Prevision of comparisons with the ALFAM2 model

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Overview

The point of this document is to look at precision of the ALFAM2 model when comparing emission between two similar conditions.

1. Prep

```
library(ALFAM2)
library(data.table)
library(ggplot2)
packageVersion('ALFAM2')
```

```
## [1] '4.2.8'
```

Read input data.

```
dat <- fread('input.csv')
```

Add other variables.

```
dat[, `:=` (app.rate.ni = 25, man.dm = 4.5, man.ph = 7.2)]
dat[, rain.rate := precipitation_mm / 1]
dat[, air.temp := temperature_celsius]
dat[, wind.2m := windspeed_m_s]
dat[, wind.sqrt := sqrt(windspeed_m_s)]
```

Get two subsets, with application starting at 12:00 and 20:00 on the same day, with emission predicted over 48 hours.

```
d1 <- dat[7:(7 + 48), ]
d2 <- dat[15:(15 + 48), ]
```

Get time in hours.

```
d1[, ct := as.numeric(difftime(time, min(time), units = 'hours'))]
d2[, ct := as.numeric(difftime(time, min(time), units = 'hours'))]
```

Take a look at the tops.

```
head(d1[, .(time, ct, app.rate.ni, man.dm, man.ph, air.temp, wind.2m)])
```

```
##                   time    ct app.rate.ni man.dm man.ph air.temp  wind.2m
##                 <POSc> <num>       <num>  <num>  <num>    <num>    <num>
## 1: 2025-05-15 12:00:00     0          25    4.5    7.2 18.75641 2.511143
## 2: 2025-05-15 13:00:00     1          25    4.5    7.2 19.38350 2.757864
## 3: 2025-05-15 14:00:00     2           25    4.5    7.2 19.68736 3.198003
## 4: 2025-05-15 15:00:00     3           25    4.5    7.2 19.54932 3.449661
## 5: 2025-05-15 16:00:00     4           25    4.5    7.2 18.98815 3.441642
## 6: 2025-05-15 17:00:00     5           25    4.5    7.2 18.01563 3.444468
```

```
head(d2[, .(time, ct, app.rate.ni, man.dm, man.ph, air.temp, wind.2m)])
```

```
##                    time    ct app.rate.ni man.dm man.ph  air.temp  wind.2m
##                  <POSc> <num>       <num>  <num>  <num>     <num>    <num>
## 1: 2025-05-15 20:00:00     0           25    4.5    7.2 13.969246 3.354596
## 2: 2025-05-15 21:00:00     1           25    4.5    7.2 12.419703 3.457194
## 3: 2025-05-15 22:00:00     2           25    4.5    7.2 11.261217 3.697640
## 4: 2025-05-15 23:00:00     3           25    4.5    7.2 10.345874 3.697640
## 5: 2025-05-16 00:00:00     4           25    4.5    7.2  9.420493 3.717327
## 6: 2025-05-16 01:00:00     5           25    4.5    7.2  8.428627 3.683218
```

Note that these inputs are different from the values shown in the screenshot in the original email message with the question!

Combine into one.

```
d1[, apptime := 'T12']
d2[, apptime := 'T20']

din <- rbind(d1, d2)
```

2. Compare parameter sets 2 and 3

Run ALFAM2 model with parameter sets 2 and 3, combine those results, and get the final values for a comparison.

```
pred2 <- alfam2(din, pars = alfam2pars02, group = 'apptime')
```

```
## Warning in alfam2(din, pars = alfam2pars02, group = "apptime"): Argument app.name is missing or dat
##     So function will return relative emission only.

## User-supplied parameters are being used.

## Warning in prepDat(dat, warn = warn): Argument prep.dum = TRUE but there are no variables to convert
##   Ignoring prep.dum = TRUE.

## Warning in alfam2(din, pars = alfam2pars02, group = "apptime"): Incorporation columns  were dropped
##     because argument time.incorp is NULL
##     So there is no incorporation.
##     Set check = FALSE to not drop, but then check output.

## Warning in alfam2(din, pars = alfam2pars02, group = "apptime"): Running with 12 parameters. Dropped
## These secondary parameters have been dropped:
##   app.mthd.os.f0
##   man.source.pig.f0
##   app.mthd.cs.f0
##   app.mthd.bc.r1
##   app.mthd.ts.r1
##   ts.cereal.hght.r1
##   app.mthd.bc.r3
##   app.mthd.cs.r3
##   incorp.shallow.f4
##   incorp.shallow.r3
##   incorp.deep.f4
##   incorp.deep.r3
```

