

Getting Functionnal-structural plant model into a pipeline: MARSHAL-pipeline

Adrien Heymans, Felicien Meunier, and Guillaume Lobet

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Introduction

The coupling of models with one another can be used to find relevant sequence of information. This can create a network of data that can be used to answer complex questions which interconnect multiscale or disciplinary frame (Passot et al. 2018). Depending of the models, the complexity of the system is significantly increase. Here, the system on which this pipeline works is a below ground system. It focuses on solving the hydraulic architecture of a root system. To illustrate the necessity of merging models together, we start by the fact that **MARSHAL** need an explicit root system architecture to add on the hydraulic part. **CRootBox** is precisely a model that compute the explicit root system architecture (Schnepf et al. 2018) and MARSHAL was designed to accept easily the CRootBox output. Dealing with models as an input for another model will also increase the dynamic approach of the overall (Passot et al. 2018). The

How to use MARSHAL in a R environment

To run this example, the marshal package is required. This package can be found on GitHub.

or by simply execute the following line in the R environment:

```
install.packages("devtools")
library(devtools)
install_github("MARSHAL-ROOT/marshall")
library(marshall)
```

MARSHAL is built upon a handful of other packages that need to be loaded. One group of function has to be loaded manually.

```
library(data.table)
library(tidyverse)
library(Matrix)
library(readxl)
library(cowplot)
library(xml2)
library(knitr)

`%!in%` <- compose(`!`, `%in%`)

source("R/io_function.R")
```

Once it is installed, the boundary condition on which the model works should be implemented.

Boundary condition of MARSHAL.

The boundary condition of MARSHAL are :

- The hydraulic properties of the roots.
- The water potential of the soil.
- The root system architecture.
- The initial pressure strength that pull water out of the collar.

Hydraulic properties of the root system

The hydraulic properties of the root system can be found in the litterature, by measuring it on root samples or with the helps of modelling tools as well. Here, the conductivities of the root come from the Doussan et al. paper (1998). To show some possibilities, three scenarios in total were built from this Doussan et al. table of conductivities (figure 1). The first, which is the original values placed along the root axes from the apex. The second, is based on the first but the maturity of the root anatomy is advanced of 5 cm towards the apex. And the third, is the opposite of the second, or in other words, the maturity of the root anatomy, insted of being advance towards the apex, is moved of 5 cm backwards.

The conductivities of the different root type.

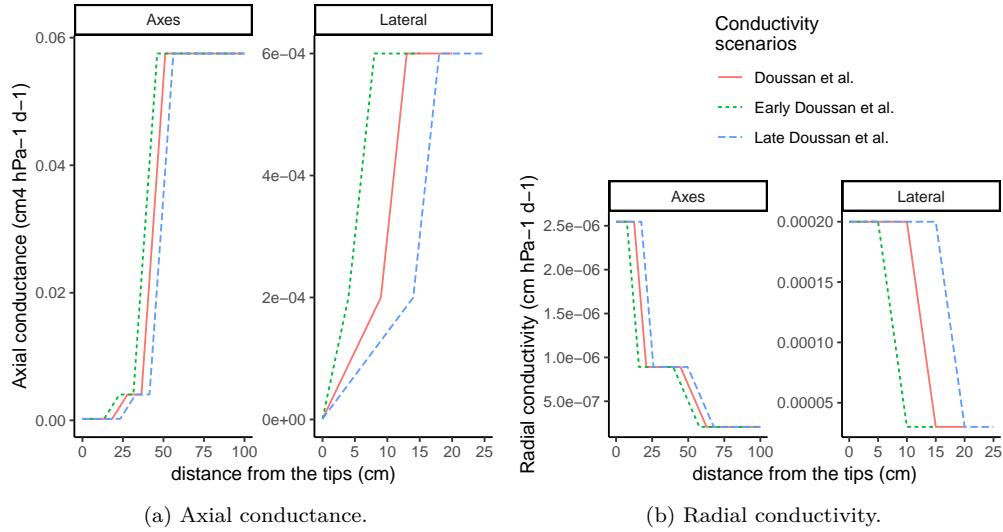


Figure 1: Conductivities properties on axes and lateral root type.

Root system architecture with CRootBox

Modelling root system architecture can be achieve with CRootBox for instance (Schnepf et al. 2018). Some examples of the parametre files for a couples of specieses are details in the *modelparameter* folder, which is linked to the CRootBox repository.

