Cold acclimation of mesophyll conductance, bundle-sheath conductance and leakiness in Miscanthus x giganteus

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Loading required packages

require(rmarkdown)  
library(modelr)  
library(dplyr)  
library(purrr)

### CAsat model

Reading data set for the combined C4-enzyme-limited photosynthesis model and the 13C discrimination model for the CAsat Measured data

d0 <- read.csv("submission 2019/deltavalues to plug in Nerea gm.csv", head = TRUE) # To load initial values

Loading initial starting values for *g*m and *g*bs for the CAsat

gbs\_gm1\_start\_df <- read.csv("submission 2019/start\_gmsat0.csv")#Loads starting values for the model  
  
gm1<- cbind(d0,gbs\_gm1\_start\_df)#Joins input data and starting values for the model

Creates a list of vectors with starting values for *g*m and *g*bs

#  
gm1\_list <- gm1 %>%  
 group\_split(.tbl = ., id) # Splits dataset by Growth and measured temperature  
  
gm1\_gbsPa <- gm1 %>%  
 group\_split(.tbl = ., id) %>%  
 map("gbsPa") %>% map\_dbl(mean) # Creates a vector with the mean values for gbs for the splitted dataset  
  
gm1\_gm <- gm1 %>%  
 group\_split(.tbl = ., id) %>%  
 map("gmPa") %>% map\_dbl(mean) # Creates a vector with the mean values for Cm for the splitted dataset  
  
gbs\_gm1\_start <- mapply(c, gm1\_gbsPa , gm1\_gm , SIMPLIFY = FALSE)

Combined C4-enzyme-limited photosynthesis and the 13C discrimination for the CAsat model

The equations with their descriptions can be found in the Supporting Information Table S1

C4\_combined\_model\_CAsat<- function (gbs\_gm,data ) {  
   
 data$dummy25<-ifelse(data$GrowthTemp=="25C",1,0)  
 data$dummy14<-ifelse(data$GrowthTemp=="14C",1,0)  
   
   
 # Variables for a  
 alpha <- 0 #Fraction of PSII active in bundle sheath cells (von Caemmerer 2000)  
   
 #Parameters with temperature dependencies  
 temp <- data$Tleaf  
 tempk <- temp + 273.15  
 R <- 0.008314  
 tk25 <- 298.15  
   
 Kc <- 121\*exp((64.2\*(tempk-tk25))/(tk25\*R\*tempk)) # Kc temperature dependency setaria Boyd et al. (2015)  
 uoc <- 0.047\*exp( (- 1.63/R)\*(1/tk25 - 1/tempk )) # uoc temperature dependency Ubierna et al. (2018)  
 Ko <- 29200\*exp((10.5\*(tempk-tk25))/(tk25\*R\*tempk)) # Ko temperature dependency setaria Boyd et al. (2015)  
   
   
 data$gbsPa <- gbs\_gm[1]  
 data$gmPa <- gbs\_gm[2]  
 data$Cm <- data$CiPa - (data$Photo/data$gmPa)  
   
 Om <- 210000\*data$Press/1000 # µmol mol-1 O2 mol fraction in the mesophyl cells (in air at equilibrium)  
 Os <- Om + (alpha \* data$Photo/(uoc\*data$gbsPa))\*data$Press  
   
 #variables for "b" in the quadratic equation for the C4 enzyme limited model  
  
 #Vpmax temperature dependency setaria Boyd 2015  
 Vpmax25 <- 300.5\*data$dummy14 + 491.7\*data$dummy25   
 deltas <- 0.25  
 hd <- 73.3  
 Ea\_Vpmax <- 94.8  
 Vpmax <- Vpmax25\*exp(Ea\_Vpmax\*((tempk-tk25)/(tk25\*R\*tempk)))\*(1+exp((tk25\*deltas-hd)/(tk25\*R)))/(1+exp((tempk\*deltas-hd)/(tempk\*R)))  
  
 #Vcmax temperature dependency Yin et al., 2011  
 k25\_Vcmax <- 58.3\*data$dummy14 + 47.1\*data$dummy25   
 Vcmax <- k25\_Vcmax\*exp((53.4\*(tempk-tk25))/(tk25\*R\*tempk))  
   
