

Understanding ALFAM2 pH response

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January 2021

```
rm(list = ls())
library(ALFAM2)
library(ggplot2)
library(dplyr)
source('.../functions/rounddf.R')
```

Get, tweak pars

```
load('.../parameters/parf.RData')
pars <- parf
pars['man.ph.r1'] <- 0.66
pars['man.ph.r3'] <- 0.24
```

Input data.

```
dat <- data.frame(ct = 168,
                  man.ph = 90:50/10,
                  TAN.app = 100)
dat$id <- 1:nrow(dat)
```

Run model.

```
pred <- ALFAM2mod(dat, pars = pars, group = 'id')
```

```
## Warning in ALFAM2mod(dat, pars = pars, group = "id"): Running with 6 parameters. Dropped 18 with no r
## These secondary parameters have been dropped: app.mthd.os.f0, app.rate.nos.f0, man.dm.f0, app.mthd.b
```

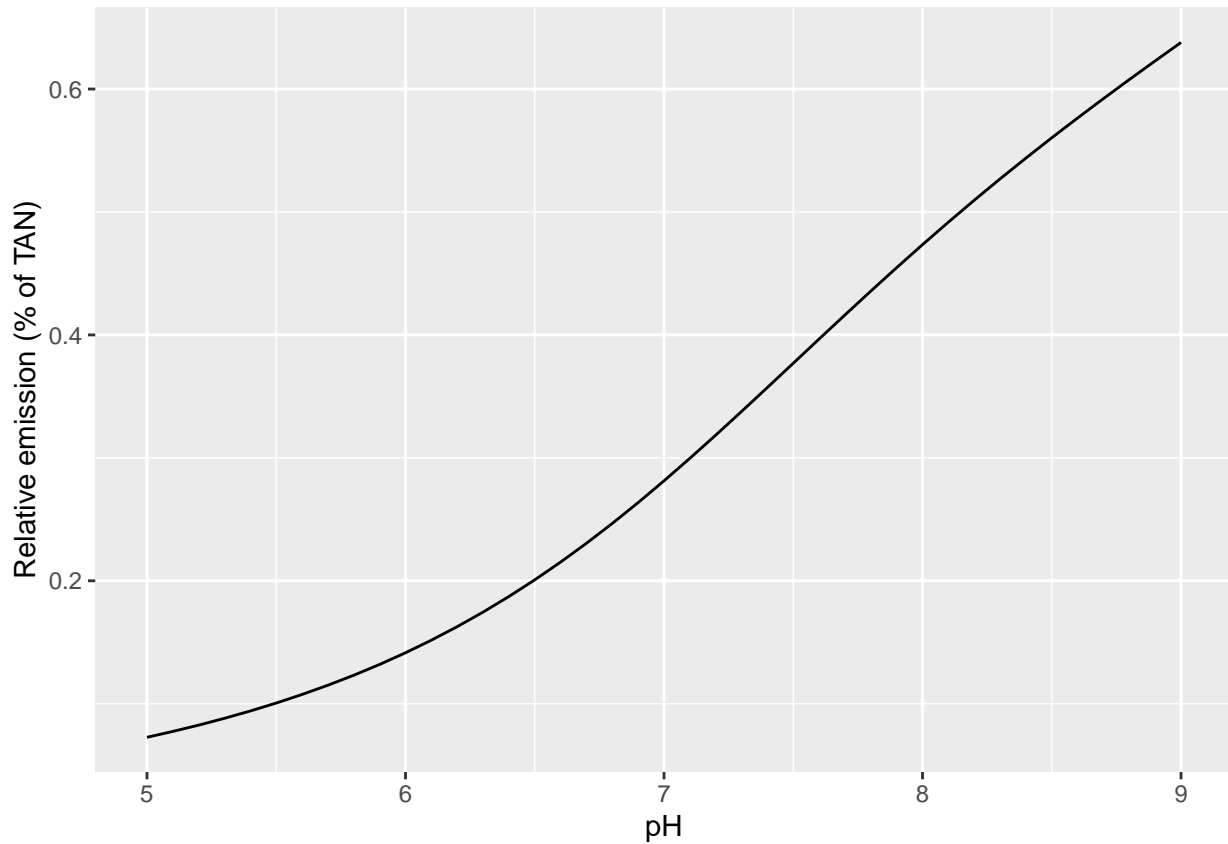
```
dat <- cbind(dat, pred[, -1:-3])
head(dat)
```

