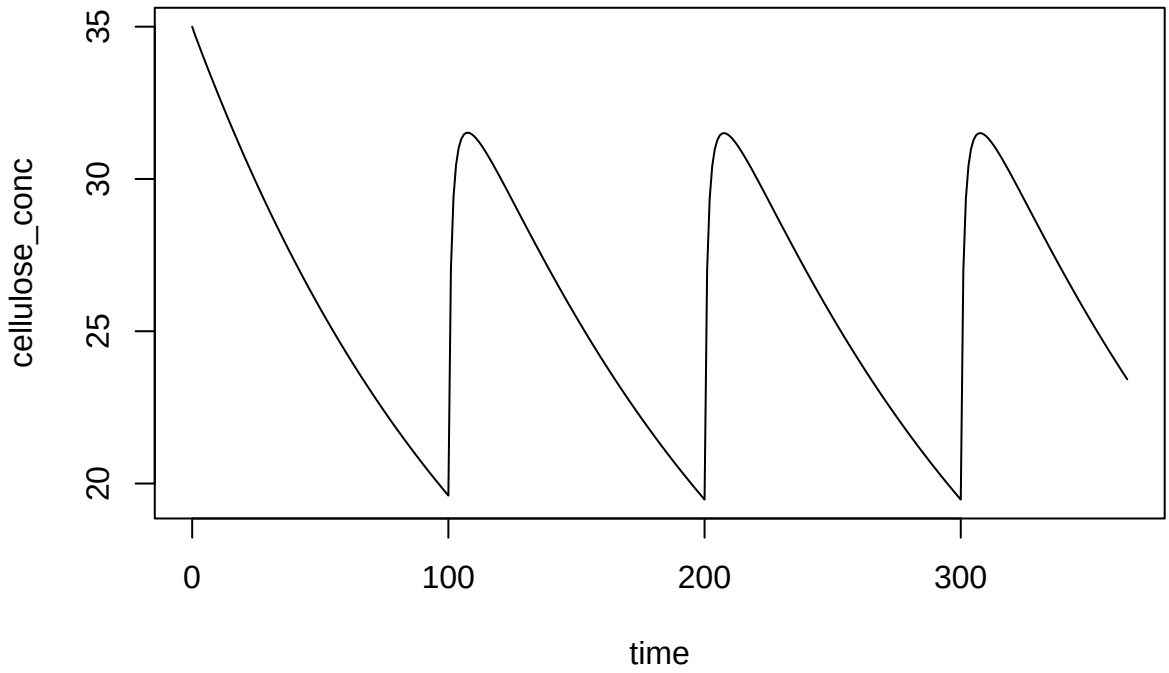

```
plot(VSd_conc ~ time, data = out2, type = 'l')
```



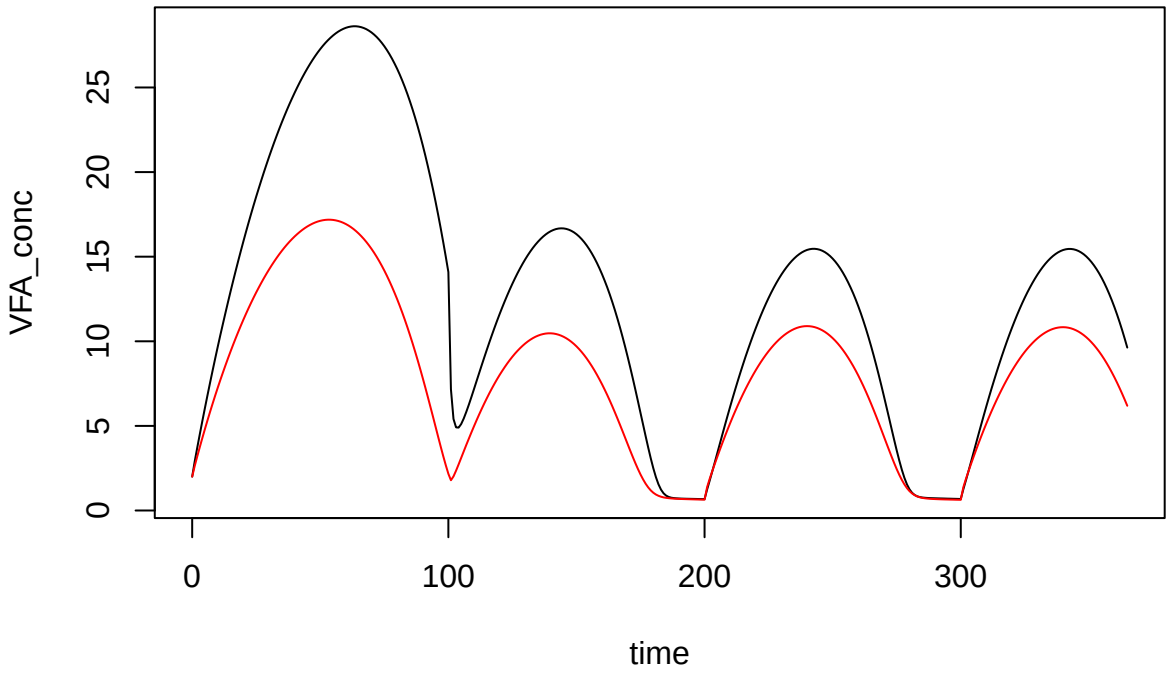

```
plot(protein_conc ~ time, data = out2, type = 'l')
```