For the purpose of the example we choose to work with three parameter files of maize:

- *Zea_mays_3_Postma_2011*
- *Zea_mays_1_Leitner_2010*
- *Zea_mays_4_Leitner_2014*

The following lines of code allows to create five unique root system architectures for each parameter files. It computes the root growth during 60 days and load every ten days the architecture information in a data table. Inside the CRootBox implementation for this example, the root growth has been restricted to the below ground level for a more realistic point of view. Furthermore, some segments were not build up to the whole root system because they were shorter than the spatial resolution of the root system.

```

# Number of repetition per root system architecture example
nrep <- 5

# List of three CrootBox parameter files for corn
param_choise <- c("Zea_mays_1_Leitner_2010",
                  "Zea_mays_3_Postma_2011",
                  "Zea_mays_4_Leitner_2014")

all_roots <- NULL
for(param_name in param_choise){
  # Load param of the selected example
  rparam <- read_rparam(path = paste0("./www/", param_name, ".rparam"))
  pparam <- read_pparam(path = paste0("./www/", param_name, ".pparam"))
  # Overwrite the param files that will be use
  write_rparam(rparam, "./www/param.rparam")
  write_pparam(pparam, "./www/param.pparam")

  for(i in c(1:nrep)){
    #####
    # Run CRootBox #
    #####
    system("www/a.exe")

    # Get all the .txt files exported by CRootBox
    fls <- list.files("./")
    fls <- fls[grep1("rootsystem.txt", fls)]

    for(f in fls){
      temp <- fread(f, header = T)
      temp$age <- strsplit(f, "_")[[1]][1]
      temp$rep <- i
      temp$ex <- param_name
      # Save the temporary data in a permanent file to use.
      all_roots <- rbind(all_roots, temp)
    }
  }
}

# Saving the root system information in a .csv
write_csv(all_roots, "all_roots.csv")

# To gain time once you have a all_roots.csv file created
# Loading the .csv file can be achieve with:
all_roots <- read.csv("all_roots.csv")

```

The figure 2 shows the root system architectures that come out CRootBox at the half of the simulation time (30 days).

Architectural phenes

Once the complete root system architecture is computed there are a number of architectural phenes that we can access.

- the area of the convex hull
- the rooting depth

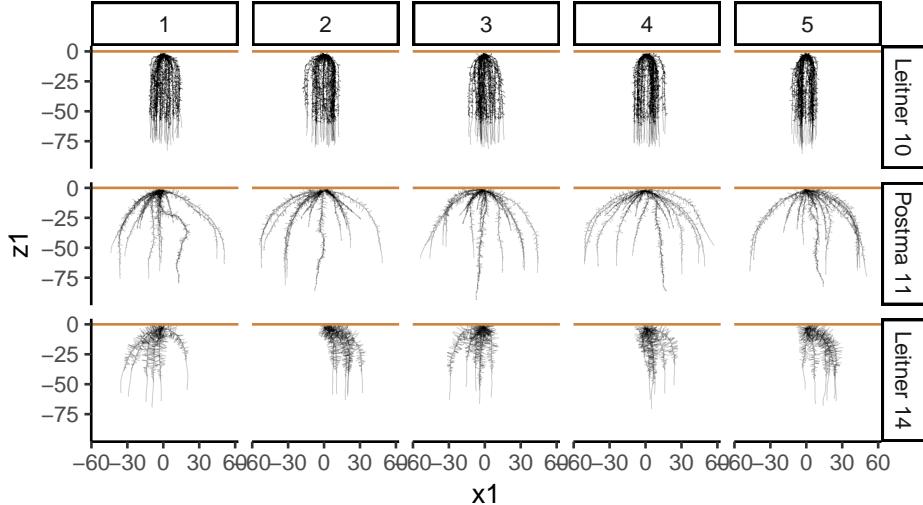


Figure 2: Projection in two dimensions of the different root systems computed with CRootBox at the age of 30 days

- the root length density along the soil profile
- the number of individual roots per root system
- the total length of the root system
- ...

here we summarize briefly with a couple of figure, the different architectural phenes which can be mesured.

