# Demo

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Some example calls of NH3/CO2/slurry pH model.

Load all functions

```
source('NH3_mods.R')
```

Use eqSpec to calculate equilibrium speciation

```
eq <- eqSpec(tot = c(H. = -0.02, NH3 = 0.1, H2CO3 = 0.1, K. = 0.03,
                     Na. = 0.02, Cl. = 0.03, HAc = 0.0242),
             temp.c = 20, of = 'all')
eq
```

```
## $m
##           H.          NH3        H2CO3          CO2           K.          Na.
## 3.906191e-08 8.545425e-04 8.861097e-06 5.316655e-03 3.000000e-02 2.000000e-02
##          Cl.          HAc           OH.          NH4.        HCO3.        CO3.2
## 3.000000e-02 3.163202e-05 2.958420e-07 9.914546e-02 9.437214e-02 3.023479e-04
##          Ac.
## 2.416837e-02
##
## $a
##           H.          NH3        H2CO3          CO2           K.          Na.
## 3.165828e-08 8.844623e-04 9.171347e-06 5.502805e-03 2.165735e-02 1.493057e-02
##          Cl.          HAc           OH.          NH4.        HCO3.        CO3.2
## 2.165735e-02 3.273954e-05 2.166467e-07 7.046144e-02 7.225524e-02 9.614624e-05
##          Ac.
## 1.814904e-02
##
## $g
##        H.       NH3     H2CO3       CO2        K.       Na.       Cl.       HAc
## 0.8104643 1.0350126 1.0350126 1.0350126 0.7219115 0.7465283 0.7219115 1.0350126
##       OH.      NH4.     HCO3.     CO3.2       Ac.
## 0.7323053 0.7106875 0.7656417 0.3179987 0.7509419
##
## $i
## [1] 0.1494478
##
## $l.m
##        H.       NH3     H2CO3       CO2        K.       Na.       Cl.       HAc
## -7.408247 -3.068266 -5.052513 -2.274362 -1.522879 -1.698970 -1.522879 -4.499873
##       OH.      NH4.     HCO3.     CO3.2       Ac.
## -6.528940 -1.003727 -1.025156 -3.519493 -1.616753
##
```

```
## $l.a
##        H.       NH3     H2CO3       CO2         K.        Na.        Cl.       HAc
## -7.499513 -3.053321 -5.037567 -2.259416 -1.664395 -1.825924 -1.664395 -4.484927
##       OH.      NH4.     HCO3.     CO3.2       Ac.
## -6.664248 -1.152048 -1.141131 -4.017068 -1.741146
##
## $l.g
##          H.          NH3       H2CO3         CO2          K.         Na.
## -0.09126614  0.01494565  0.01494565  0.01494565 -0.14151601 -0.12695373
##         Cl.          HAc         OH.        NH4.       HCO3.       CO3.2
## -0.14151601  0.01494565 -0.13530780 -0.14832132 -0.11597444 -0.49757462
##         Ac.
## -0.12439365
##
## $tot
##      H.     NH3   H2CO3      K.     Na.     Cl.     HAc
## -0.0200  0.1000  0.1000  0.0300  0.0200  0.0300  0.0242
##
## $totk
##           H.          NH3        H2CO3          CO2           K.          Na.
## -0.020000000  0.100000000  0.094683345  0.005316655  0.030000000  0.020000000
##          Cl.          HAc
##  0.030000000  0.024200000
##
## $cb
## [1] 1.197548e-09
##
## $i.its
## [1] 2
##
## $p.CO2
## [1] 0.1406605
##
## $p.NH3.NH3
## [1] 1.146077e-05
```

Some info on arguments: tot = molalities (concentration in mol/kg water) of "components" (elements here, but not below, each represented by a "master species"), temp.c = temperature in C, of = output format ('all' is the most complete).