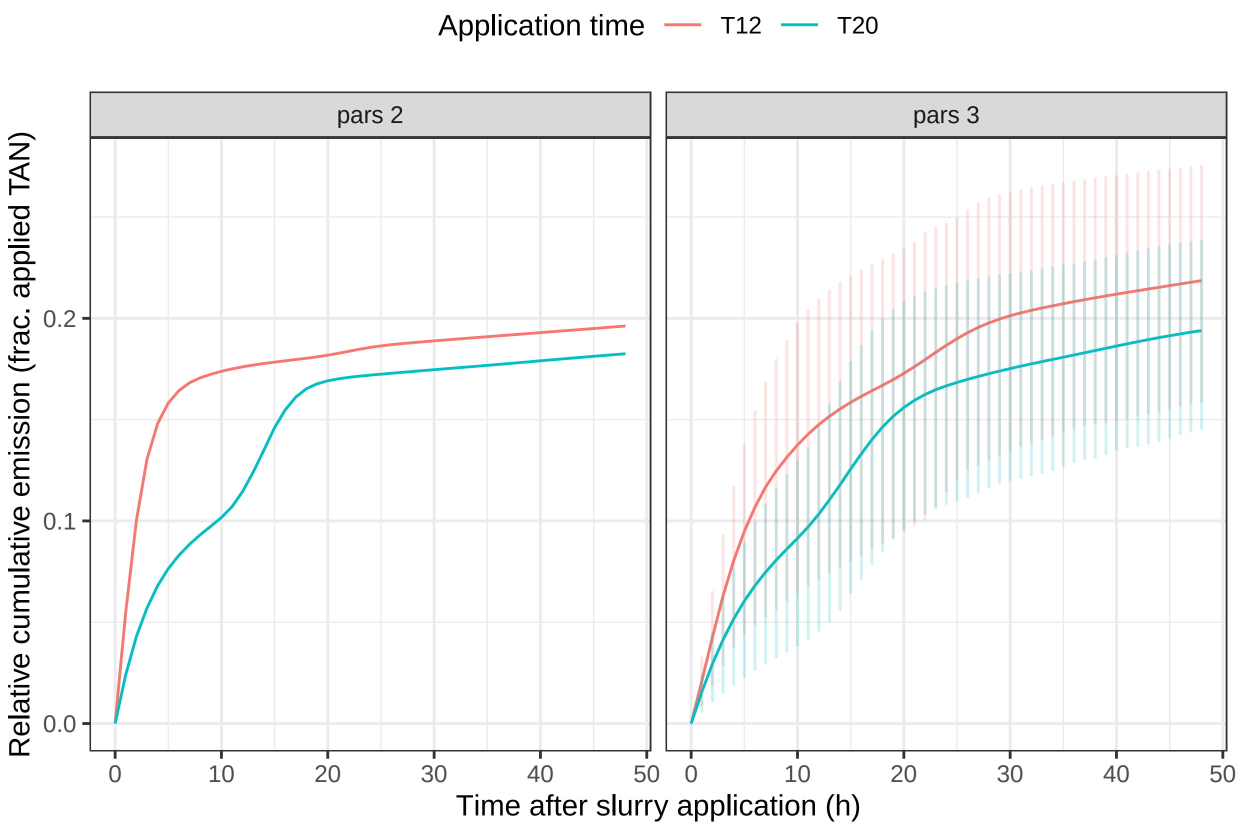
```
pred3 <- alfam2(din, pars = alfam2pars03, group = 'apptime', conf.int = 0.9)
```

```
## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Argument app.na
##     So function will return relative emission only.

## Default parameters (Set 3) are being used.

## Warning in prepDat(dat, warn = warn): Argument prep.dum = TRUE but there are no variables to convert
##   Ignoring prep.dum = TRUE.

## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Incorporation
##     because argument time.incorp is NULL
##     So there is no incorporation.
##     Set check = FALSE to not drop, but then check output.

## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Running with 1
## These secondary parameters have been dropped:
##   app.mthd.os.f0
##   app.mthd.cs.f0
##   man.source.pig.f0
##   app.mthd.bc.r1
##   app.mthd.ts.r1
##   app.mthd.cs.r3
##   incorp.deep.r3
##   incorp.shallow.f4
##   incorp.deep.f4
```

```
setDT(pred2)
setDT(pred3)

pred2[, parset := 'pars 2']
pred3[, parset := 'pars 3']

preds <- rbind(pred2, pred3, fill = TRUE)

pend <- preds[ct == 48, ]
pend <- dcast(pend, parset ~ apptime, value.var = 'er')
pend[, ediff := 100 * (T12 - T20)]
```