The convex hull

The convex hull is one of the most commun known traits to works with. It gives a qualitative information about root exploration. To find the convex hull with an explicit root system in 3D is straight forwards. Thanks to the chull function, we are able to identify all the coordinates that make the convex hull and the Polygon function in the sp package allows us to determine the area of the convex hull.

```
root_20 <- all_roots%>%
  filter(age %in% c("20", "40", "60"))
pol_ch = poly_area<- NULL
for(i in unique(all_roots$ex)){
  for(j in unique(all_roots$rep)){
    for(ag in unique(root_20$age)){
      for(xy in c("x", "y")){# get the convex hull from two sides
        tmp <- root_20%>%
          filter(ex == i, rep == j, age == ag)%>%
          select(paste0(xy, "2"), z2, ex, rep, age)
        # select(x2,z2, ex, rep, age)
        first_col <- tmp[,1]
        x <- matrix(c(first_col, tmp$z2), nc = 2)
        # Get the incices of the unique points lying on the convex hull
        ch <- chull(x= first_col, y = tmp$z2)
        ch <- c(ch, ch[1])

        # Area of the convex hull
        xy.coords <- cbind(first_col, tmp$z2)
        chull.coords <- xy.coords[ch,]
```

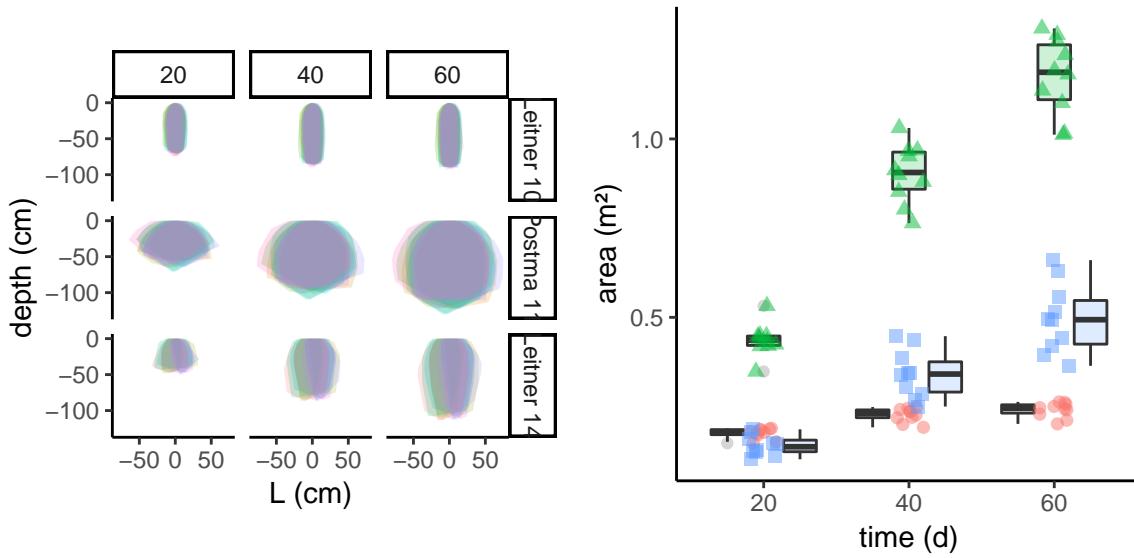


Figure 3: Area of the convex hull for the different root system architecture examples. \triangle = Postma 2011, \square

Thanks to the details information, we can measure some root phenes along the z axis. The maximal rooting depth is an interesting phenotypic value. This can even be used in other models such as hydrus1D to estimate

```
# Summarise the total root length and the rooting depth information.
RLD <- all_roots %>%
  mutate(age = as.numeric(age)) %>%
  group_by(age, rep, ex) %>%
  summarise(root = sum(length),
            rooting_depth = min(z2))

RLD2 <- all_roots %>%
  mutate(age = as.numeric(age)) %>%
  group_by(age, rz1 = round(z1/2)*2, # on every two cm of the profile
```

