Calculation of fractional VOC losses from silage using 2012 model

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Overview

This document presents calculation of fraction VOC losses from silage fed to cattle based on the model described in Hafner et al. (2012). All calculations were carried out in R.

Initial steps

Load model from Hafner et al. (2012).

```
source('../model/FAConvDiffMod_v8.R')
```

Set constants. Diffusivity in clear air (m2/s) (`d.a`) and Henry's law constant (aq:g, g / m3 in aq phase per g / m3 gas phase). Henry's law constant parameters from NIST Chemistry Webbook (Sander, 2011).

```
d.a <- c(`Acetic acid` = 1.2E-5, Acetaldehyde = 1.3E-5, `Propyl acetate` = 1.3E-5, Ethanol = 1.2E-5)

k.h.p <- matrix(c(-12.6,  6300,
                  -17.31, 5920,
                  -17.6,  5700,
                  -15.78, 6248),
              ncol = 2, byrow = TRUE,
              dimnames = list(c('Acetic acid', 'Acetaldehyde', 'Propyl acetate', 'Ethanol'),
                              c('int', 'itemp')))
k.h.p
```

```
##                   int itemp
## Acetic acid    -12.60  6300
## Acetaldehyde   -17.31  5920
## Propyl acetate -17.60  5700
## Ethanol        -15.78  6248
```

1. Feedout loss

Assumptions:

- 15 cm removed every 12 hours
- Loss only from outer 15 cm
- Density was 232 kg/m3, based on Muck and Holmes (2000) Table 1 average (WI bunker silos)
- Dry matter 34%, from same source
- Gas-phase diffusion-dispersion coefficient `ksg` is 2E-5 m2/s from Hafner et al. (2012, Fig. 1)
- Temperature is set to the average of monthly averages for the contiguous US from 1991 through 2020
- Wind speed is lower than the climatological normal average of about 4 m/s, due to obstructions and resistance close to the ground, giving a surface mass transfer coefficient value of 0.01 m/s

Set silage properties and management. These follow assumptions listed above.

```
dm <- 0.34
rho.d <- 232
thk <- 0.15
t.outs <- 12 * 3600
```

Transport properties.

```
k.sg <- 2E-5
h.m <- 0.01
```

Weather

```
temp.c
```

```
## [1] 11.8212
```

```
temp.k <- temp.c + 273.15
```

```
k.h <- exp(k.h.p[, 'int'] + k.h.p[, 'itemp']/temp.k)
k.h
```

```
##    Acetic acid   Acetaldehyde Propyl acetate        Ethanol
##    13460.25962       31.94542       11.04548      466.39006
```

```
floss <- data.frame(rep = c('Acetic acid', 'Acetaldehyde', 'Propyl acetate', 'Ethanol'),
                    group = c('Acid', 'Aldehyde', 'Ester', 'Alcohol'),
                    store = NA, mix = NA, feed = NA, total = NA)
```

Acetic acid loss

```
stage <- 'store'
rep <- 'Acetic acid'
out <- facd.mod(c.d = 1, d.a = d.a[rep], dm = dm, e.d=100, h.m = h.m, k.h = k.h[rep],
                l = thk, k.sg = k.sg, temp.c = temp.c, t.outs = t.outs, rho.d = rho.d)
out$ts
```

```
##                 t       j.surf     emis     f.lost  c.b.v.s
## Acetic acid 43200 6.073741e-05 3.545084 0.01018702 860.9552
```

```
floss[floss$rep == rep, stage] <- out$ts$f.lost
```

Predicted loss: 1%.

Ethanol loss

```
rep <- 'Ethanol'
out <- facd.mod(c.d = 1, d.a = d.a[rep], dm = dm, e.d=100, h.m = h.m, k.h = k.h[rep],
                l = thk, k.sg = k.sg, temp.c = temp.c, t.outs = t.outs, rho.d = rho.d)
out$ts
```

```
##             t       j.surf     emis     f.lost  c.b.v.s
## Ethanol 43200 0.0003974237 30.46997 0.08755739 195.2129
```

```
floss[floss$rep == rep, stage] <- out$ts$f.lost
```

Predicted loss: 8.8%.

Propyl acetate

```
rep <- 'Propyl acetate'
out <- facd.mod(c.d = 1, d.a = d.a[rep], dm = dm, e.d=100, h.m = h.m, k.h = k.h[rep],
                l = thk, k.sg = k.sg, temp.c = temp.c, t.outs = t.outs, rho.d = rho.d)
out$ts
```

```
##                    t      j.surf     emis    f.lost c.b.v.s
## Propyl acetate 43200 0.002375863 218.3688 0.6274965 27.7321
```

```
floss[floss$rep == rep, stage] <- out$ts$f.lost
```

Predicted loss: 62.7%.