Here are the results. First cumulative emission over time.

```
ggplot(preds, aes(ct, er, colour = apptime)) +
  geom_line() +
  geom_errorbar(aes(ymin = er.lwr, ymax = er.upr, width = 0), alpha = 0.2) +
  facet_wrap(~ parset) +
  theme_bw() +
  theme(legend.position = 'top') +
  labs(x = 'Time after slurry application (h)',
       y = 'Relative cumulative emission (frac. applied TAN)',
       colour = 'Application time')
```



Error bars are 90% confidence intervals.

Difference between 12:00 and 20:00 as percentage of applied TAN.

```
print(pend)
```

```
## Key: <parset>
##    parset       T12       T20    ediff
##    <char>     <num>     <num>    <num>
## 1: pars 2 0.1962045 0.1825097 1.369486
## 2: pars 3 0.2186139 0.1939791 2.463477
```

3. Confidence interval on comparison with parameter set 3

Run ALFAM2 model, returning all 100 sets of results (100 “plausible parameter sets”, see paper), and get final times.

```
pred3c <- alfam2(din, pars = alfam2pars03, group = 'apptime', conf.int = 'all')
```

```
## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Argument app.na
##     So function will return relative emission only.

## Default parameters (Set 3) are being used.

## Warning in prepDat(dat, warn = warn): Argument prep.dum = TRUE but there are no variables to convert
##   Ignoring prep.dum = TRUE.

## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Incorporation
##     because argument time.incorp is NULL
##     So there is no incorporation.
##     Set check = FALSE to not drop, but then check output.
## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Running with 1
## These secondary parameters have been dropped:
##   app.mthd.os.f0
##   app.mthd.cs.f0
##   man.source.pig.f0
##   app.mthd.bc.r1
##   app.mthd.ts.r1
##   app.mthd.cs.r3
##   incorp.deep.r3
##   incorp.shallow.f4
##   incorp.deep.f4
```

```
setDT(pred3c)
pend3c <- pred3c[ct == 48, ]
```

Reshape and get difference for each parameter set, and then confidence interval from quantiles.

```
pw <- dcast(pend3c, par.id ~ apptime, value.var = 'er')
pw[, dd := T12 - T20]
print(100 * quantile(pw$dd, c(0.05, 0.5, 0.95)))
```

```
##       5%      50%      95%
## 1.312387 2.245726 3.548143
```

So 90% CI is [1.3, 3.5] % of applied TAN. This is relatively high precision in my opinion. In includes the uncertainty in parameter values that come from variability in measurements among institutions. It might seem strange that we have high confidence in a positive difference here in the comparison (higher emission at 12:00 than 20:00) when the error bars in the plot above overlap quite a bit. The explanation is that we have more confidence in relative effects than in absolute emission, probably mainly due to the nature of the measurement data.

