bala\_c4test\_remkoedits\_v1.R

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# source("functions/functions.R")  
### ACi model for Vpmax and Vc max only  
c4\_aci<- function (Ci, PPFD = 1500, Tleaf = 25, VPMAX25 = 120, Vcmax = 60,   
 Vpr = 80, alpha = 0, gbs = 0.003, O2 = 210, JMAX25 = 400,   
 x = 0.4, THETA = 0.7, RD0 = 1, RTEMP = 25, TBELOW = 0,   
 DAYRESP = 1, FRM = 0.5, Rd= 1, ...)   
{  
 Vcmax <- Vcmax  
 Vpmax <- VPMAX25  
 Jmax <- JMAX25  
 TK <- Tleaf + 273.15  
 low\_gammastar <- 0.00019305  
 Kc <- 650   
 Kp <- 80   
 Ko <- 450   
 K <- Kc \* (1 + O2/Ko)  
 Rd<- Rd  
 Rm <- FRM \* Rd  
 Vp <- pmin(Ci \* Vpmax/(Ci + Kp), Vpr)  
 a.c <- 1 - (alpha \* Kc)/(0.047 \* Ko)  
 b.c <- -((Vp - Rm + gbs \* Ci) + (Vcmax - Rd) + gbs \* K +   
 alpha \* low\_gammastar/0.047 \* (low\_gammastar \* Vcmax +   
 Rd \* Kc/Ko))  
 c.c <- (Vcmax - Rd) \* (Vp - Rm + gbs \* Ci) - (Vcmax \* gbs \*   
 low\_gammastar \* O2 + Rd \* gbs \* K)  
   
 A.enzyme <- (-b.c - sqrt(b.c^2 - 4 \* a.c \* c.c))/(2 \* a.c)  
   
 Qp2 <- PPFD \* (1 - 0.15)/2  
   
 J <- (1/(2 \* THETA)) \* (Qp2 + Jmax - sqrt((Qp2 + Jmax)^2 -   
 4 \* THETA \* Qp2 \* Jmax))  
   
 a.j <- 1 - 7 \* low\_gammastar \* alpha/(3 \* 0.047)  
   
 b.j <- -((x \* J/2 - Rm + gbs \* Ci) + ((1 - x) \* J/3 - Rd) +   
 gbs \* (7 \* low\_gammastar \* O2/3) + alpha \* low\_gammastar/0.047 \*   
 ((1 - x) \* J/3 + Rd))  
 c.j <- ((x \* J/2 - Rm + gbs \* Ci) \* ((1 - x) \* J/3 - Rd) -   
 gbs \* low\_gammastar \* O2 \* ((1 - x) \* J/3 - 7 \* Rd/3))  
   
   
 A.light <- (-b.j - sqrt(b.j^2 - 4 \* a.j \* c.j))/(2 \* a.j)  
   
 An <- pmin(A.enzyme, A.light)  
   
 Ac <- A.enzyme  
   
 Aj <- A.light  
   
   
 shape2 <- 0.999  
 Ad <- (Ac + Aj - sqrt((Ac + Aj)^2 - 4 \* shape2 \* Ac \* Aj))/(2 \* shape2) - Rd  
 Ac <- Ac - Rd  
 Aj <- Aj - Rd  
   
 df <- data.frame (ALEAF = Ad, Ci = Ci,An = An, Ac = Ac, Aj = Aj, Vp = Vp,   
 Rd = Rd, Tleaf = Tleaf, PPFD = PPFD)  
 return(df)  
   
}  
  
## fiting the model  
  
fitc4 <- function(dat, varnames = list(ALEAF = "Photo", Tleaf = "Tleaf",   
 Ci = "Ci", PPFD = "PPFD", Rd= "Rd"))  
{   
 m <- as.list(match.call())  
 a <- as.list(formals(fitc4))  
 f <- names(formals(c4\_aci))  
 extrapars <- setdiff(names(m), c(names(a), ""))  
 for (i in seq\_along(extrapars)) {  
 if (extrapars[i] %in% f) {  
 val <- eval(m[[extrapars[i]]])  
 formals(c4\_aci)[extrapars[i]] <- val  
 }  
 else {  
 warning("Parameter ", extrapars[i], " not recognized.")  
 }  
 }  
   
 acifun\_wrap <- function(Ci, ...) {  
 r <- c4\_aci(Ci = Ci,...)  
 r$ALEAF  
 }  
   
 aciSS <- function(VPMAX25, Vcmax) {  
 Photo\_mod <- acifun\_wrap(dat$Ci, PPFD = dat$PPFD,VPMAX25=VPMAX25,Vcmax = Vcmax, JMAX25 = 400, Rd = dat$Rd, Tleaf = dat$Tleaf)  
 SS <- sum((dat$ALEAF - Photo\_mod)^2)  
 return(SS)  
 }  
   
 aciSS(vpmax\_guess, vcmax\_guess)  
   