Here is some info on the ouput from eqSpec

```
names(eq)
```

```
##  [1] "m"         "a"         "g"         "i"         "l.m"       "l.a"
##  [7] "l.g"       "tot"       "totk"      "cb"        "i.its"     "p.CO2"
## [13] "p.NH3.NH3"
```

m = molalities of species (conc. in mol/kg water), a = activities of species, g = activity coefficients, i = ionic strength, l.m = log molalities, l.a = log activities, tot = molalities of components (e.g., H2CO3 = TIC, NH3 = TAN), totk = similar to tot but here H2CO3 (i.e., H2CO3, HCO3-, and CO3-2 species) and CO2 (only CO2 (aq)) are listed separately–totk is only used to get totals for kinetic model where there are two IC components, cb = charge (un)balance, i.its = iterations used for ionic strength to stabilize, p.CO2 = equilibrium CO2 partial pressure

```
str(eq)
```

```
## List of 13
##  $ m        : Named num [1:13] 3.91e-08 8.55e-04 8.86e-06 5.32e-03 3.00e-02 ...
##   ..- attr(*, "names")= chr [1:13] "H." "NH3" "H2CO3" "CO2" ...
##  $ a        : Named num [1:13] 3.17e-08 8.84e-04 9.17e-06 5.50e-03 2.17e-02 ...
##   ..- attr(*, "names")= chr [1:13] "H." "NH3" "H2CO3" "CO2" ...
##  $ g        : Named num [1:13] 0.81 1.035 1.035 1.035 0.722 ...
##   ..- attr(*, "names")= chr [1:13] "H." "NH3" "H2CO3" "CO2" ...
##  $ i        : num 0.149
##  $ l.m      : Named num [1:13] -7.41 -3.07 -5.05 -2.27 -1.52 ...
##   ..- attr(*, "names")= chr [1:13] "H." "NH3" "H2CO3" "CO2" ...
##  $ l.a      : Named num [1:13] -7.5 -3.05 -5.04 -2.26 -1.66 ...
##   ..- attr(*, "names")= chr [1:13] "H." "NH3" "H2CO3" "CO2" ...
##  $ l.g      : Named num [1:13] -0.0913 0.0149 0.0149 0.0149 -0.1415 ...
##   ..- attr(*, "names")= chr [1:13] "H." "NH3" "H2CO3" "CO2" ...
##  $ tot      : Named num [1:7] -0.02 0.1 0.1 0.03 0.02 0.03 0.0242
##   ..- attr(*, "names")= chr [1:7] "H." "NH3" "H2CO3" "K." ...
##  $ totk     : Named num [1:8] -0.02 0.1 0.09468 0.00532 0.03 ...
##   ..- attr(*, "names")= chr [1:8] "H." "NH3" "H2CO3" "CO2" ...
##  $ cb       : num 1.2e-09
##  $ i.its    : num 2
##  $ p.CO2    : num 0.141
##  $ p.NH3.NH3: num 1.15e-05
```

```
eq
```

```
## $m
##           H.          NH3        H2CO3          CO2           K.          Na.
## 3.906191e-08 8.545425e-04 8.861097e-06 5.316655e-03 3.000000e-02 2.000000e-02
##          Cl.          HAc           OH.          NH4.        HCO3.        CO3.2
## 3.000000e-02 3.163202e-05 2.958420e-07 9.914546e-02 9.437214e-02 3.023479e-04
##          Ac.
## 2.416837e-02
##
## $a
##           H.          NH3        H2CO3          CO2           K.          Na.
## 3.165828e-08 8.844623e-04 9.171347e-06 5.502805e-03 2.165735e-02 1.493057e-02
##          Cl.          HAc           OH.          NH4.        HCO3.        CO3.2
## 2.165735e-02 3.273954e-05 2.166467e-07 7.046144e-02 7.225524e-02 9.614624e-05
##          Ac.
## 1.814904e-02
##
## $g
##        H.       NH3     H2CO3       CO2        K.       Na.       Cl.       HAc
## 0.8104643 1.0350126 1.0350126 1.0350126 0.7219115 0.7465283 0.7219115 1.0350126
##       OH.      NH4.     HCO3.     CO3.2       Ac.
## 0.7323053 0.7106875 0.7656417 0.3179987 0.7509419
##
## $i
## [1] 0.1494478
##
## $l.m
##        H.       NH3     H2CO3       CO2        K.       Na.       Cl.       HAc
## -7.408247 -3.068266 -5.052513 -2.274362 -1.522879 -1.698970 -1.522879 -4.499873
```

```
##       OH.      NH4.     HCO3.     CO3.2       Ac.
## -6.528940 -1.003727 -1.025156 -3.519493 -1.616753
##
## $l.a
##        H.       NH3     H2CO3       CO2         K.       Na.       Cl.       HAc
## -7.499513 -3.053321 -5.037567 -2.259416 -1.664395 -1.825924 -1.664395 -4.484927
##       OH.      NH4.     HCO3.     CO3.2       Ac.
## -6.664248 -1.152048 -1.141131 -4.017068 -1.741146
##
## $l.g
##          H.          NH3       H2CO3         CO2          K.          Na.
## -0.09126614  0.01494565  0.01494565  0.01494565 -0.14151601 -0.12695373
##         Cl.          HAc          OH.         NH4.       HCO3.       CO3.2
## -0.14151601  0.01494565 -0.13530780 -0.14832132 -0.11597444 -0.49757462
##         Ac.
## -0.12439365
##
## $tot
##      H.     NH3   H2CO3      K.     Na.     Cl.     HAc
## -0.0200  0.1000  0.1000  0.0300  0.0200  0.0300  0.0242
##
## $totk
##           H.          NH3        H2CO3          CO2          K.          Na.
## -0.020000000  0.100000000  0.094683345  0.005316655  0.030000000  0.020000000
##          Cl.          HAc
##  0.030000000  0.024200000
##
## $cb
## [1] 1.197548e-09
##
## $i.its
## [1] 2
##
## $p.CO2
## [1] 0.1406605
##
## $p.NH3.NH3
## [1] 1.146077e-05
```

