

Excel: True story.

M	O	P	Q	R	AC	AD	AE	AF	AH
CO2	V1	V2	BP	stream	CO2	C1	C2	G	C
ppmv	HS	liq		temp	BscF				final
647.6	30	30	1.05	289.5	0.9722	28.88	27.47	1690	676.1
1079.5	28	32	0.98	289.5	0.9722	48.14	42.73	2715	1018.2
885.7	29	31	0.99	289.5	0.9722	39.50	35.42	2243	868.4

1. What has been calculated?
2. Where's the mistake?

The same Excel spreadsheet calculation in R:

```
M <- c(647.6, 1079.5, 885.7) # CO2 ppmv
O <- c(30, 28, 29) # V1 HS
P <- c(30, 32, 31) # V2 (liquid)
Q <- c(1.05, 0.98, 0.99) # BP
R <- c(289.5, 289.5, 289.5) # stream temp
AC <- (2.7182818^(-58.0931+(90.5069*(100/R)) +
  (22.294*log(R/100)))) * 0.001 *
  (0.0821*273.15*1000 - 1636.75+12.0408*273.15 -
  3.27957*0.01*273.15^2 +
  3.16528*1e-5*273.15^3) # CO2 BscF
AD <- M/(0.0821*273.15) # C1
AE <- M*Q*AC*1/(0.0821*293.15) # C2
AF <- (AD*O) + (AE*P) # G
AH <- (AF/P)*12 # C final
```

Names help a little...

```
conc_CO2gas <- c(647.6, 1079.5, 885.7)
vol_headsp <- c(30, 28, 29 )
vol_liquid <- c(30, 32, 31 )
air_pressure <- c(1.05, 0.98, 0.99 )
lab_temp <- c(289.5, 289.5, 289.5)
air_gas_coef <- rep(0.9721713,3)
gas_constant_R <- 0.0821
conc_CO2g_lab <- conc_CO2gas / (gas_constant_R * 273.15)
conc_CO2aq_lab <- conc_CO2gas * air_pressure * air_gas_coef /
  (gas_constant_R * 293.15)
mol_CO2tot_lab <-
  (conc_CO2g_lab*vol_headsp) + (conc_CO2aq_lab*vol_liquid)
conc_CO2aq_field <- (mol_CO2tot_lab/vol_liquid) * 12
```

What if R let you include units?

```
library(unitted)
conc_CO2gas <- u(c(647.6, 1079.5, 885.7), "uatm atm^-1")
vol_headsp <- u(c(30, 28, 29), "mL")
vol_liquid <- u(c(30, 32, 31), "mL")
air_pressure <- u(c(1.05, 0.98, 0.99), "atm")
lab_temp <- u(c(289.5, 289.5, 289.5), "K")
air_gas_coef <- u(rep(0.9721713,3), "")
gas_constant_R <- u(0.0821, "L atm K^-1 mol^-1")
conc_CO2g_lab <- conc_CO2gas / (gas_constant_R * lab_temp)
conc_CO2aq_lab <- conc_CO2gas * air_pressure * air_gas_coef /
  (gas_constant_R * lab_temp) *
  u(1/1000, "atm uatm^-1") * u(1000, "umol mol^-1")
```

What if R were smart about units?

```
mol_CO2tot_lab <-  
  (conc_CO2g_lab*vol_headsp) + (conc_CO2aq_lab*vol_liquid)  
  
## Error: Trying to add objects with conflicting units:  
## mL mol uatm atm^-2 L^-1, mL umol L^-1  
  
# Fix conc_CO2g_lab:  
conc_CO2g_lab <- conc_CO2g_lab *  
  air_pressure * u(1/1000,"atm uatm^-1") * u(1000,"umol mol^-1")  
# Try again:  
mol_CO2tot_lab <-  
  ((conc_CO2g_lab*vol_headsp) + (conc_CO2aq_lab*vol_liquid))  
# Great! Finish the calculation:  
conc_CO2aq_field <- (mol_CO2tot_lab/vol_liquid) *  
  u(12, "ugC umol^-1")
```

library(unitted). Coming to an R session near you.

```
u(data.frame(conc_CO2g_lab, conc_CO2aq_lab, conc_CO2aq_field))
```

```
##   conc_CO2g_lab conc_CO2aq_lab conc_CO2aq_field
## U      umol L^-1      umol L^-1      ugC L^-1
## 1         28.61         27.81         677.1
## 2         44.51         43.27         986.6
## 3         36.89         35.87         844.5
```