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




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



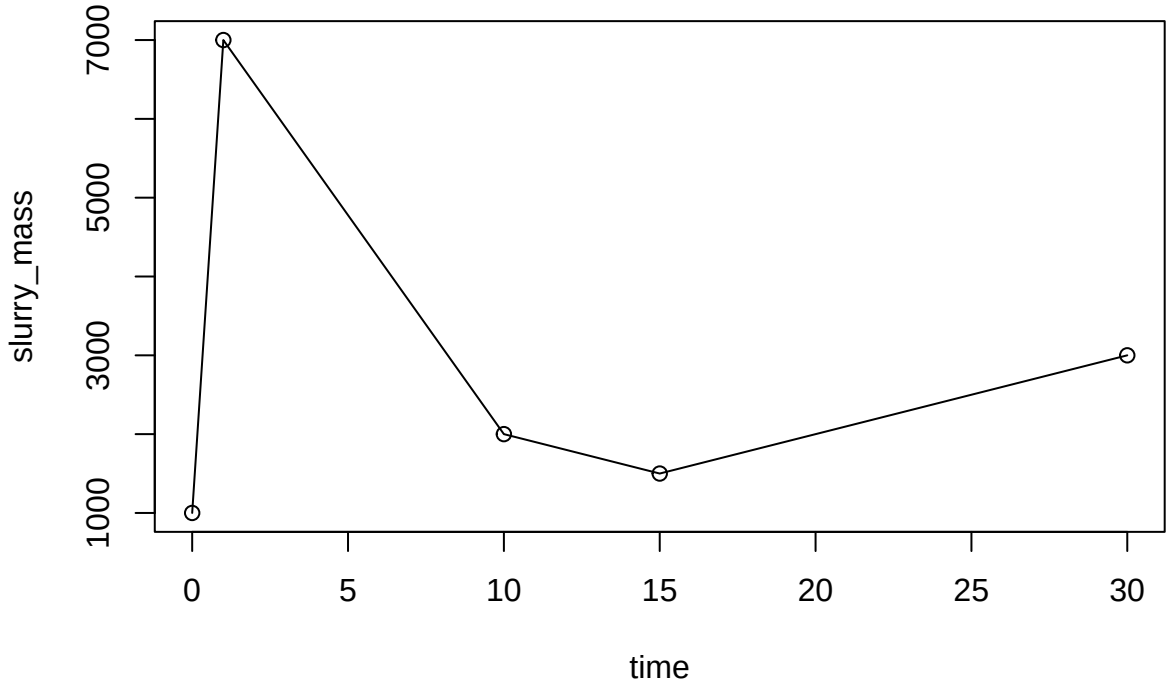
This flexibility comes from an approach similar to what we used for microbial groups.

3. Time-variable inputs part 1

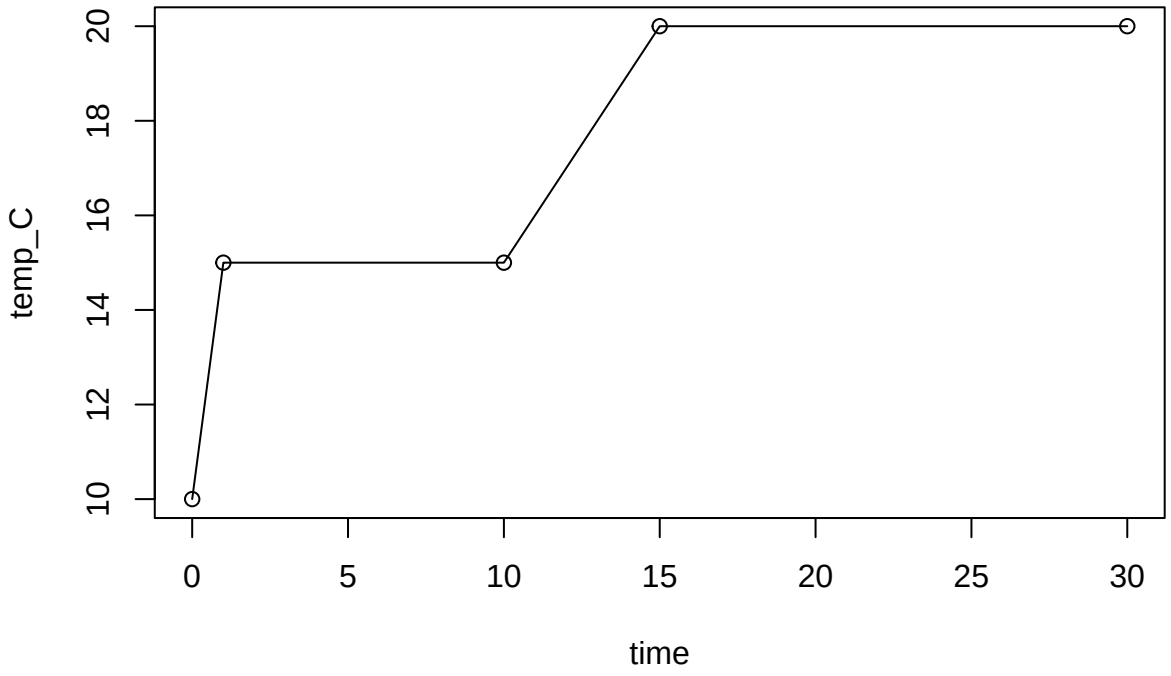
The `abm()` function can handle variability over time in any inputs now. Here slurry mass and temperature will vary.

```r
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')
```