 #Rubisco specificity setaria Boyd 2015  
 sco <- 1310\*exp(-31.1\*(tempk-tk25)/(tk25\*R\*tempk))  
 sm\_gamma <- 0.5/sco #Half the reciprocal of the Rubisco specificity (von Caemmerer, 2000)  
 big\_gamma <- sm\_gamma\*Os  
   
 #Kp temperature dependency setaria Boyd 2015  
 kp <- 7.44 \* exp((36.3 \* (tempk - tk25))/(tk25 \*R\* tempk))   
   
 Rlight <- data$Rlight  
 Rm <- .5 \* data$Rlight #  
   
 data$Vp <- (data$Cm\*Vpmax)/(data$Cm+kp)   
   
   
 #Quadratic coefficients to calculate A  
 a <- 1 - ((alpha\*Kc)/(uoc\*Ko))  
 b <- -( (data$Vp - Rm + data$gbsPa \* data$Cm) + (Vcmax - Rlight) + data$gbsPa\*(Kc \* (1 + (Om/Ko))) +   
 ( (alpha/uoc)\*(sm\_gamma \* Vcmax + Rlight \* Kc/Ko)) )  
 c <- (Vcmax - Rlight)\*(data$Vp - Rm + data$gbsPa\*data$Cm) - (Vcmax\*data$gbsPa \* sm\_gamma \* Om + Rlight\* data$gbsPa\*(Kc\*(1+(Om/Ko))) )  
   
 data$Amod <- (-b - sqrt(b^2 - 4\*a\*c))/2\*a  
   
  
  
 #discrimination factors for D13C model  
 f<-11.6 #fractionation during photorespiration  
 a\_b<- 2.9 #fractionation during difussion through the leaf boundary layer  
 a\_s <- 4.4 #13C fractionation due to diffusion in air  
 a\_w <- 1.8 #Summed discriminations against 13C during liquid phase diffusion and dissolution  
 a\_b<- 2.9 #fractionation during difussion through the leaf boundary layer  
 s <- 1.8 #Fractionation during leakage of CO2 out of the bundle-sheath cells   
   
   
   
 data$Cbs <- data$Cm + (data$Vp - data$Photo - Rm)/ data$gbsPa # Equation 4.5 von caemmerer 2000  
   
   
 Vc <- (data$Cbs\*Vcmax)/(data$Cbs+Kc\*(1+(Os/Ko))) # Equation 4.7 von caemmerer 2000  
 Vo <- 2\*big\_gamma\*Vc/data$Cbs# Equation 4.8 von caemmerer 2000  
   
   
 data$b3p<-30 # fractionation by Rubisco   
 data$b3<-data$b3p-((data$e\*Rlight + f\*Vo\*0.5) /Vc)  
   
 # Net fractionation by CO2 dissolution, hydration, and PEPc activity  
 data$b4p <- -(9.483\*1000)/ (273 + data$Tleaf) + 23.89 +2.2 # data$b4' temp dependency  
 data$b4 <- data$b4p - ((data$e\*Rm)/data$Vp)   
  
 data$a\_bar\_Ci <- with(data = data, ( a\_b\*(CaPa-CL) + a\_s\*(CL-CiPa) ) / (CaPa-CiPa) )  
 alpha\_ac <- 1 + data$a\_bar\_Ci /1000   
   
 g\_ac <- data$CndCO2  
 data$t <- alpha\_ac\*data$E/(2\*g\_ac)   
   
 data$phi <- (data$gbsPa \* (data$Cbs - data$Cm)) / data$Vp  
   
 data$D13C\_mod <- with( data = data, 1/(1-t) \* ( a\_b\*(CaPa-CL)/CaPa + a\_s\*(CL-CiPa)/CaPa) +   
 (1+t)/(1-t) \* ( a\_w \*(CiPa - Cm)/CaPa + (data$b4 + phi\*(data$b3\* Cbs/(Cbs - Cm)- s)) \* Cm / ((1 + (phi\*Cm)/(Cbs - Cm))\*CaPa ) ))  
  
 return(data)  
   
 }

Measuring distance between observed and modeled values

measure\_distance <- function(gbs\_gm,data) {   
 diff\_A <- data$Photo - C4\_combined\_model\_CAsat(gbs\_gm, data)$Amod   
 diff\_D13C <- data$Dobs - C4\_combined\_model\_CAsat(gbs\_gm, data)$D13C\_mod  
 sum((diff\_A/data$Photo)^2, (diff\_D13C/data$Dobs)^2)  
}

