

Codos: CO2 Correction Tools

Installation

You can install the released version of codos from CRAN with:

```
install.packages("codos")
```

And the development version from GitHub with:

```
# install.packages("devtools")
devtools::install_github("special-uor/codos", "dev")
```

Note: Some of the equations on this document are not displayed properly (due to a server issue), check out the README.pdf.

Background:

Vapour-pressure deficit (vpd)

vpd is given by mean daily growing season temperature, tmp [°C] and moisture index, mi [-]. Using the CRU TS 4.04 dataset (University of East Anglia Climatic Research Unit et al. 2020) we found the following relation:

$$vpd = 4.589 \times \exp(0.0611 \times tmp - 0.87 \times mi)$$

The steps performed were:

1. Generate a monthly climatology for the period between 1961 and 1990 (inclusive). Variables used: cld, pre, tmn, tmx, vap.

```
# Monthly climatology for `tmn`
codos::monthly_clim("cru_ts4.04.1901.2019.tmn.dat.nc", "tmn", 1961, 1990)
```

Output file:

```
"cru_ts4.04.1901.2019.tmn.dat-clim-1961-1990.nc"
```

2. Interpolate the monthly data to daily. Variables used: cld, pre, tmn, tmx, vap.

```
# Monthly to daily interpolation for `tmn`
codos::nc_int("cru_ts4.04.1901.2019.tmn.dat-clim-1961-1990.nc", "tmn")
```

Output file:

```
"cru_ts4.04.1901.2019.tmn.dat-clim-1961-1990-int.nc"
```

3. Calculate daily temperature, tmp. Variables used: tmn and tmx.

```
codos::daily_temp(tmin = list(filename = "cru_ts4.04.1901.2019.tmn.dat-clim-1961-1990-int.nc",
                                id = "tmn"),
                  tmax = list(filename = "cru_ts4.04.1901.2019.tmx.dat-clim-1961-1990-int.nc",
                                id = "tmx"),
                  output_filename = "cru_ts4.04-clim-1961-1990-daily.tmp.nc")
```

4. Calculate mean growing season for daily temperature

```
codos::nc_gs("cru_ts4.04-clim-1961-1990-daily.tmp.nc", "tmp", thr = 0)
```

Output file:

```
"cru_ts4.04-clim-1961-1990-daily.tmp-gs.nc"
```

5. Calculate potential evapotranspiration (pet)

Install SPLASH (unofficial R package) as follows:

```
remotes::install_github("villegar/splash", "dev")
```

Or, download from the official source: <https://bitbucket.org/labprentice/splash>.

```
elv <- codos::nc_var_get("halfdeg.elv.nc", "elv")$data
tmp <- codos::nc_var_get("cru_ts4.04.1901.2019.daily.tmp.nc", "tmp")$data
cld <- codos::nc_var_get("cru_ts4.04.1901.2019.cld.dat-clim-1961-1990-int.nc",
                        "cld")$data

codos::splash_evap(output_filename = "cru_ts4.04-clim-1961-1990-pet.nc",
                  elv, # Elevation, 720x360 grid
                  sf = 1 - cld / 100,
                  tmp,
                  year = 1961, # Reference year
                  lat = codos::lat,
                  lon = codos::lon)
```

Output file:

```
"cru_ts4.04-clim-1961-1990-pet.nc"
```

6. Calculate moisture index (mi)

$$MI_{i,j} = \frac{\text{Total precipitation}}{\text{Total PET}}$$

```
pet <- codos::nc_var_get("cru_ts4.04-clim-1961-1990-pet.nc",
                        "pet")$data
pre <- codos::nc_var_get("cru_ts4.04.1901.2019.pre.dat-new-clim-1961-1990-int.nc",
                        "pre")$data
codos::nc_mi(output_filename = "cru_ts4.04-clim-1961-1990-mi.nc",
             pet, # potential evapotranspiration
             pre) # precipitation
```

Output file:

```
"cru_ts4.04-clim-1961-1990-mi.nc"
```

7. Approximate vpd

```
tmp <- codos::nc_var_get("cru_ts4.04-clim-1961-1990-daily.tmp.nc",
                        "tmp")$data
vap <- codos::nc_var_get("cru_ts4.04.1901.2019.vap.dat-clim-1961-1990-int.nc",
                        "vap")$data
output_filename <- file.path(path, "cru_ts4.04-clim-1961-1990-vpd-tmp.nc")
codos::nc_vpd(output_filename, tmp, vap)
```