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

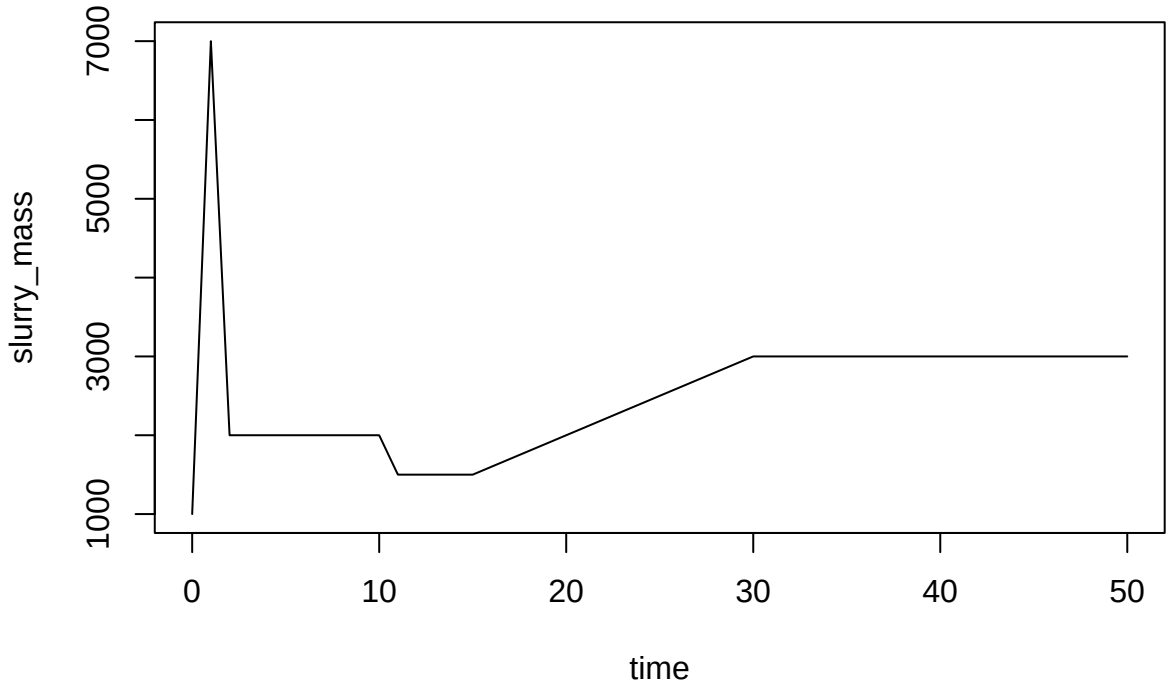


This data frame goes in the `var_pars` argument, which must be a list. The data frame must have a `slurry_mass` column if it is used–it is not possible to use an `abm_regular()`-like approach with variable temperature etc.

```
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'))
```

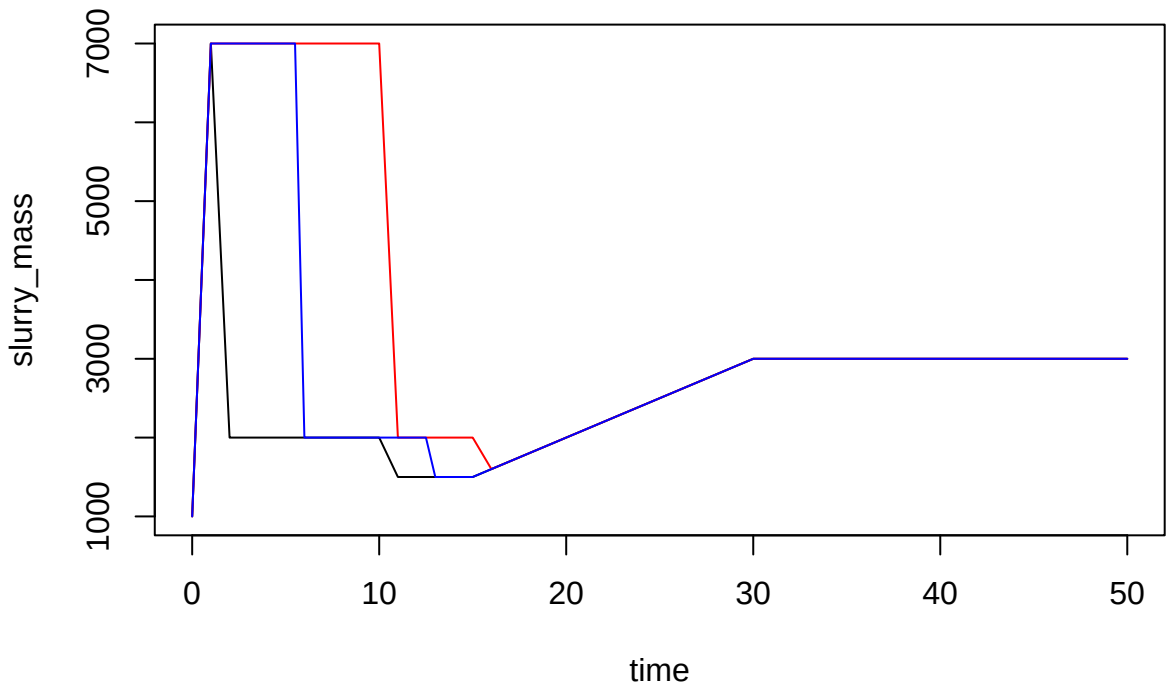
```
devtools::load_all()
```

```
## i Loading ABM
```