Writing the dataset with the results for the CAsat model created using the optim function

results\_gmsat0 <- map2\_df(.x = gbs\_gm1\_start,   
 .y = gm1\_list,  
 .f = ~ data.frame (C4\_combined\_model\_CAsat(gbs\_gm = Reduce(cbind,   
 optim(.x, measure\_distance, data =.y)$par), data =.y),  
 Sum.diff = optim(.x, measure\_distance, data = .y)$value) )   
  
write.csv(results\_gmsat0, "submission 2019/results\_gmsat0.csv", row.names = FALSE)

### CAlim model

Reading data set for the ombined C4-enzyme-limited photosynthesis model and the 13C discrimination model for the CAlim

Loading initial starting values for *g*m and *g*bs for the CAlim

gbs\_gm2\_start\_df <- read.csv( "submission 2019/start\_gmCAlim0.csv")# Loads starting values for the model  
  
gm2<- cbind(d0,gbs\_gm2\_start\_df)# Joins input data and starting values for the model

Creates a list of vectors with starting values for gm and gbs

gm2\_list <- gm2 %>%  
 group\_split(.tbl = ., id) # Splits dataset by Growth and measured temperature  
  
gm2\_gbsPa <- gm2 %>%  
 group\_split(.tbl = ., id) %>%  
 map("gbsPa") %>% map\_dbl(mean) # Creates a vector with the mean values for gbs for the splitted dataset  
  
gm2\_gm <- gm2 %>%  
 group\_split(.tbl = ., id) %>%  
 map("gmPa") %>% map\_dbl(mean) # Creates a vector with the mean values for Cm for the splitted dataset  
  
gbs\_gm2\_start <- mapply(c, gm2\_gbsPa , gm2\_gm , SIMPLIFY = FALSE) #Creates a list of vectors with paired values of gbs and Cm

Combined C4-enzyme-limited photosynthesis and the 13C discrimination for the CAlim model

The equations with their descriptions can be found in the Supporting Information Table S1

C4\_combined\_model\_CAlim<- function (gbs\_gm,data ) {  
   
 data$dummy25<-ifelse(data$GrowthTemp=="25C",1,0)  
 data$dummy14<-ifelse(data$GrowthTemp=="14C",1,0)  
   
 # Variables for a  
 alpha <- 0   
   
 #Parameters with temperature dependencies  
 temp <- data$Tleaf  
 tempk <- temp + 273.15  
 R <- 0.008314  
 tk25 <- 298.15  
   
 Kc <- 121\*exp((64.2\*(tempk-tk25))/(tk25\*R\*tempk))   
 uoc <- 0.047\*exp( (- 1.63/R)\*(1/tk25 - 1/tempk ))   
 Ko <- 29200\*exp((10.5\*(tempk-tk25))/(tk25\*R\*tempk))   
   
 data$gbsPa <- gbs\_gm[1]  
 data$gmPa <- gbs\_gm[2]  
 data$Cm <- data$CiPa - data$Photo / data$gmPa  
   
 Om <- 210000\*data$Press/1000   
 Os <- Om + (alpha \* data$Photo/(uoc\*data$gbsPa))\*data$Press  
   
 #variables for "b" in the quadratic equation for the C4 enzyme limited model  
   
 #Vpmax temperature dependcy setaria Boyd 2015  
 Vpmax25 <- 300.5\*data$dummy14 + 491.7\*data$dummy25   
 deltas <- 0.25  
 hd <- 73.3  
 Ea\_Vpmax <- 94.8  
 Vpmax <- Vpmax25\*exp(Ea\_Vpmax\*((tempk-tk25)/(tk25\*R\*tempk)))\*  
 (1+exp((tk25\*deltas-hd)/(tk25\*R)))/(1+exp((tempk\*deltas-hd)/(tempk\*R)))  
   
 #Vcmax temperature dependency Yin et al., 2011  
 k25\_Vcmax <- 58.3\*data$dummy14 + 47.1\*data$dummy25   
 Vcmax <- k25\_Vcmax\*exp((53.4\*(tempk-tk25))/(tk25\*R\*tempk))  
   