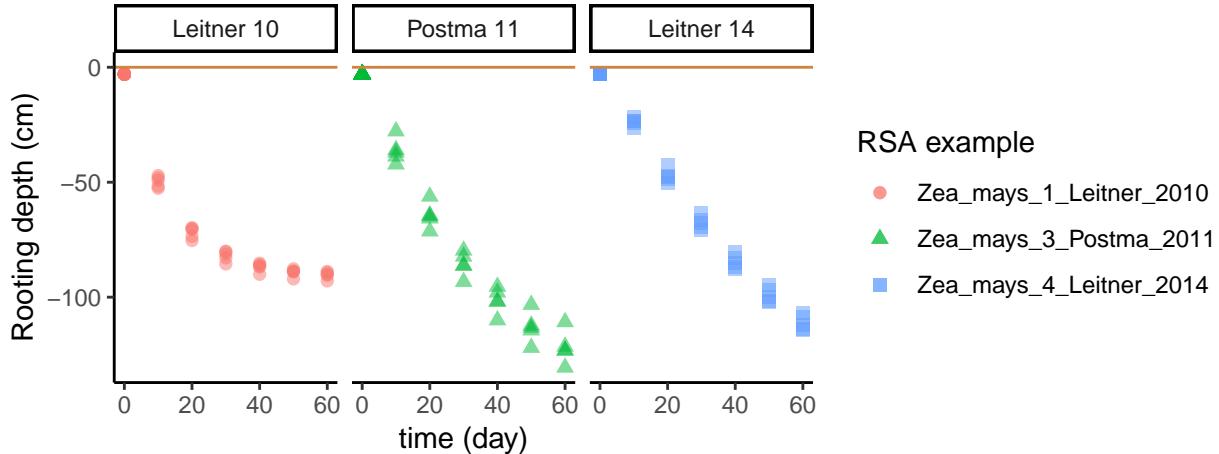


Figure 4: Rooting depth of the different root system examples

```
ex)%>%
summarise(root = sum(length)/nrep)
```

The root lengths

Root length density is a major phenotypic trait measured in field when below ground information are requested. Here we computed the total root length every ten days. So, we can observe that after 60 days, the total root length is more or less the same for the three RSA example, which can be approximate to a similar carbon investment in the root system at that time. King et al. (2003) showed that a more homogenous vertical distribution of the roots should pay back in terms of carbon investments for water uptake. In the **result** section this assumption is developed.

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```

Number of roots.

Although the total root length reaches a close value of ten meter for all the different root systems after 60 days, there is a huge gap in term of number of roots between each of the root system architecture (figure 6).

The water soil potential

The pressure head of the water potential within the soil is created from the following line of code. Here, there are three soil scenarios with three different coefficients for the drying function.

The drying function is :

$$\psi_i = \alpha \times \frac{(Z_i + L)^{10} \times T_i}{L^{10} \times T_{end}} - 230$$

- ψ_i = water potential in the soil at i cm below the surface.
- α = drying coefficient of the soil (-300 = "humid", -7000 = "dry" and -15.000 = "arid").
- Z_i = the depth (cm)
- L = the maximal soil profile depth.
- T = the simulation time (day)
- -230 is the water potential in the soil at the field capacity for a silty soil.

```
# Take the same time variable as the one that were implemented in CRootBox.
full_time <- sort(unique(as.numeric(all_roots$age)))
time_step = full_time[2] - full_time[1]
```