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

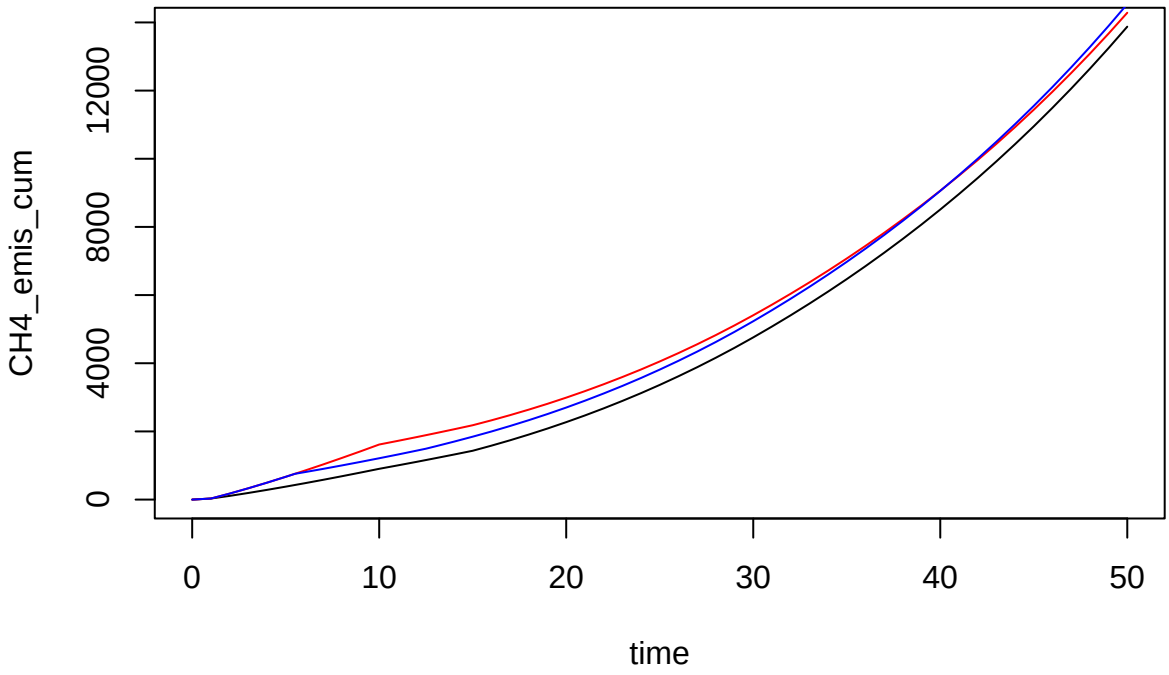
```
            mic_pars = mic_pars,
            sub_pars = sub_pars,
            chem_pars = chem_pars,
            var_pars = var_pars,
            add_pars = list(approx_method = 'mid'))
```

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



Here there is an effect of slurry mass and temperature.

```
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.