4. Comparison to average approach

Calculate difference based on average inputs.

```
datave <- data.table(apptime = c('T12', 'T20'), ct = 48, app.rate.ni = 25, man.dm = 4.5, man.ph = 7.2,
                     wind.sqrt = sqrt(c(3.23, 3.11)), air.temp = c(12.07, 11.65))
```

```
pred2ave <- alfam2(datave, pars = alfam2pars02, group = 'apptime')
```

```
## Warning in alfam2(datave, pars = alfam2pars02, group = "apptime"): Argument app.name is missing or d
##     So function will return relative emission only.
```

```
## User-supplied parameters are being used.
```

```
## Warning in prepDat(dat, warn = warn): Argument prep.dum = TRUE but there are no variables to convert
##   Ignoring prep.dum = TRUE.
```

```
## Warning in alfam2(datave, pars = alfam2pars02, group = "apptime"): Incorporation columns  were dropp
##     because argument time.incorp is NULL
##     So there is no incorporation.
##     Set check = FALSE to not drop, but then check output.
```

```
## Warning in alfam2(datave, pars = alfam2pars02, group = "apptime"): Running with 10 parameters. Dropp
## These secondary parameters have been dropped:
##   app.mthd.os.f0
##   man.source.pig.f0
##   app.mthd.cs.f0
##   app.mthd.bc.r1
##   wind.2m.r1
##   app.mthd.ts.r1
##   ts.cereal.hght.r1
##   rain.rate.r2
##   app.mthd.bc.r3
##   app.mthd.cs.r3
##   incorp.shallow.f4
##   incorp.shallow.r3
##   incorp.deep.f4
##   incorp.deep.r3
```

```
pred3ave <- alfam2(datave, pars = alfam2pars03, group = 'apptime', conf.int = 0.9)
```

```
## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Argument app.na
##     So function will return relative emission only.

## Default parameters (Set 3) are being used.

## Warning in prepDat(dat, warn = warn): Argument prep.dum = TRUE but there are no variables to convert
##   Ignoring prep.dum = TRUE.

## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Incorporation
##     because argument time.incorp is NULL
##     So there is no incorporation.
##     Set check = FALSE to not drop, but then check output.

## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Running with 1
## These secondary parameters have been dropped:
##   app.mthd.os.f0
##   app.mthd.cs.f0
##   man.source.pig.f0
##   app.mthd.bc.r1
##   app.mthd.ts.r1
##   rain.rate.r2
##   app.mthd.cs.r3
##   incorp.deep.r3
##   incorp.shallow.f4
##   incorp.deep.f4
##   rain.rate.r5
```