Output file:

```
"cru_ts4.04-clim-1961-1990-vpd-tmp.nc"
```

8. Find the coefficients for the following equation

$$\text{vpd} = a \times \exp(k\text{Tmp} \times \text{tmp} - k\text{MI} \times \text{mi})$$

```
mi <- codos::nc_var_get("cru_ts4.04-clim-1961-1990-mi.nc", "mi")$data
Tmp <- codos::nc_var_get("cru_ts4.04-clim-1961-1990-daily.tmp-gs.nc", "tmp")$data
vpd <- codos::nc_var_get("cru_ts4.04-clim-1961-1990-vpd-tmp-gs.nc", "vpd")$data

# Apply ice mask
mi[codos::ice_mask] <- NA
Tmp[codos::ice_mask] <- NA
vpd[codos::ice_mask] <- NA

# Filter low temperatures, Tmp < 5
mi[Tmp < 5] <- NA
Tmp[Tmp < 5] <- NA

# Create data frame
df <- tibble::tibble(Tmp = c(Tmp),
                     vpd = c(vpd),
                     MI = c(mi))

# Filter grid cells with missing Tmp, vpd, or MI
df <- df[!is.na(df$Tmp) & !is.na(df$vpd) & !is.na(df$MI), ]

# Linear approximation
lmod <- lm(log(vpd) ~ Tmp + MI, data = df)
# Non-linear model
exp_mod <- nls(vpd ~ a * exp(kTmp * Tmp - kMI * MI),
              df,
              start = list(a = exp(coef(lmod)[1]),
                           kTmp = coef(lmod)[2],
                           kMI = coef(lmod)[3]),
              control = list(maxiter = 200))
```

Summary statistics:

```
summary(exp_mod)
#>
#> Formula: vpd ~ a * exp(kTmp * Tmp - kMI * MI)
#>
#> Parameters:
#>      Estimate Std. Error t value Pr(>|t|)
#> a      4.589148   0.019843   231.3   <2e-16 ***
#> kTmp    0.061108   0.000174   351.2   <2e-16 ***
#> kMI     0.870229   0.002585   336.7   <2e-16 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> Residual standard error: 2.241 on 60291 degrees of freedom
#>
#> Number of iterations to convergence: 8
```

```
#> Achieved convergence tolerance: 7.419e-06
coefficients(exp_mod)
#>          a          kTmp          kMI
#> 4.58914835 0.06110768 0.87022950
```

Corrected m_i from reconstructed m_i

The following equations were used:

$$f = e/1.6 = D/[c_a(1 - \chi)]$$

$$\chi = \frac{\xi \times \text{vpd}^{1/2} + \text{vpd}}{c_a / (c_a + 9.7)}$$

$$\xi = [\beta(K + \Gamma^*) / (1.6\eta^*)]^{1/2}$$

where:

- e ratio of water lost to carbon fixed [-]
- vpd vapour pressure deficit [Pa]
- c_a ambient CO2 partial pressure [Pa]
- χ ratio of leaf-internal to ambient CO2 partial pressures [-]
- ξ stomatal sensitivity factor [Pa^{1/2}]
- Γ^* photorespiratory compensation point [Pa]: a function of temperature and elevation
- β ratio of cost factors for carboxylation and transpiration = 146 [-]
- K effective Michaelis constant of Rubisco [Pa]: a function of temperature and elevation
- η^* viscosity of water relative to its value at 25°C [-]

And the equilibrium relation:

$$f(T_{c1}, M_{l1}, c_{a,1}) = f(T_{c0}, M_{l0}, c_{a,0})$$

where:

- T_{c1} past temperature (assume equal to reconstructed value) [K]
- M_{l1} past MI (unknown) [-]
- $c_{a,1}$ past ambient CO2 partial pressure [Pa], adjusted for elevation
- T_{c0} present temperature [K]
- M_{l0} reconstructed MI [-]
- $c_{a,1}$ 'recent' ambient CO2 partial pressure [Pa], adjusted for elevation

Steps in the solution:

1. Evaluate $f(T_{c0}, M_{l0}, c_{a,0})$
2. Equate this to:

$$[\xi(T_{c1}, z) \times \text{vpd}_1^{1/2} + \text{vpd}_1] / [c_{a,1}(z) / (c_{a,1}(z) + 9.7)]$$

where:

- z is elevation
- vpd_1 is past vapour pressure deficit

And solve for vpd_1 .

3. Convert vpd_1 back to MI (at temperature T_{c1}), to yield an estimate of M_{l1} .

Using `codas`, all the steps translate to a simple function call

```
corrected_mi <- codos::corrected_mi(present_t,  
                                   past_temp,  
                                   recon_mi,  
                                   modern_co2,  
                                   past_co2)
```

Note that this function takes temperatures in [°C] and ambient CO₂ partial pressures in [μ mol/mol] (unless, `scale_factor` is overwritten, e.g. `scale_factor = 1` to use ambient CO₂ partial pressures in [Pa]).

More details:

```
?codos::corrected_mi
```

References

University of East Anglia Climatic Research Unit, Ian C. Harris, Philip D. Jones, and Tim Osborn. 2020. *CRU TS4.04: Climatic Research Unit (CRU) Time-Series (TS) Version 4.04 of High-Resolution Gridded Data of Month-by-Month Variation in Climate (Jan. 1901- Dec. 2019)*. Centre for Environmental Data Analysis. <https://catalogue.ceda.ac.uk/uuid/89e1e34ec3554dc98594a5732622bce9>.