```
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
```

```
##   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        50
```

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

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

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

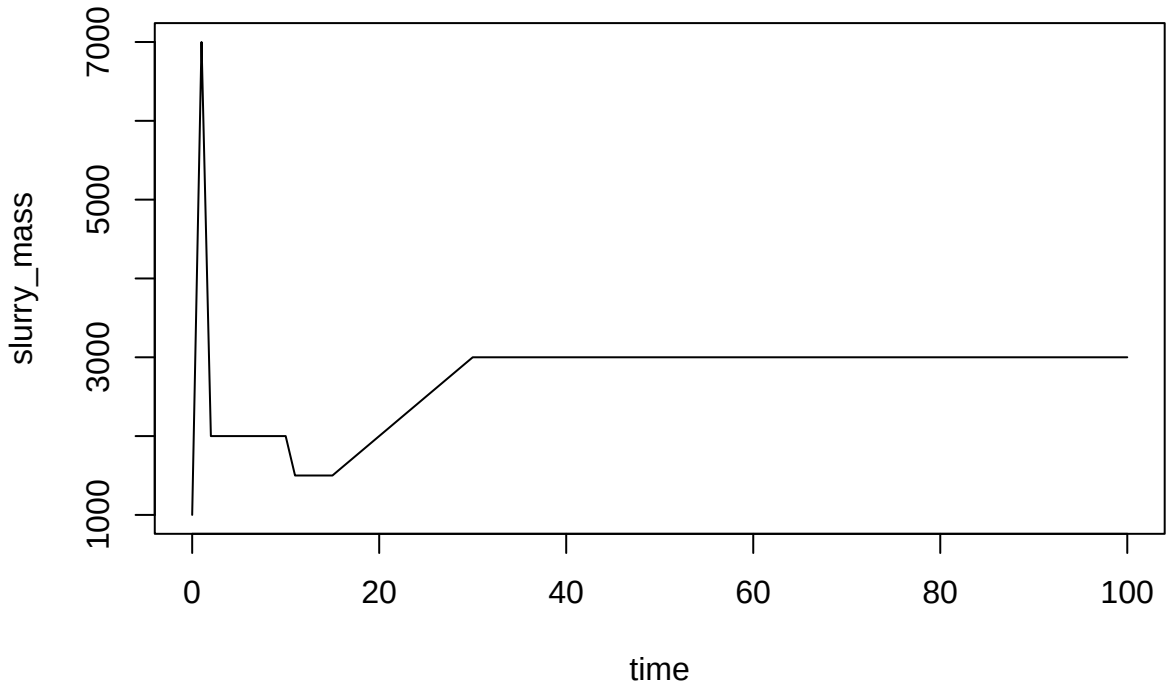
```
## [[1]]
## VSd
##   0
```

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

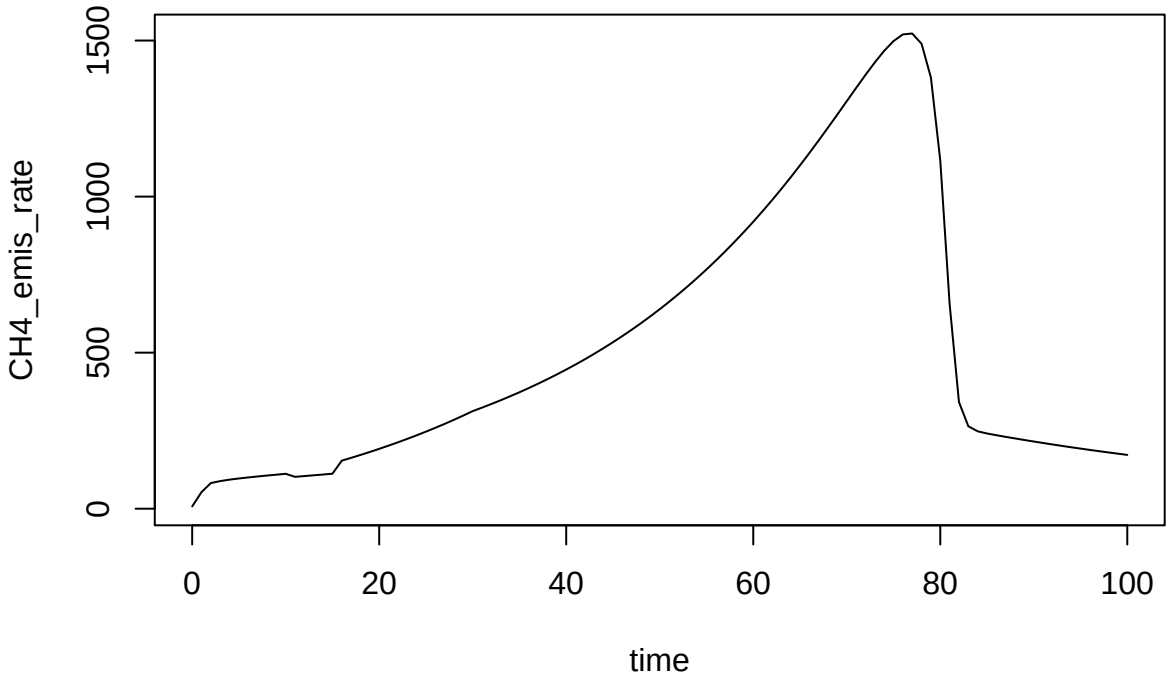
```
## i Loading ABM
```