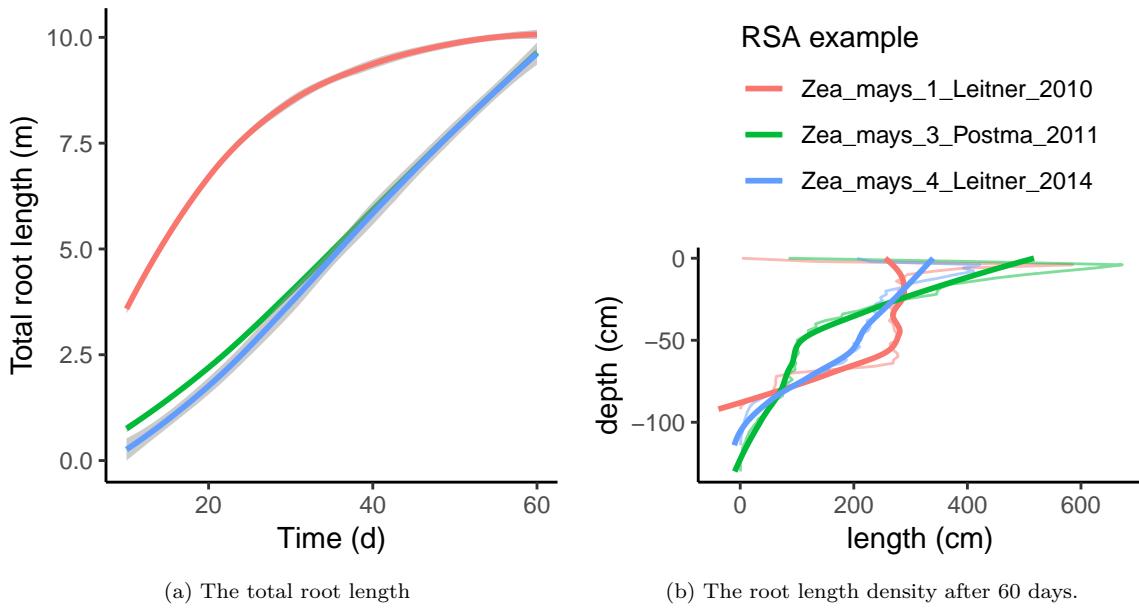


Figure 5: The root lenght

```

endTime = max(full_time)
ntimesteps = endTime/time_step

# Creating some values for the water potential in the soil along the profile depth.
profile_depth <- 150
z <- seq(profile_depth, 0, by = 5)
value <- sort(rep(full_time, length(z)))
psi <- rep(-230, length(value))
z <- rep(z, ntimesteps)

soil <- NULL
# Making three scenarios
for(i in c(-300, -7000, -15000)){
  soil_tmp <- cbind(z, value, psi)%>%
    as.tibble()%>%
    mutate(psi = i*((z+profile_depth)^(10))*value)/
      ((profile_depth^10)*endTime)-230,
    humid = i)
  soil_tmp <- soil_tmp%>%
    mutate(id = 1:nrow(soil_tmp))
  soil<- rbind(soil, soil_tmp)
}

```

The water potential at the collar

Expressed in hecto-Pascal, the pressure head define the transpiration strength that drags the water out of the root system. here we take the default value of -15.000 hPa

```
# Water potential at the collar (hPa)
tpots <- -15000
```

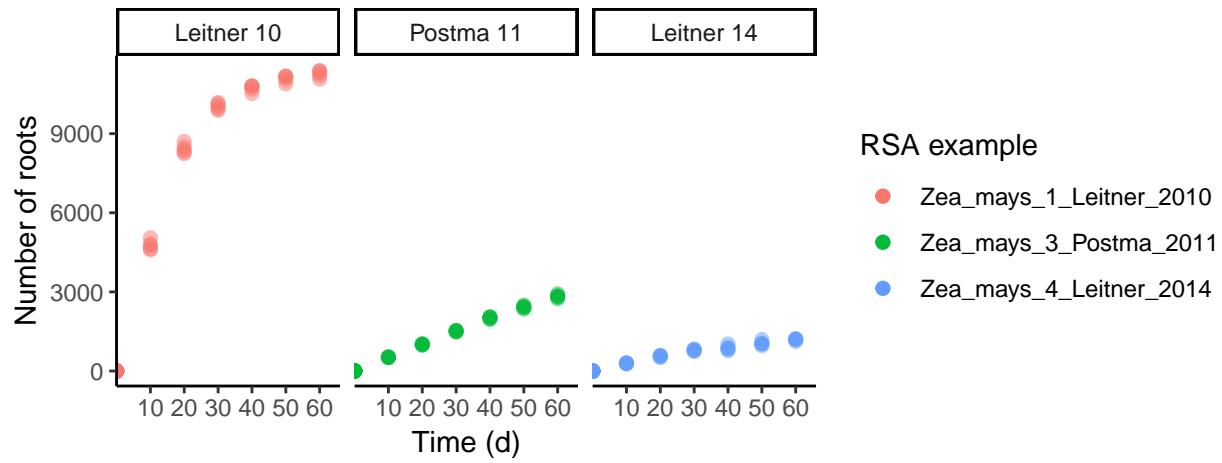


Figure 6: Number of different roots for each of the root system examples.