 d <- 0.3  
 n <- 20  
   
 gg <- expand.grid(VPMAX25 = seq(vpmax\_guess \* (1 - d),vpmax\_guess\* (1 + d), length = n),Vcmax = seq(vcmax\_guess \* (1 - d),vcmax\_guess\* (1 + d), length = n))  
 ##   
 m <- with(gg, mapply(aciSS,VPMAX25=VPMAX25, Vcmax = Vcmax))  
 ii <- which.min(m)  
   
 vpmax\_guess <- gg$VPMAX25[ii]  
 vcmax\_guess<- gg$Vcmax[ii]  
   
   
 nlsfit <- nls(ALEAF ~ acifun\_wrap(Ci, PPFD = PPFD, VPMAX25= VPMAX25,Vcmax = Vcmax),   
 data = dat, control = nls.control(maxiter = 500, minFactor = 1/10000),   
 start = list(VPMAX25= vpmax\_guess,Vcmax = vcmax\_guess))  
   
 p <- coef(nlsfit)  
 acirun <- c4\_aci(Ci = dat$Ci, VPMAX25 = p[[1]], Vcmax = p[[2]], PPFD = dat$PPFD, Tleaf = dat$Tleaf, Rd= dat$Rd)  
   
 acirun$Ameas <- dat$ALEAF  
 acirun$Ci <- dat$Ci  
 names(acirun)[names(acirun) == "ALEAF"] <- "Amodel"  
 avars <- match(c("Ci", "Ameas", "Amodel"), names(acirun))  
 acirun <- acirun[, c(avars, setdiff(1:ncol(acirun), avars))]  
   
 l <- list()  
 l$df <- acirun[order(acirun$Ci), ]  
 l$pars <- summary(nlsfit)$coefficients[, 1:2]  
 l$nlsfit <- nlsfit  
 formals(c4\_aci)$Tleaf<- mean(dat$Tleaf)  
 formals(c4\_aci)$PPFD <- mean(dat$PPFD)  
 formals(c4\_aci)$VPMAX25 <- l$pars[1]  
 formals(c4\_aci)$Vcmax <- l$pars[2]  
 l$c4\_aci <- c4\_aci  
 l$Vpmax\_guess <- vpmax\_guess  
 l$Vcmax\_guess <- vcmax\_guess  
   
 class(l) <- "c4acifit"  
 return(l)  
}  
  
print.c4acifit <- function (x, ...){  
 cat("Result of C4 fitaci.\n\n")  
 cat("Data and predictions:\n")  
 print(x$df)  
 cat("\nEstimated parameters:\n")  
 print(x$pars)  
  
 cat("\n\n")  
 cat("Parameter settings:\n")  
 fm <- formals(x$c4\_aci)  
 pars <- c("Vpr", "THETA")  
 fm <- fm[pars]  
 cat(paste0(names(fm), " = ", unlist(fm), "\n"))  
}  
  
  
  
  
plot.c4acifit <- function (x, what = c("data", "model"), xlim = NULL, ylim = NULL,   
 whichA = c("Ac", "Vp", "Amin"), add = FALSE, pch = 19, addzeroline = TRUE,   
 addlegend = !add, lwd = c(1, 2),   
 ...)   
{  
 if (is.null(ylim))   
 ylim <- with(x$df, c(min(Ameas), 1.1 \* max(Ameas)))  
 if (is.null(xlim))   
 xlim <- with(x$df, c(0, max(Ci)))  
 if (length(lwd) == 1)   
 lwd <- c(lwd, lwd)  
 Ci <- with(x$df, seq(min(Ci), max(Ci), length = 101))  
 pred <- x$c4\_aci(Ci = Ci)  
 if (!add) {  
 with(x$df, plot(Ci, Ameas, type = "n", ylim = ylim, xlim = xlim,   
 xlab = expression(italic(C)[i] ~ ~(ppm)), ylab = expression(italic(A)[net] ~   
 ~(mu \* mol ~ m^-2 ~ s^-1)), ...))  
 }  
 if ("data" %in% what)   
 with(x$df, points(Ci, Ameas, pch = pch, ...))  
 if ("model" %in% what) {  
 if ("Vp" %in% whichA)   
 with(pred, points(Ci, Vp - Rd, type = "l", col = "blue",   
 lwd = lwd[1]))  
 if ("Ac" %in% whichA)   
 with(pred, points(Ci, Ac - Rd, type = "l", col = "red",   
 lwd = lwd[1]))  
 if ("Amin" %in% whichA)   
 with(pred, points(Ci, ALEAF, type = "l", col = "black",   
 lwd = lwd[2]))  
 }  
  
 if (addzeroline)   
 abline(h = 0, lty = 3)  
 if (addlegend) {  
 legend("bottomright", c(expression(italic(A)[c]), expression(italic(V)[p]),   
 "Limiting rate"), lty = 1, lwd = c(1, 1, 2), col = c("red",   
 "blue", "black"))  
 }  
}