 #Rubisco specificity setaria Boyd 2015  
 sco <- 1310\*exp(-31.1\*(tempk-tk25)/(tk25\*R\*tempk))  
 sm\_gamma <- 0.5/sco #Half the reciprocal of the Rubisco specificity von Caemmerer, (2000)  
 big\_gamma <- sm\_gamma\*Os  
   
 #Kp temperature dependency setaria Boyd 2015  
 kp <- 30 \* exp((27.2 \* (tempk - tk25))/(tk25 \*R\* tempk))  
   
   
 Rlight <- data$Rlight  
 Rm <- .5 \* data$Rlight   
   
   
   
 #kca temperature dependency setaria Boyd 2015  
 k25 <- 23.2\*data$dummy14 + 39.8\*data$dummy25   
 Ea <- 40.9  
 deltas <- 0.21  
 hd <- 64.5  
 kca <- k25\*exp(Ea\*(tempk-tk25)/(tk25\*R\*tempk))\*  
 ((1+exp((tk25\*deltas-hd)/(tk25\*R)))/(1+exp((tempk\*deltas-hd)/(tempk\*R))))   
   
 Vh <- data$Cm\*kca  
   
 KH <- 2.9799\*exp(-2400\*((1/tempk)-(1/298.15)))  
   
 Kf <- 0.0389858 \* exp((74.8936\*( tempk-298.15))/(298.15\*0.008314\*tempk))  
 Kr <- 0.00332955 \* exp((65.2704\*( tempk-298.15))/(298.15\*0.008314\*tempk))  
   
 CO2 <- data$Cm/KH  
   
 x <- Kr/Kf\*(Vh/CO2)  
 y <- Vpmax-Vh + kp \* Kr/Kf \*(Vh/CO2)  
 z <- -Vh\*kp  
   
   
 HCO3 <- (-y + sqrt(y^2 - 4\*x\*z))/(2\*x)  
   
 data$Vp <- (HCO3\*Vpmax)/(HCO3+kp)   
   
 #Quadratic coefficients to calculate A  
 a <- 1 - ((alpha\*Kc)/(uoc\*Ko))  
 b <- -( (data$Vp - Rm + data$gbsPa \* data$Cm) + (Vcmax - Rlight) + data$gbsPa\*(Kc \* (1 + (Om/Ko))) +   
 ( (alpha/uoc)\*(sm\_gamma \*Vcmax + Rlight \* Kc/Ko)) )  
 c <- (Vcmax - Rlight)\*(data$Vp - Rm + data$gbsPa\*data$Cm) -   
 (Vcmax\*data$gbsPa \* sm\_gamma \* Om + Rlight\* data$gbsPa\*(Kc\*(1+(Om/Ko))) )  
   
 data$Amod <- (-b - sqrt(b^2 - 4\*a\*c))/2\*a  
   
   
 #discrimination factors for D13C model  
 f<-11.6 #fractionation during photorespiration  
 a\_b<- 2.9 #fractionation during difussion through the leaf boundary layer  
 a\_s <- 4.4 #13C fractionation due to diffusion in air  
 a\_w <- 1.8 #Summed discriminations against 13C during liquid phase diffusion and dissolution  
 a\_b<- 2.9 #fractionation during difussion through the leaf boundary layer  
 s <- 1.8 #Fractionation during leakage of CO2 out of the bundle-sheath cells   
   
   
 data$Cbs <- data$Cm + (data$Vp - data$Photo - Rm)/ data$gbsPa # Equation 4.5 von caemmerer 2000  
   
   
 Vc <- (data$Cbs\*Vcmax)/(data$Cbs+Kc\*(1+(Os/Ko))) # Equation 4.7 von caemmerer 2000  
 Vo <- 2\*big\_gamma\*Vc/data$Cbs# Equation 4.8 von caemmerer 2000  
   
   
   
 data$b3p <- 30 # fractionation by Rubisco   
 data$b3<-data$b3p-((data$e\*Rlight + f\*Vo\*0.5) /Vc)  
   