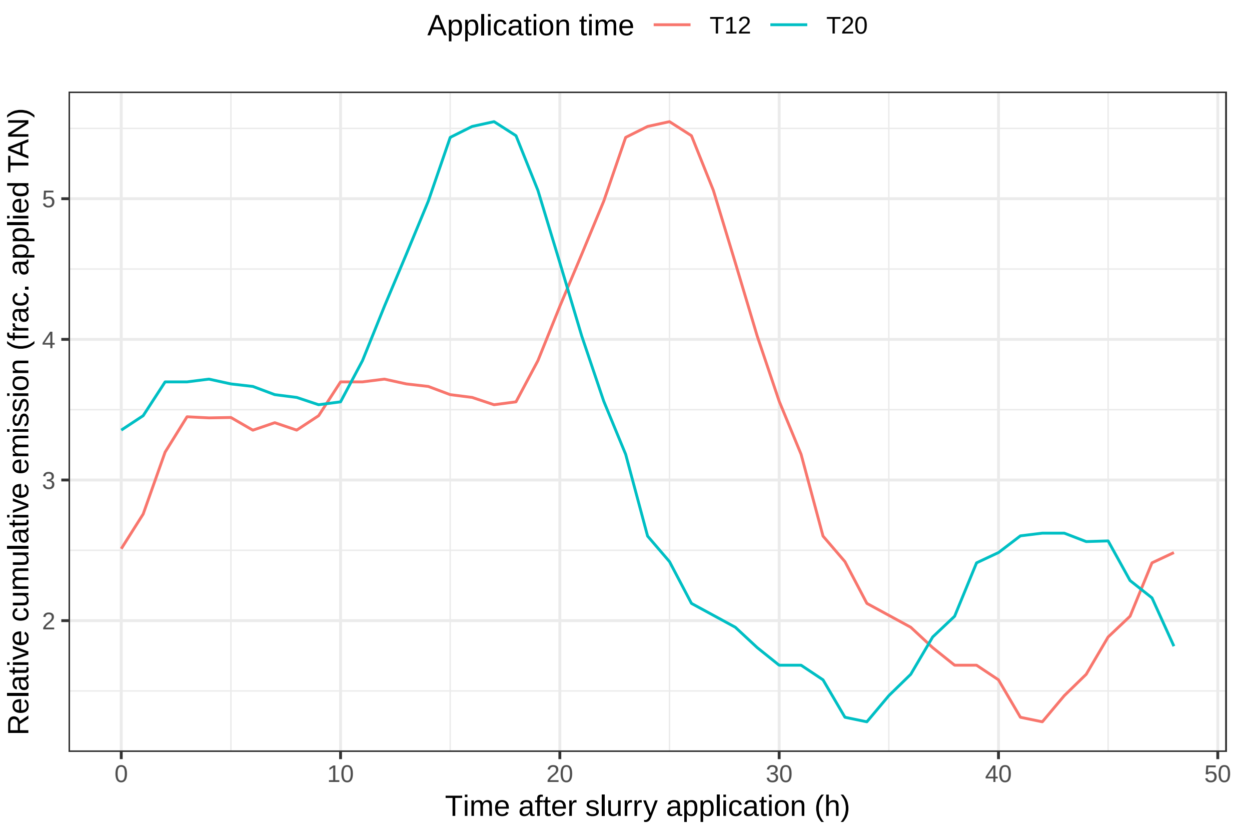
```
setDT(pred2ave)
setDT(pred3ave)

pred2ave[, parset := 'pars 2']
pred3ave[, parset := 'pars 3']

preds <- rbind(pred2ave, pred3ave, fill = TRUE)

pave <- dcast(preds, parset ~ apptime, value.var = 'er')
pave[, ediff := 100 * (T12 - T20)]
pave
```

```
## Key: <parset>
##    parset       T12       T20     ediff
##    <char>     <num>     <num>     <num>
## 1: pars 2 0.1789281 0.1771386 0.1789439
## 2: pars 3 0.1871136 0.1810322 0.6081352
```

Why is the difference so much smaller when based on average inputs? The answer is that the difference in total emission with the hourly data is mainly due to what happens in the first 12 hours or so. That is according to the ALFAM2 model. But the CI in the previous section should give some confidence that this interpretation is meaningful.

