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(AceticAcid = 1.2E-5, Acetaldehyde = 1.3E-5, PropylAcetate = 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('AceticAcid', 'Acetaldehyde', 'PropylAcetate', 'Ethanol'),
                                c('int', 'itemp')))
k.h.p
```

```
##                   int itemp
## AceticAcid    -12.60  6300
## Acetaldehyde  -17.31  5920
## PropylAcetate -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 was 20 degrees C, close to the 1971-2000 climatological normal average presented in Table 1 in Montes et al. 2010 (packed silage)

- 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 <- 20
temp.k <- temp.c + 273.15
```

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

```
##    AceticAcid  Acetaldehyde PropylAcetate       Ethanol
##   7264.134365     17.893539      6.321589    252.982629
```

Acetic acid loss

```
cmpd <- 'AceticAcid'
out <- facd.mod(c.d = 1, d.a = d.a[cmpd], dm = dm, e.d=100, h.m = h.m, k.h = k.h[cmpd],
                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
## AceticAcid 43200 8.776241e-05 5.415568 0.01556198 690.6423
```

Predicted loss: 1.6%.

Ethanol loss

```
cmpd <- 'Ethanol'
out <- facd.mod(c.d = 1, d.a = d.a[cmpd], dm = dm, e.d=100, h.m = h.m, k.h = k.h[cmpd],
                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 0.0005345844 42.13073 0.1210653 146.531
```

Predicted loss: 12.1%.

Propyl acetate

```
cmpd <- 'PropylAcetate'
out <- facd.mod(c.d = 1, d.a = d.a[cmpd], dm = dm, e.d=100, h.m = h.m, k.h = k.h[cmpd],
                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
## PropylAcetate 43200 0.002320986 273.1455 0.7849009 15.98861
```

Predicted loss: 78.5%.

Acetaldehyde

```
cmpd <- 'Acetaldehyde'
out <- facd.mod(c.d = 1, d.a = d.a[cmpd], dm = dm, e.d=100, h.m = h.m, k.h = k.h[cmpd],
                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 0.001997303 169.8795 0.4881594 38.7974
```

Predicted loss: 48.8%.

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)

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

```
cmpd <- 'AceticAcid'
out <- facd.mod(c.d = 1, d.a = d.a[cmpd], dm = dm, e.d=100, h.m = h.m, k.h = k.h[cmpd],
                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
## AceticAcid 21600 9.001991e-05 2.760419 0.02453706 229.0172
```

Predicted loss: 2.5%.

Ethanol loss

```
cmpd <- 'Ethanol'
out <- facd.mod(c.d = 1, d.a = d.a[cmpd], dm = dm, e.d=100, h.m = h.m, k.h = k.h[cmpd],
                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 0.0005517134 21.67991 0.1927103 48.92509
```

Predicted loss: 19.3%.

Propyl acetate

```
cmpd <- 'PropylAcetate'
out <- facd.mod(c.d = 1, d.a = d.a[cmpd], dm = dm, e.d=100, h.m = h.m, k.h = k.h[cmpd],
                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
## PropylAcetate 21600 0.0005387787 108.9318 0.9682829 1.236297
```

Predicted loss: 96.8%.

Acetaldehyde

```
cmpd <- 'Acetaldehyde'
out <- facd.mod(c.d = 1, d.a = d.a[cmpd], dm = dm, e.d=100, h.m = h.m, k.h = k.h[cmpd],
                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 0.001562991 83.86904 0.7455025 9.920727
```

Predicted loss: 74.6%.