 # Net fractionation by CO2 dissolution, hydration, and PEPc activity  
 data$b4p <- -(9.483\*1000)/ (273 + data$Tleaf) + 23.89 +2.2 #data$b4' temp dependency  
 data$b4 <- data$b4p\*(1-data$Vp/Vh)+ (1.1+1.1)\*data$Vp/Vh - ((data$e\*Rm)/data$Vp)  
   
   
 data$a\_bar\_Ci <- with(data = data, ( a\_b\*(CaPa-CL) + a\_s\*(CL-CiPa) ) / (CaPa-CiPa) )  
 alpha\_ac <- 1 + data$a\_bar\_Ci /1000   
   
 g\_ac <- data$CndCO2  
 data$t <- alpha\_ac\*data$E/(2\*g\_ac)   
   
 data$phi <- (data$gbsPa \* (data$Cbs - data$Cm)) / data$Vp  
   
 data$D13C\_mod <- with( data = data, 1/(1-t) \* ( a\_b\*(CaPa-CL)/CaPa + a\_s\*(CL-CiPa)/CaPa) +   
 (1+t)/(1-t) \* ( a\_w \*(CiPa - Cm)/CaPa +   
 (data$b4 + phi\*(data$b3\* Cbs/(Cbs - Cm)- s)) \* Cm / ((1 + (phi\*Cm)/(Cbs - Cm))\*CaPa ) ))  
   
 return(data)  
   
}

Measuring distance between observed and modeled values

measure\_distance2 <- function(gbs\_gm,data) {   
 diff\_A <- data$Photo - C4\_combined\_model\_CAlim(gbs\_gm, data)$Amod   
 diff\_D13C <- data$Dobs - C4\_combined\_model\_CAlim(gbs\_gm, data)$D13C\_mod  
 sum((diff\_A/data$Photo)^2, (diff\_D13C/data$Dobs)^2)  
}

Writing the dataset with the results for the CAsat model created using the optim function

results\_gmCAlim<- map2\_df(.x = gbs\_gm2\_start,  
 .y = gm2\_list,  
 .f = ~ data.frame (C4\_combined\_model\_CAlim(gbs\_gm = Reduce(cbind,   
 optim(.x, measure\_distance2, data = .y)$par),data =.y),  
 Sum.diff = optim(.x, measure\_distance2, data = .y)$value) )  
  
write.csv(results\_gmCAlim, "submission 2019/results\_gmCAlim.csv", row.names = FALSE)

#### CAlim+PPDK model

Reading data set for the ombined C4-enzyme-limited photosynthesis model and the 13C discrimination model for the CAlim+PPDK

gbs\_gm3\_start\_df <- read.csv("submission 2019/start\_gmPPDKlim0.csv")#Loads starting values for the model  
  
gm3<- cbind(d0,gbs\_gm3\_start\_df)#Joins input data and starting values for the model

Creates a list of vectors with starting values for gm and gbs for the CAlim+PPDK model

gm3\_list <- gm3 %>%  
 group\_split(.tbl = ., id) # Splits dataset by Growth and measured temperature  
  
  
gm3\_gbsPa <- gm3 %>%  
 group\_split(.tbl = ., id) %>%  
 map("gbsPa") %>% map\_dbl(mean) # Creates a vector with the mean values for gbs for the splitted dataset  
  
gm3\_gm <- gm3 %>%  
 group\_split(.tbl = ., id) %>%  
 map("gmPa") %>% map\_dbl(mean) # Creates a vector with the mean values for Cm for the splitted dataset  
  
gbs\_gm3\_start <- mapply(c, gm3\_gbsPa , gm3\_gm , SIMPLIFY = FALSE) #Creates a list of vectors with paired values of gbs and Cm

Combined C4-enzyme-limited photosynthesis and the 13C discrimination for the CAlim+PPDK model

The equations with their descriptions can be found in the Supporting Information Table S1

C4\_combined\_model\_CAPPDKlim<- function (gbs\_gm,data ) {  
   
 data$dummy25<-ifelse(data$GrowthTemp=="25C",1,0)  
 data$dummy14<-ifelse(data$GrowthTemp=="14C",1,0)  
   
 # Variables for a  
 alpha <- 0   
   
 #Parameters with temperature dependencies  
 temp <- data$Tleaf  
 tempk <- temp + 273.15  
 R <- 0.008314  
 tk25 <- 298.15  
   