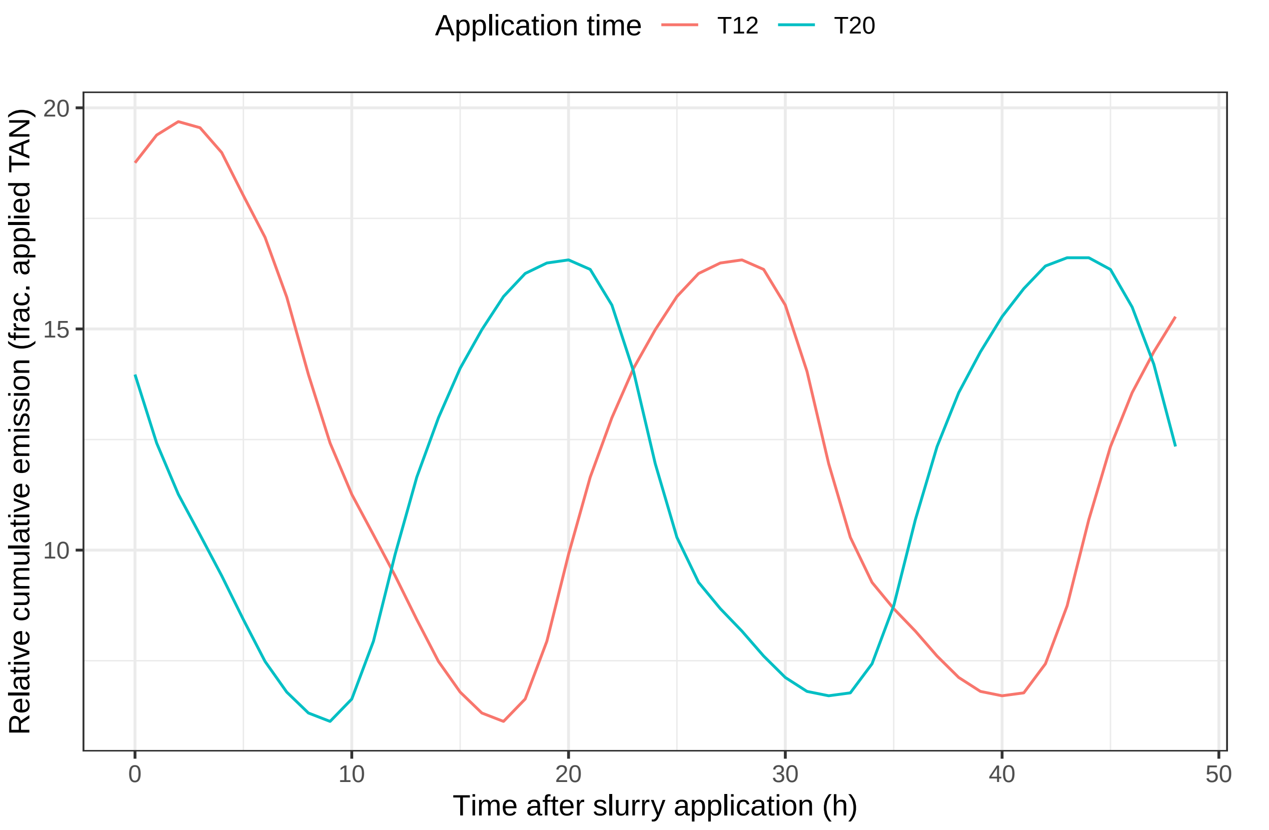
Wind speed actually starts higher for application at 20:00.

```
ggplot(din, aes(ct, wind.2m, colour = apptime)) +
  geom_line() +
  theme_bw() +
  theme(legend.position = 'top') +
  labs(x = 'Time after slurry application (h)',
       y = 'Relative cumulative emission (frac. applied TAN)',
       colour = 'Application time')
```



But air temperature is lower for around 12 hours.

```
ggplot(din, aes(ct, air.temp, colour = apptime)) +
  geom_line() +
  theme_bw() +
  theme(legend.position = 'top') +
  labs(x = 'Time after slurry application (h)',
       y = 'Relative cumulative emission (frac. applied TAN)',
       colour = 'Application time')
```



We can take a closer look at model parameters and pools to understand the effects of these differences. Here we'll get confidence intervals for some outputs of interest. Only parameter set 3 is used here.