Acetaldehyde

```
rep <- 'Acetaldehyde'
out <- facd.mod(c.d = 1, d.a = d.a[rep], dm = dm, e.d=100, h.m = h.m, k.h = k.h[rep],
                l = thk, k.sg = k.sg, temp.c = temp.c, t.outs = t.outs, rho.d = rho.d)
out$ts
```

```
##                  t      j.surf     emis    f.lost  c.b.v.s
## Acetaldehyde 43200 0.001532993 128.0485 0.3679554 51.63453
```

```
floss[floss$rep == rep, stage] <- out$ts$f.lost
```

Predicted loss: 36.8%.

2. Feeding loss

Assumptions:

- Average of 20 cm silage in feed lanes for 6 hours
- Density is 75 kg/m3, based roughly on Hafner et al. (2012)
- Dry matter 34%, from Muck and Holmes 2000 Table 1
- Gas-phase diffusion-dispersion coefficient `ksg` is 3.3E-5 m2/s from Hafner et al. (2012, median best-fit value listed on p 139, right side)
- Temperature same as with feedout above
- Surface mass transfer coefficient value of 0.01 m/s from Hafner et al. (2012)

The first assumption has substantial uncertainty, since depth and exposure time depend on feed frequency and consumption rate, and depth varies over time.

Silage properties and management, based on above assumptions.

```
dm <- 0.34
rho.d <- 75
thk <- 0.15
t.outs <- 6 * 3600
```

Transport properties

```
k.sg <- 3.3E-5
h.m <- 0.01
```

Acetic acid loss

```r
stage <- 'feed'
rep <- 'Acetic acid'
out <- facd.mod(c.d = 1, d.a = d.a[rep], dm = dm, e.d=100, h.m = h.m, k.h = k.h[rep],
                l = thk, k.sg = k.sg, temp.c = temp.c, t.outs = t.outs, rho.d = rho.d)
out$ts
```

```
##                   t       j.surf     emis     f.lost  c.b.v.s
## Acetic acid 21600 6.212896e-05 1.802342 0.01602081 284.7069
```

```r
floss[floss$rep == rep, stage] <- out$ts$f.lost
```

Predicted loss: 1.6%.

Ethanol loss

```r
rep <- 'Ethanol'
out <- facd.mod(c.d = 1, d.a = d.a[rep], dm = dm, e.d=100, h.m = h.m, k.h = k.h[rep],
                l = thk, k.sg = k.sg, temp.c = temp.c, t.outs = t.outs, rho.d = rho.d)
out$ts
```

```
##             t       j.surf     emis    f.lost  c.b.v.s
## Ethanol 21600 0.0004101008 15.66651 0.1392579 65.14838
```

```r
floss[floss$rep == rep, stage] <- out$ts$f.lost
```

Predicted loss: 13.9%.

Propyl acetate

```r
rep <- 'Propyl acetate'
out <- facd.mod(c.d = 1, d.a = d.a[rep], dm = dm, e.d=100, h.m = h.m, k.h = k.h[rep],
                l = thk, k.sg = k.sg, temp.c = temp.c, t.outs = t.outs, rho.d = rho.d)
out$ts
```

```
##                    t      j.surf     emis    f.lost  c.b.v.s
## Propyl acetate 21600 0.001196595 99.23447 0.8820842 4.596228
```

```r
floss[floss$rep == rep, stage] <- out$ts$f.lost
```

Predicted loss: 88.2%.

Acetaldehyde

```r
rep <- 'Acetaldehyde'
out <- facd.mod(c.d = 1, d.a = d.a[rep], dm = dm, e.d=100, h.m = h.m, k.h = k.h[rep],
                l = thk, k.sg = k.sg, temp.c = temp.c, t.outs = t.outs, rho.d = rho.d)
out$ts
```

```
##                  t      j.surf     emis   f.lost  c.b.v.s
## Acetaldehyde 21600 0.001493056 65.46206 0.581885 16.35838
```

```r
floss[floss$rep == rep, stage] <- out$ts$f.lost
```

Predicted loss: 58.2%.

Mixing losses

Set to 10% of feed losses

```r
floss$mix <- floss$feed / 10
```

Total losses

```r
floss$total <- 1 - (1 - floss$store) * (1 - floss$mix) * (1 - floss$feed)
```

Summary of fractional loss values

```r
floss
```

```
##               rep    group      store         mix       feed      total
## 1    Acetic acid     Acid 0.01018702 0.001602081 0.01602081 0.02760499
## 2   Acetaldehyde Aldehyde 0.36795543 0.058188499 0.58188499 0.75110999
## 3 Propyl acetate    Ester 0.62749651 0.088208419 0.88208419 0.95995042
## 4        Ethanol  Alcohol 0.08755739 0.013925788 0.13925788 0.22555922
```