```
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)
```

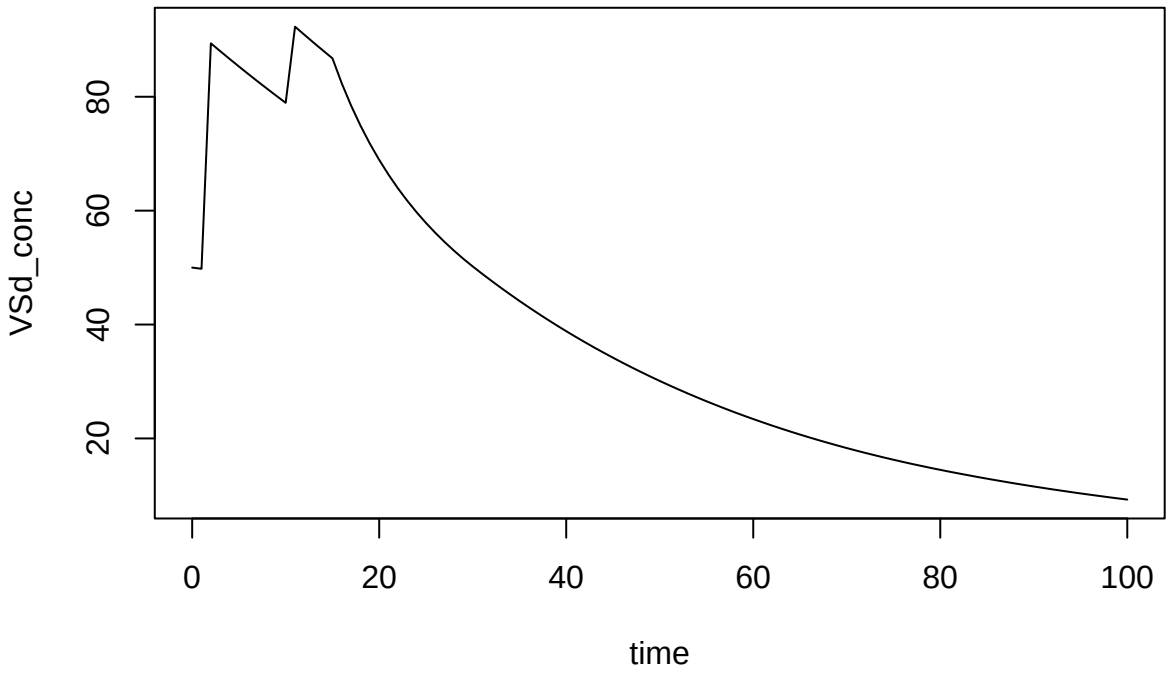
```
plot(slurry_mass ~ time, data = out4a, type = 'l')
```



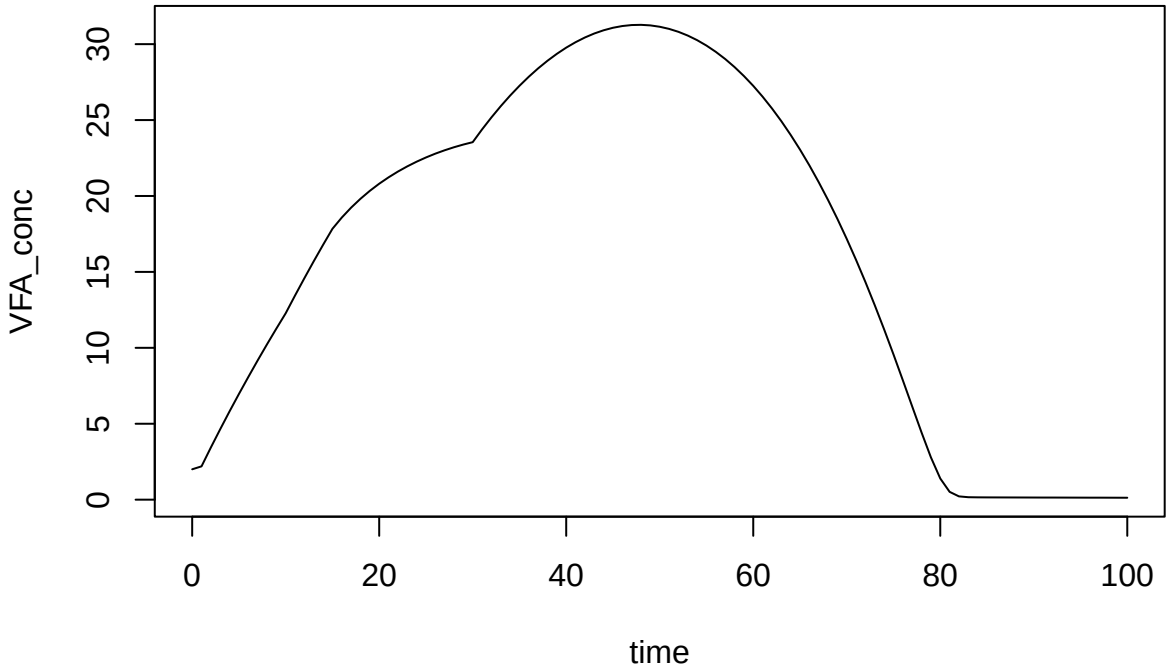

```
plot(CH4_emis_rate ~ time, data = out4a, type = 'l')
```




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