 Kc <- 121\*exp((64.2\*(tempk-tk25))/(tk25\*R\*tempk))   
 uoc <- 0.047\*exp( (- 1.63/R)\*(1/tk25 - 1/tempk ))   
 Ko <- 29200\*exp((10.5\*(tempk-tk25))/(tk25\*R\*tempk))   
   
 data$gbsPa <- gbs\_gm[1]  
 data$gmPa <- gbs\_gm[2]  
 data$Cm <- data$CiPa - data$Photo / data$gmPa  
   
 Om <- 210000\*data$Press/1000   
 Os <- Om + (alpha \* data$Photo/(uoc\*data$gbsPa))\*data$Press  
   
 #variables for "b" in the quadratic equation for the C4 enzyme limited model  
   
 #Vpmax temperature dependcy setaria Boyd 2015  
 Vpmax25 <- 300.5\*data$dummy14 + 491.7\*data$dummy25   
 deltas <- 0.25  
 hd <- 73.3  
 Ea\_Vpmax <- 94.8  
 Vpmax <- Vpmax25\*exp(Ea\_Vpmax\*((tempk-tk25)/(tk25\*R\*tempk)))\*  
 (1+exp((tk25\*deltas-hd)/(tk25\*R)))/(1+exp((tempk\*deltas-hd)/(tempk\*R)))  
   
 #Vcmax temperature dependency setaria Yin et al., 2011  
 k25\_Vcmax <- 58.3\*data$dummy14 + 47.1\*data$dummy25   
 Vcmax <- k25\_Vcmax\*exp((53.4\*(tempk-tk25))/(tk25\*R\*tempk))  
   
 # PPDK temperature dependency setaria Boyd et al (2015)  
 k25\_VPPDKmax <- 58.1\*data$dummy14 + 47.2\*data$dummy25   
 data$Vpr <- k25\_VPPDKmax\*exp((56.7\*(tempk-tk25))/(tk25\*R\*tempk))  
   
   
 #Rubisco specificity setaria Boyd 2015  
 sco <- 1310\*exp(-31.1\*(tempk-tk25)/(tk25\*R\*tempk))  
 sm\_gamma <- 0.5/sco #Half the reciprocal of the Rubisco specificity (von Caemmerer, 2000)  
 big\_gamma <- sm\_gamma\*Os  
   
 #Kp temperature dependency setaria Boyd 2015  
 kp <- 30 \* exp((27.2 \* (tempk - tk25))/(tk25 \*R\* tempk))   
   
   
 Rlight <- data$Rlight  
 Rm <- .5 \* data$Rlight  
  
   
 #kca temperature dependency setaria Boyd 2015  
 k25 <- 23.2\*data$dummy14 + 39.8\*data$dummy25   
 Ea <- 40.9  
 deltas <- 0.21  
 hd <- 64.5  
 kca <- k25\*exp(Ea\*(tempk-tk25)/(tk25\*R\*tempk))\*  
 ((1+exp((tk25\*deltas-hd)/(tk25\*R)))/(1+exp((tempk\*deltas-hd)/(tempk\*R)) ))   
   
 Vh <- data$Cm\*kca  
   
 KH <- 2.9799\*exp(-2400\*((1/tempk)-(1/298.15)))  
   
 Kf <- 0.0389858 \* exp((74.8936\*( tempk-298.15))/(298.15\*0.008314\*tempk))  
 Kr <- 0.00332955 \* exp((65.2704\*( tempk-298.15))/(298.15\*0.008314\*tempk))  
   
 CO2 <- data$Cm/KH  
   
 x <- Kr/Kf\*(Vh/CO2)  
 y <- Vpmax-Vh + kp \* Kr/Kf \*(Vh/CO2)  
 z <- -Vh\*kp  
   
   
 HCO3 <- (-y + sqrt(y^2 - 4\*x\*z))/(2\*x)  
   
   
 data$Vp\_app <- (HCO3\*Vpmax)/(HCO3+kp)  
   
 data$Vp <- min(data$Vp\_app, data$Vpr)   
   