If you specify a pH, KOH or HAc (acetic acid) will be added to match it, so this call is essentially identical

```
eq <- eqSpec(tot = c(H. = -0.02, NH3 = 0.1, H2CO3 = 0.1,
                     K. = 0.03, Na. = 0.02, Cl. = 0.03,
                     HAc = 0.0),
             temp.c = 20, pH = 7.5, of = 'all')
```

Here we will extract total component concentrations for use in kinetic model (only difference from tot argument in call above is partitioning of H2CO3)

```
itot <- eq$totk
```

itot is initial total concentration of components (including distribution of IC between H2CO3 and CO2, which are not necessarily in equilibrium in simulation below)

```
itot
```

```
##           H.          NH3        H2CO3          CO2          K.          Na.
```

```
## -0.020000000  0.100000000  0.118775663  0.006661572  0.030000000  0.020000000
##          Cl.           HAc
##  0.030000000  0.000000000
```

Now for the emission model (note that there is also an equilibrium version eqEmisDiffMod()) Next call predicts changes in solution chemistry as CO2 and NH3 are emitted from surface, assuming no carbonic anhydrase (that what the "kin" is for–kinetic)

May take 30 sec to run

```
pred <- kinEmisDiffMod(c.thk = c(rep(1E-5, 5), rep(1E-4, 5), rep(9.45E-4, 10)),
                       h.m = 1E-3, p.CO2.a = 4E-6,
                       times = c(0:5*600, 1:12*3600), temp.c = 20, tot = itot)
```

Some info on arguments: c.thk = a vector of cell thicknesses in m (more and smaller is more accurate and slower), h.m = convective mass transfer coefficient in air for NH3 (m/s), p.CO2.a = ambient CO2 partial pressure (atm), temp.c = temperature in C, tot = molalities of components (usual length 8 vector and MUST be in order: "H.", "NH3", "H2CO3", "CO2", "K.", "Na.", "Cl.", "HAc")