```
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))
```

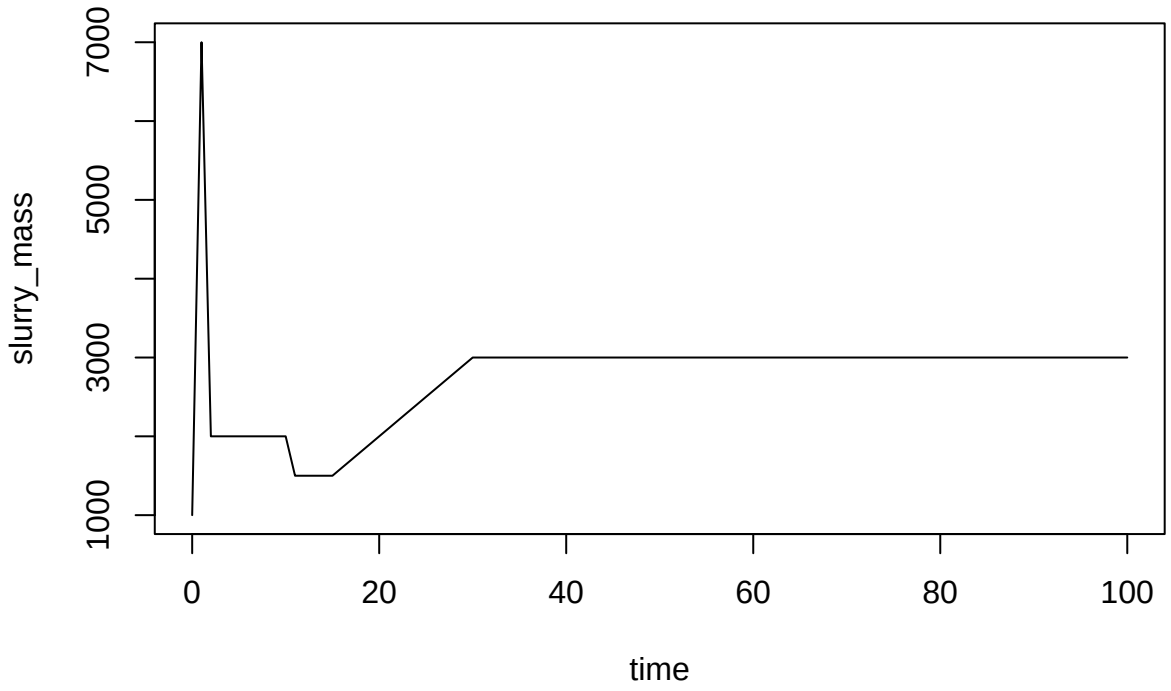
Some microbial parameters for a shift in temperature optima, "adaptation" for example.

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

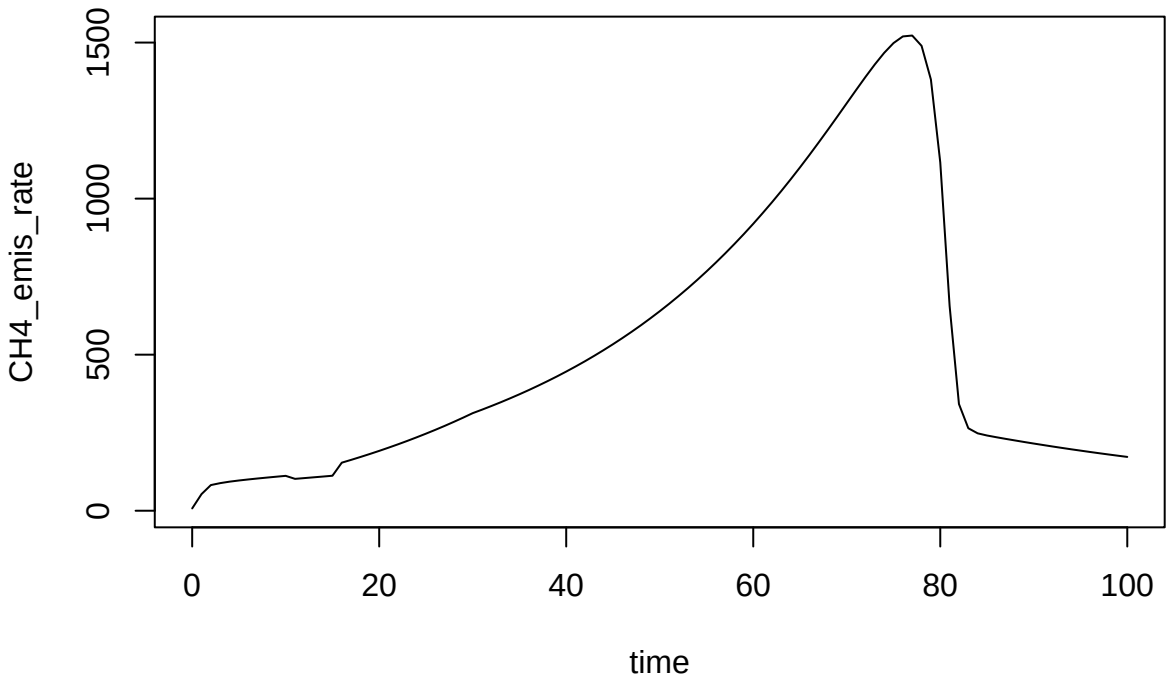
```
##   time slurry_mass  pH sub_fresh          T_opt
## 1    0        1000 7.0        50 20, 20, 30, 46
## 2    1        7000 6.9        50 22, 22, 32, 48
## 3   10        2000 6.8       100 24, 24, 34, 50
## 4   15        5000 6.7        50 26, 26, 36, 52
## 5   30        3000 6.6        50 28, 28,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

