**SUMMARY**

The following comments relate to def.calc.sdg.R.

**MOLES OF GAS IN HEADSPACE WATER**

The equation for calculating the dissolved CO2 in equilibrium with eqCO2 is:

The units for the inputs, as formatted in the NEON-dissolved-gas repo, are:

* HCO2 in mol m-3 Pa-1,
* eqCO2 in ppmv
* baro in kPa

To resolve the equation in units of mol L-1, the following dimensional analysis is required:

The constant for the unit conversion condenses to 0.000001, which is equal to cPresConv in the def.calc.sdg.R function. This is consistent with the equation for calculating the dissolved gas concentration of the equilibrated headspace water in the dissGas package, which reads as:

This is all good, except that the comment for cPresConv reads “conversion factor from kPa to Pa”. This really confused me because the conversion from kPa to Pa is actually 1000. In fact, cPresConv actually accounts for three separate unit conversions:

1. ppmv to parts
   1. I don’t know if ‘parts’ is really a unit, but ppmv needs to be divided by 1 million
2. kPa to Pa
3. m3 to L

If we argue that the kPa -> Pa and m3 -> L conversion cancel out, then cPresConv really represents the conversion of ppmv to ‘parts’.

**MOLES OF GAS IN HEADSPACE GAS**

The moles of CO2 in the headspace gas can be calculated from the Ideal Gas Law.

where P is the CO2 partial pressure in the headspace gas. The units for the inputs, as formatted in the NEON-dissolved-gas repo, are:

* P, which is labeled “baro” in the package: kPa
* V, which is labeled “volGas” in the package: mL
* R: L kPa K-1 mol-1
* T, which is labeled “waterTemp” in the package and converted to K via the constant “cKelvin”: K

To resolve the equation, as presented in def.calc.sdg.jb.V2.R, in units of mol, the following dimensional analysis is required:

As above, the unit conversions condense to 1/1000000 for the conversion of ppmv to parts (again, not sure ‘parts’ is really a unit). As above, I think the comment provided for cPresConv should be revised.

**MOLES OF GAS IN REFERENCE AIR**

Same comment as above