Info on the ouput Complete output

```
names(pred)
```

```
##  [1] "times"    "pos"      "tot.k"    "tot.f"    "act"      "mol"
##  [7] "ph"       "kin.CO2"  "emis"     "exe.time" "n.calls"  "pars"
## [13] "summ"
```

times = times, pos = cell positions (cell centers), tot.k = molalities of components that change with time (NH3, CO2, H2CO3) and note that msp stands for "master species", tot.f = molalities of compnents that are fixed (all other components are not transported, because there is no emission, and this model does not include "multi-component diffusion"), act = activities of each species, ph = pH at all locations and times, kin.CO2 = CO2 (aq) hydration rate (I think. . . need to check), emis = emission rates and cumulatives (a data frame). str(pred)

Extact times

```
tt <- pred$times
```

position (center of cells) converted to mm

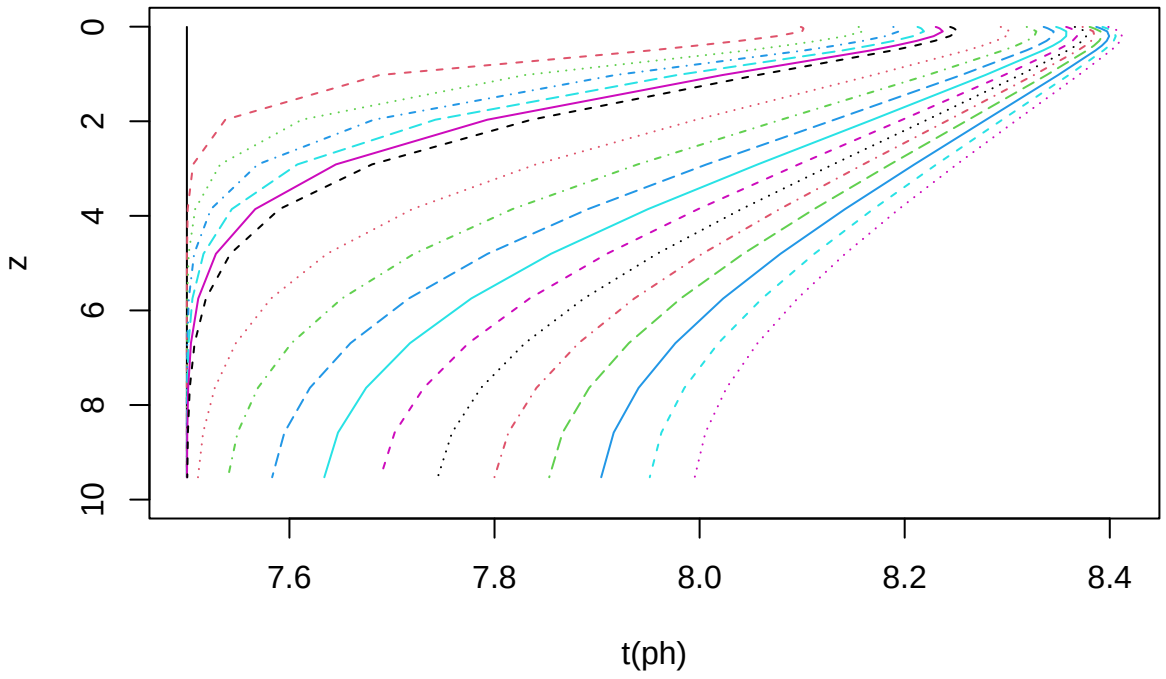
```
z <- pred$pos*1000
```

and pH

```
ph <- pred$ph
```

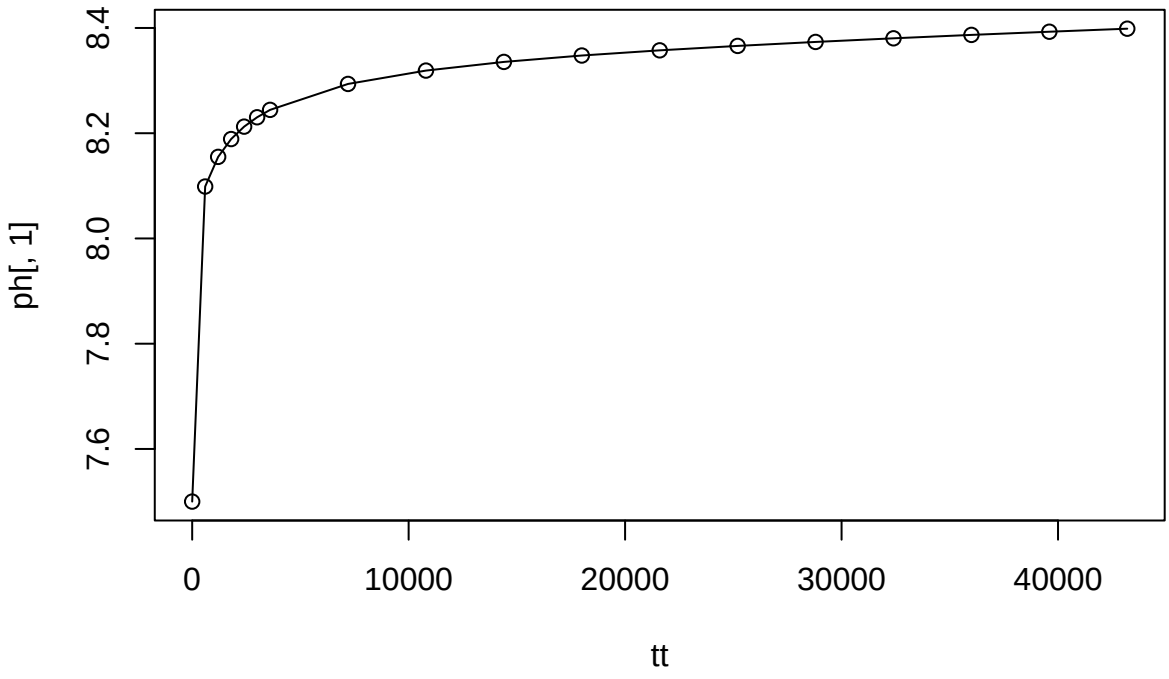
Plot pH

```
matplot(t(ph), z, type = 'l', ylim = c(10, 0))
```