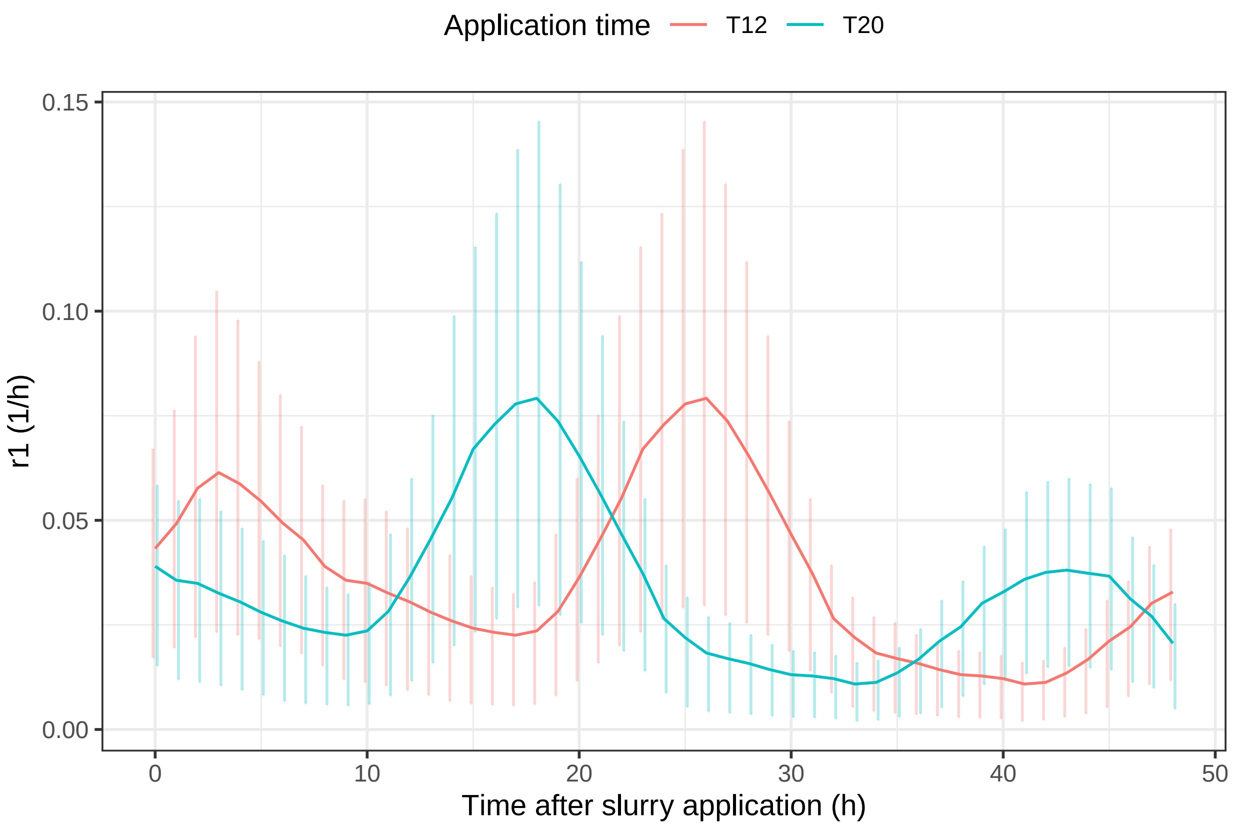
```
pred3p <- alfam2(din, pars = alfam2pars03, group = 'apptime',
                 conf.int = 0.9, var.ci = c('f', 's', 'er', 'r1', 'r2'))
```

```
## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Argument app.na
##     So function will return relative emission only.

## Default parameters (Set 3) are being used.

## Warning in prepDat(dat, warn = warn): Argument prep.dum = TRUE but there are no variables to convert
##   Ignoring prep.dum = TRUE.

## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Incorporation 
##     because argument time.incorp is NULL
##     So there is no incorporation.
##     Set check = FALSE to not drop, but then check output.

## Warning in alfam2(dat = dat, pars = pars, add.pars = add.pars, app.name = app.name, : Running with 1
## These secondary parameters have been dropped:
##   app.mthd.os.f0
##   app.mthd.cs.f0
##   man.source.pig.f0
##   app.mthd.bc.r1
##   app.mthd.ts.r1
##   app.mthd.cs.r3
##   incorp.deep.r3
##   incorp.shallow.f4
##   incorp.deep.f4
```

```r
setDT(pred3p)
```