##	ct	man.ph	TAN.app	id	f0	r1	r2	r3	f4
## 1	168	9.0	100	1	0.3511408	0.8015409	0.07650173	0.003746867	1
## 2	168	8.9	100	2	0.3511408	0.6885345	0.07650173	0.003545425	1
## 3	168	8.8	100	3	0.3511408	0.5914604	0.07650173	0.003354813	1
## 4	168	8.7	100	4	0.3511408	0.5080725	0.07650173	0.003174449	1
## 5	168	8.6	100	5	0.3511408	0.4364412	0.07650173	0.003003781	1
## 6	168	8.5	100	6	0.3511408	0.3749089	0.07650173	0.002842289	1
##	f	s	j	e	e.int	er			
## 1	3.035254e-63	36.21316	0.3796836	63.78684	63.78684	0.6378684			
## 2	5.337169e-55	37.71055	0.3707705	62.28945	62.28945	0.6228945			
## 3	6.456199e-48	39.23038	0.3617239	60.76962	60.76962	0.6076962			
## 4	7.835790e-42	40.77666	0.3525199	59.22334	59.22334	0.5922334			
## 5	1.319508e-36	42.35364	0.3431331	57.64636	57.64636	0.5764636			
## 6	4.072860e-32	43.96554	0.3335385	56.03446	56.03446	0.5603446			

```
dat$red0.5 <- c(dat$er[1:(nrow(dat) - 10)] - dat$er[-1:-10], rep(NA, 10))
dat$rr0.5 <- 100 * dat$red0.5 / dat$er
```

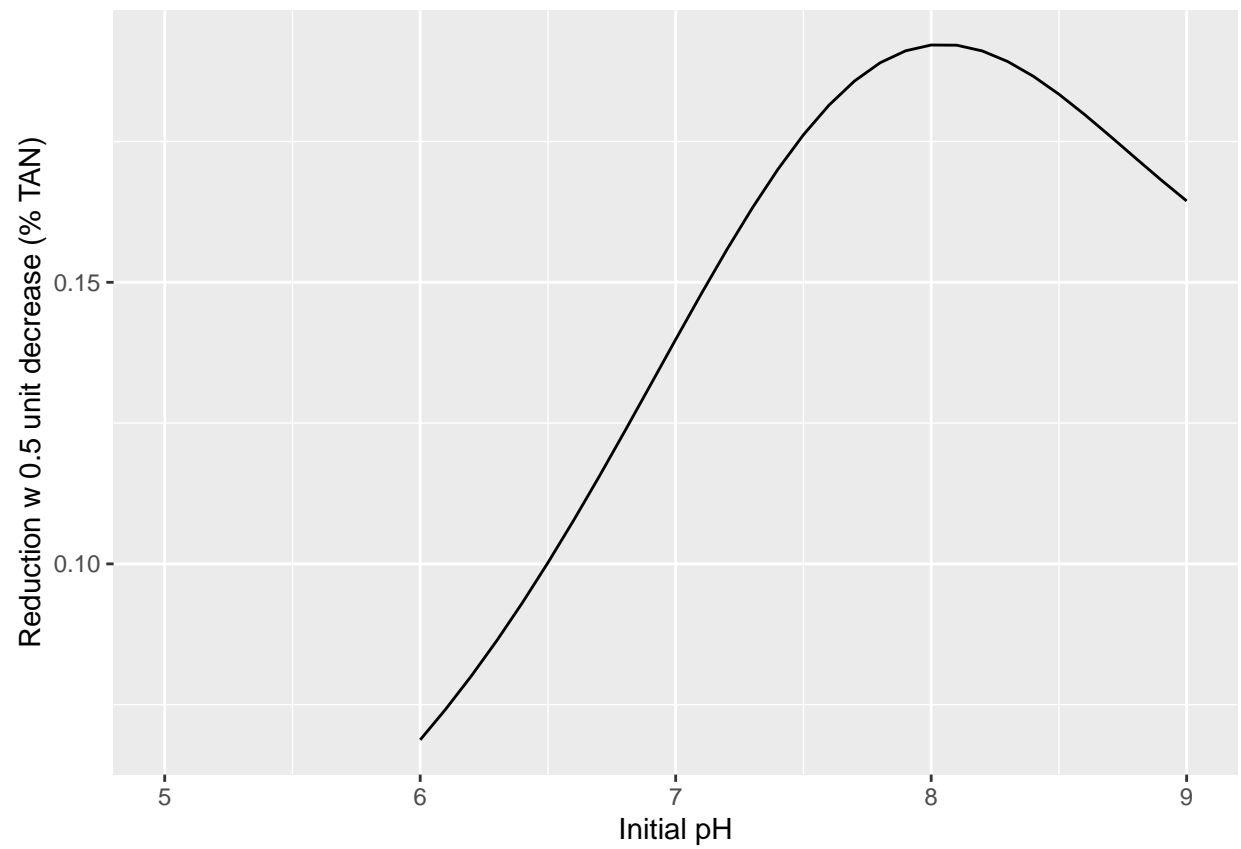
Plot.

```
ggplot(dat, aes(man.ph, er)) +
  geom_line() +
  labs(x = 'pH', y = 'Relative emission (% of TAN)')
```



```
ggplot(dat, aes(man.ph, red0.5)) +
  geom_line() +
  labs(x = 'Initial pH', y = 'Reduction w 0.5 unit decrease (% TAN)')
```

Warning: Removed 10 row(s) containing missing values (geom_path).



```
ggplot(dat, aes(man.ph, rred0.5)) +  
  geom_line() +  
  labs(x = 'Initial pH', y = 'Relative reduction w 0.5 unit decrease (% untreated emis.)')
```

```
## Warning: Removed 10 row(s) containing missing values (geom_path).
```