"Surface" pH over time

```
plot(tt, ph[, 1], type = 'o')
```




Get fluxes

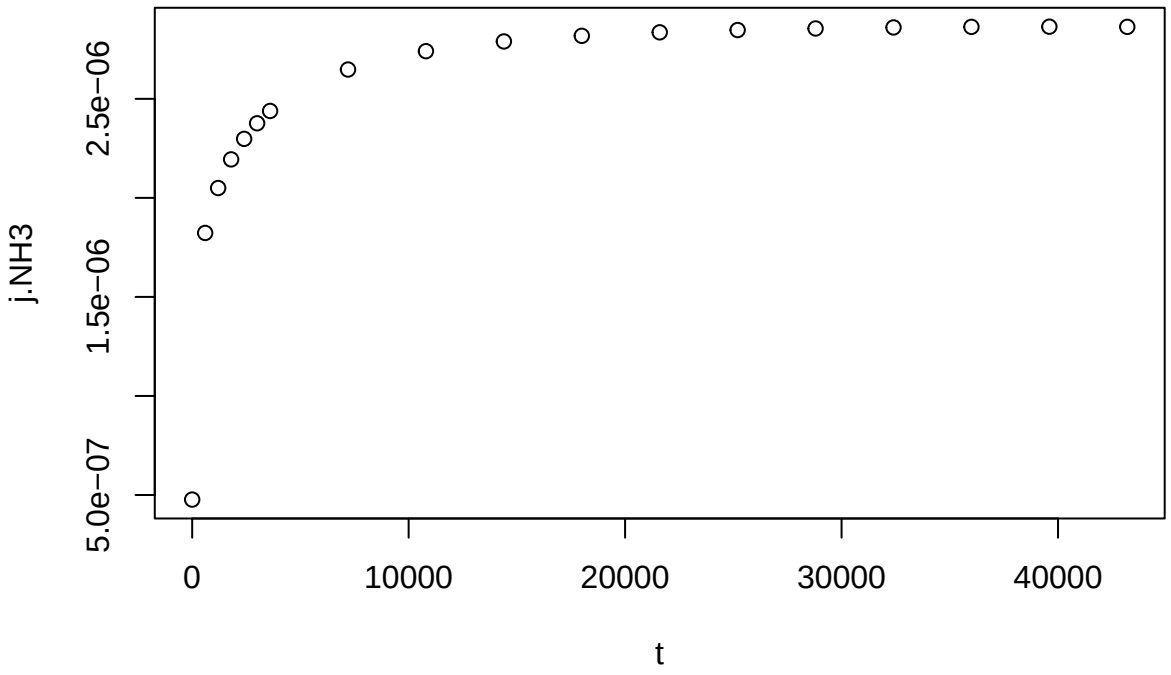
```
pred$emis
```

```
##           t        j.NH3        j.CO2        e.NH3       e.CO2    e.NH3.rel
## 0         0 4.769401e-07 4.557667e-03 0.0000000000 0.000000000 0.0000000000
## 600     600 1.822962e-06 9.738549e-06 0.0009024633 0.008915497 0.0009024633
## 1200   1200 2.049607e-06 8.201373e-06 0.0020704250 0.014233645 0.0020704250
```

```
## 1800   1800 2.194284e-06 7.418364e-06 0.0033462950 0.018898793 0.0033462950
## 2400   2400 2.297832e-06 6.923425e-06 0.0046954424 0.023191989 0.0046954424
## 3000   3000 2.376499e-06 6.574302e-06 0.0060987331 0.027235969 0.0060987331
## 3600   3600 2.438783e-06 6.310321e-06 0.0075440466 0.031097688 0.0075440466
## 7200   7200 2.647830e-06 5.452464e-06 0.0167590255 0.052029393 0.0167590255
## 10800 10800 2.740499e-06 5.037332e-06 0.0264772148 0.070844197 0.0264772148
## 14400 14400 2.789642e-06 4.770487e-06 0.0364398912 0.088469836 0.0364398912
## 18000 18000 2.818012e-06 4.573661e-06 0.0465381728 0.105273518 0.0465381728
## 21600 21600 2.835616e-06 4.415350e-06 0.0567174553 0.121443702 0.0567174553
## 25200 25200 2.847236e-06 4.280142e-06 0.0669481526 0.137089441 0.0669481526
## 28800 28800 2.855131e-06 4.160060e-06 0.0772131110 0.152278756 0.0772131110
## 32400 32400 2.860280e-06 4.051039e-06 0.0875014413 0.167056398 0.0875014413
## 36000 36000 2.863205e-06 3.950480e-06 0.0978043528 0.181456893 0.0978043528
## 39600 39600 2.864170e-06 3.856627e-06 0.1081142411 0.195507529 0.1081142411
## 43200 43200 2.863314e-06 3.768425e-06 0.1184242689 0.209230801 0.1184242689
##         e.CO2.rel      p.CO2.s      p.NH3.s
## 0     0.000000000 0.1762452869 1.147280e-05
## 600   0.007107536 0.0003805818 4.385137e-05
## 1200  0.011347225 0.0003211404 4.930331e-05
## 1800  0.015066334 0.0002908621 5.278353e-05
## 2400  0.018488919 0.0002717232 5.527436e-05
## 3000  0.021712826 0.0002582229 5.716671e-05
## 3600  0.024791433 0.0002480150 5.866494e-05
## 7200  0.041478428 0.0002148424 6.369357e-05
## 10800 0.056477805 0.0001987896 6.592272e-05
## 14400 0.070529166 0.0001884709 6.710485e-05
## 18000 0.083925254 0.0001808597 6.778731e-05
## 21600 0.096816310 0.0001747380 6.821077e-05
## 25200 0.109289272 0.0001695096 6.849030e-05
## 28800 0.121398368 0.0001648661 6.868021e-05
## 32400 0.133179273 0.0001606504 6.880406e-05
## 36000 0.144659513 0.0001567619 6.887443e-05
## 39600 0.155860841 0.0001531326 6.889763e-05
## 43200 0.166801191 0.0001497219 6.887704e-05
```

Plot NH3 flux

```
plot(j.NH3 ~ t, data = pred$emis)
```




and cumulative emission

```
plot(e.NH3 ~ t, data = pred$emis)
```