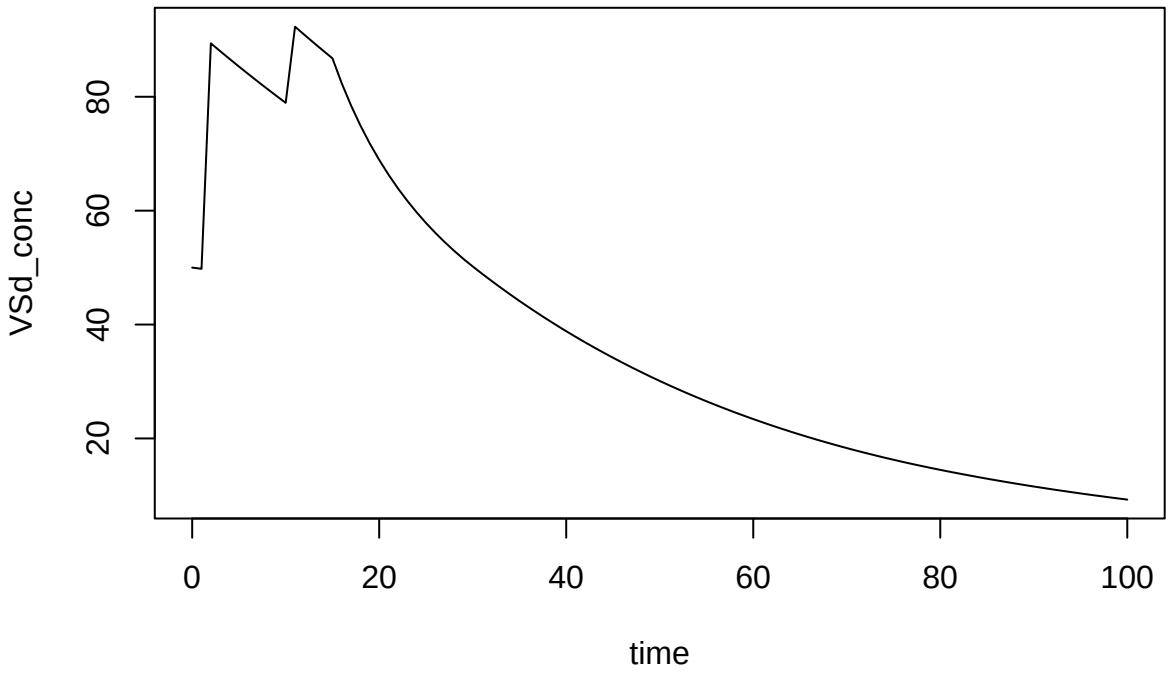
```
plot(slurry_mass ~ time, data = out4b, type = 'l')
```



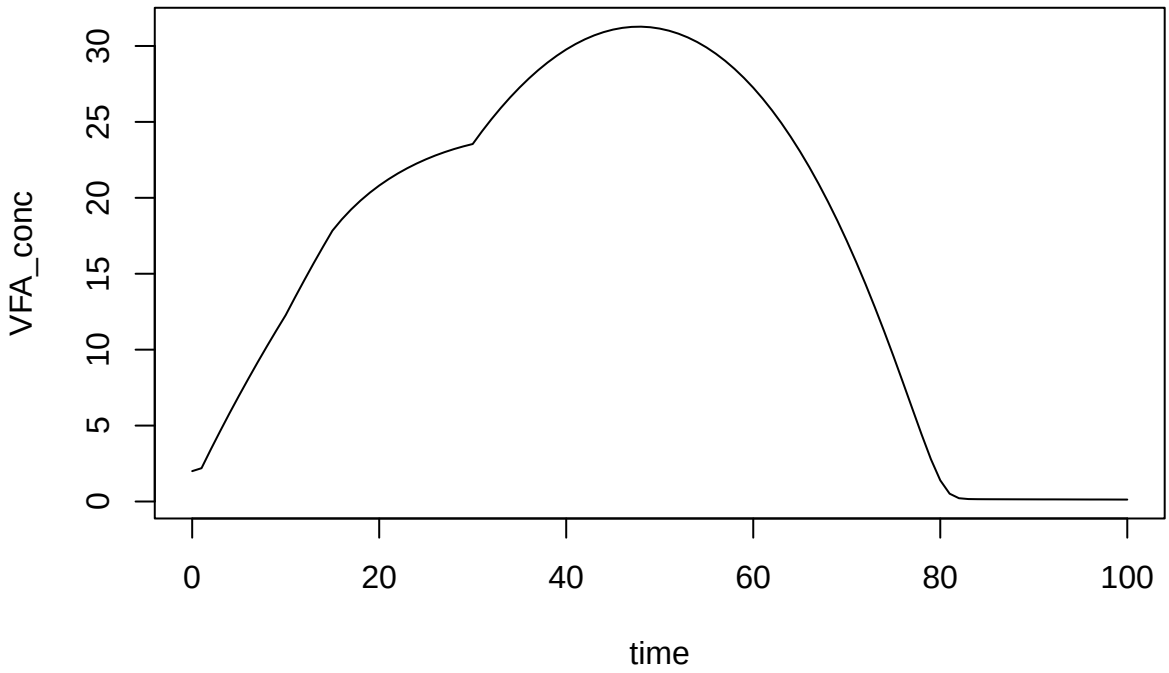
```
plot(CH4_emis_rate ~ time, data = out4b, type = 'l')
```




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




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



5. 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.

6. Inhibition

```
ilwr <- matrix(
  c(1, 0.1, 3, 0.1,
    1, 0.1, 3, 0.1,
    1, 0.1, 3, 0.01,
    4, 0.1, 3, 0.1),
  nrow = length(grps),
  byrow = TRUE,
  dimnames = list(
    c('m0', 'm1', 'm2', 'sr1'),
    c('NH4.', 'NH3', 'VFA', 'HVFA')
  )
)

iupr <- matrix(
  c(4, 0.5, 7, 0.3,
    4, 0.5, 7, 0.3,
    4, 0.5, 7, 0.03,
    8, 0.5, 9, 0.3),
  nrow = length(grps),
  byrow = TRUE,
  dimnames = list(
    c('m0', 'm1', 'm2', 'sr1'),
    c('NH4.', 'NH3', 'VFA', 'HVFA')
  )
)

inhib_pars <- list(
```

```
  ilwr = ilwr,
  iupr = iupr
)
```

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

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

```
## i Loading ABM
```

```
out5 <- 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,
            inhib_pars = inhib_pars,
            var_pars = var_pars
)
```