 #Quadratic coefficients to calculate A  
 a <- 1 - ((alpha\*Kc)/(uoc\*Ko))  
 b <- -( (data$Vp - Rm + data$gbsPa \* data$Cm) + (Vcmax - Rlight) + data$gbsPa\*(Kc \* (1 + (Om/Ko))) +   
 ( (alpha/uoc)\*(sm\_gamma \* Vcmax + Rlight \* Kc/Ko)) )  
 c <- (Vcmax - Rlight)\*(data$Vp - Rm + data$gbsPa\*data$Cm) -   
 (Vcmax\*data$gbsPa \* sm\_gamma \* Om + Rlight\* data$gbsPa\*(Kc\*(1+ (Om/Ko))) )  
   
 data$Amod <- (-b - sqrt(b^2 - 4\*a\*c))/2\*a  
   
   
 #discrimination factors for D13C model  
 f<-11.6 #fractionation during photorespiration  
 a\_b<- 2.9 #fractionation during difussion through the leaf boundary layer  
 a\_s <- 4.4 #13C fractionation due to diffusion in air  
 a\_w <- 1.8 #Summed discriminations against 13C during liquid phase diffusion and dissolution  
 a\_b<- 2.9 #fractionation during difussion through the leaf boundary layer  
 s <- 1.8 #Fractionation during leakage of CO2 out of the bundle-sheath cells   
   
 data$Cbs <- data$Cm + (data$Vp - data$Photo - Rm)/ data$gbsPa # Equation 4.5 von caemmerer  
   
   
 Vc <- (data$Cbs\*Vcmax)/(data$Cbs+Kc\*(1+(Os/Ko))) # Equation 4.7 von caemmerer  
 Vo <- 2\*big\_gamma\*Vc/data$Cbs# Equation 4.8 sussane von caemmerer  
   
   
   
 data$b3p<-30 # fractionation by Rubisco   
 data$b3<-data$b3p-((data$e\*Rlight + f\*Vo\*0.5) /Vc)  
   
 # Net fractionation by CO2 dissolution, hydration, and PEPc activity  
 data$b4p <- -(9.483\*1000)/ (273 + data$Tleaf) + 23.89 +2.2 #data$b4' temp dependency  
 data$b4 <- data$b4p\*(1-data$Vp/Vh)+ (1.1+1.1)\*data$Vp/Vh - ((data$e\*Rm)/data$Vp)  
   
   
 data$a\_bar\_Ci <- with(data = data, ( a\_b\*(CaPa-CL) + a\_s\*(CL-CiPa) ) / (CaPa-CiPa) )  
 alpha\_ac <- 1 + data$a\_bar\_Ci /1000   
   
 g\_ac <- data$CndCO2  
 data$t <- alpha\_ac\*data$E/(2\*g\_ac)  
   
 data$phi <- (data$gbsPa \* (data$Cbs - data$Cm)) / data$Vp  
   
 data$D13C\_mod <- with( data = data, 1/(1-t) \* ( a\_b\*(CaPa-CL)/CaPa + a\_s\*(CL-CiPa)/CaPa) +   
 (1+t)/(1-t) \* ( a\_w \*(CiPa - Cm)/CaPa + (data$b4 + phi\*(data$b3\* Cbs/(Cbs - Cm)- s)) \* Cm / ((1 + (phi\*Cm)/(Cbs - Cm))\*CaPa ) ))  
   
 return(data)  
   
}

Measuring distance between observed and modeled values

measure\_distance3 <- function(gbs\_gm,data) {   
 diff\_A <- data$Photo - C4\_combined\_model\_CAPPDKlim(gbs\_gm, data)$Amod   
 diff\_D13C <- data$Dobs - C4\_combined\_model\_CAPPDKlim(gbs\_gm, data)$D13C\_mod  
 sum((diff\_A/data$Photo)^2, (diff\_D13C/data$Dobs)^2)  
}

Writing the dataset with the results for the CAlim+PPDK model created using the optim function

results\_gmCA\_PPDKlim<- map2\_df(.x = gbs\_gm3\_start,  
 .y = gm3\_list,  
 .f = ~ data.frame (C4\_combined\_model\_CAPPDKlim(gbs\_gm = Reduce(cbind,   
 optim(.x, measure\_distance3, data = .y)$par), data =.y),  
 Sum.diff = optim(.x, measure\_distance3, data = .y)$value) )  
  
write.csv(results\_gmCA\_PPDKlim, "submission 2019/results\_gmCA\_PPDKlim.csv", row.names = FALSE)