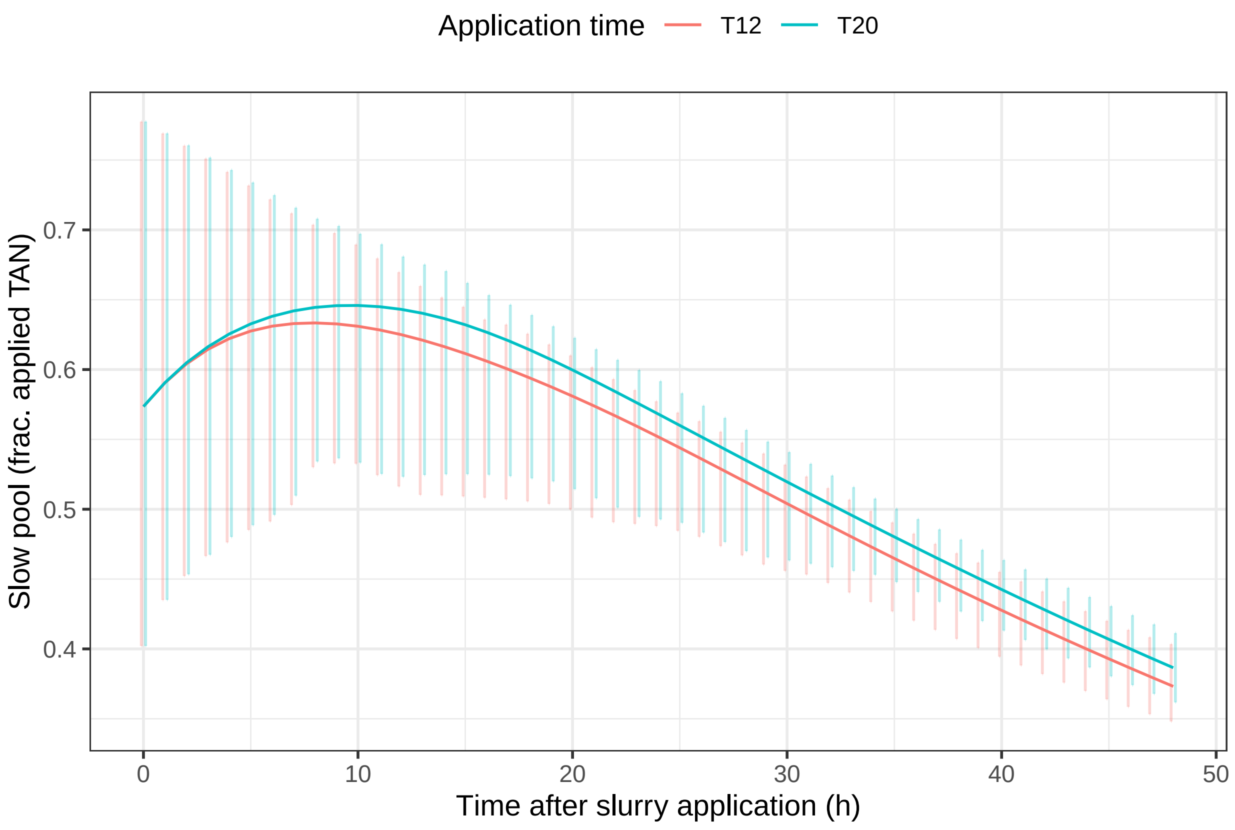
We can see that the lower initial temperature makes for a substantially lower rate of volatilization from the fast pool.

```r
pred3p[, xd := ct]
pred3p[apptime == 'T12', xd := xd - 0.1]
pred3p[apptime == 'T20', xd := xd + 0.1]
ggplot(pred3p, aes(ct, r1, colour = apptime)) +
  geom_errorbar(aes(x = xd, ymin = r1.lwr, ymax = r1.upr, width = 0), alpha = 0.3) +
  geom_line() +
  theme_bw() +
  theme(legend.position = 'top') +
  labs(x = 'Time after slurry application (h)',
       y = 'r1 (1/h)',
       colour = 'Application time')
```



And that means more TAN gets into the slow pool and stays there, with application at 20:00.

```r
ggplot(pred3p, aes(ct, s, colour = apptime)) +
  geom_errorbar(aes(x = xd, ymin = s.lwr, ymax = s.upr, width = 0), alpha = 0.3) +
  geom_line() +
  theme_bw() +
  theme(legend.position = 'top') +
  labs(x = 'Time after slurry application (h)',
       y = 'Slow pool (frac. applied TAN)',
       colour = 'Application time')
```



Really, the small difference in emission predicted with average inputs is not very meaningful. It could have a different sign than the hourly results. One argument for hour-of-day application decisions is that the timing of weather changes matter. But of course timing of weather changes are not reflected in average inputs at all.