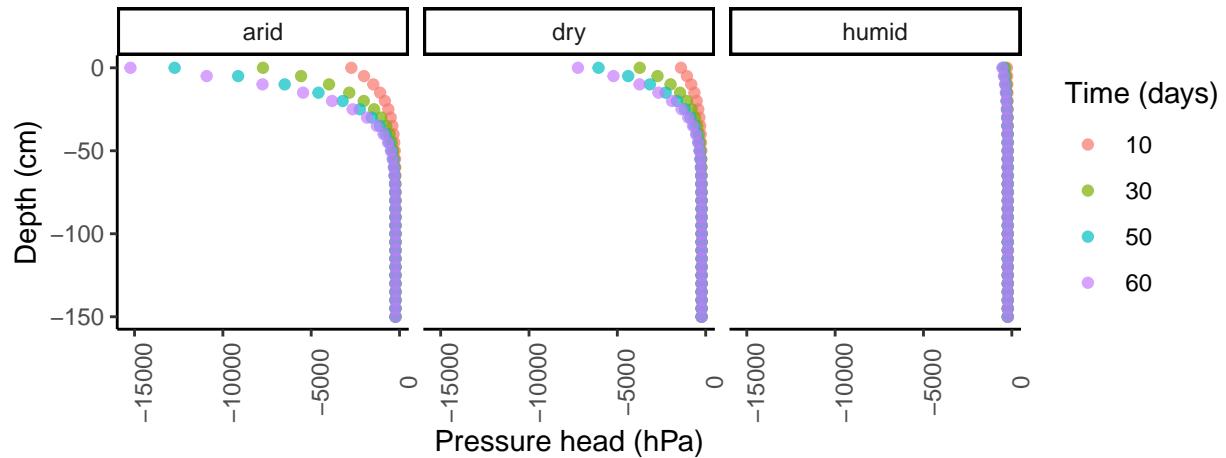


Figure 7: Water potential evolution during the simulation time along the soil profile

MARSHAL

MARSHAL provide an estimation of the conductance of the whole root system, the actual and the potential transpiration. Here we call the MARSHAL function `getSUF` that will solve the hydraulic part of the root system for each soil, conductivities, root system architecture scenarios and at each time step of the process.

```
new_all_roots <- NULL
results<- NULL
k <- 1
# -----
# Computing the root system hydraulic architecture
# -----

#-----
# Total of simulation that will be initiate
# all <- length(unique(all_roots$rep)) * length(unique(conductivities$scenario)) *
#           length(unique(all_roots$age)) * length(unique(all_roots$ex)) *
#           length(unique(soil$humid))
# pb = txtProgressBar(min = 0, max = all, initial = 0, style = 3)
#-----

# Loop to run MARSHAL with the selected simulation parameters.

for(exa in unique(all_roots$ex)){# Example of RSA
  for(re in unique(all_roots$rep)){ # repetition
    for(ag in sort(as.numeric(unique(all_roots$age)))){# age of the RS
      for(sen in unique(conductivities$scenario)){ # hydraulic properties
        for(hum in unique(soil$humid)){ # Scenario of water potential in the soil

          # Progression bar (optional)
          # setTxtProgressBar(pb,k)

          # Select specific Soil for the simulation
          temp_soil <- soil %>%
            filter(value == ag,
                  humid == hum)%>%
            select(-value, -humid)
          # Select specific root system for the simulation
          temp_root <- all_roots %>%
            filter(age == ag,
                  rep == re,
                  ex == exa)%>%
            as.tibble()%>%
            select(-ex)
          # Select specific conductivities
          temp_conduct <- conductivities%>%
            filter(scenario == sen)%>%
            select(-scenario)

          # -----
          # Run MARSHAL
          # -----

          hydraulics <- getSUF(temp_root,
                                temp_conduct,
                                temp_soil,
```

```

        hetero = T,
        Psi_collar = tpots)

# Aggregate output from MARSHAL
results <- rbind(results, data.frame(krs = hydraulics$krs,
                                      tact = hydraulics$tact,
                                      tpot = hydraulics$tpot,
                                      tp = tpots,
                                      scenario = sen,
                                      age = ag,
                                      rep = re,
                                      ex = exa,
                                      humid = hum,
                                      simulation = k))

# Keep the information about the very detail hydrological parameter on
# all the root segment only for one repetition of the plant per simulation.
if(re >= nrep-1){
  # Format dataset to be compatible with MARSHAL output
first <- temp_root[temp_root$node1ID == 0,]
nodals_ids <- unique(temp_root$branchID[temp_root$type == 4 |
                                             temp_root$type == 5])
for(no in nodals_ids){
  temp <- temp_root%>%
    filter(branchID == no)
  temp <- temp[1,]
  connection <- data.frame(node1ID = 0,
                             node2ID = temp$node1ID,
                             branchID = temp$branchID,
                             x1 = first$x1, y1 = first$y1, z1 = first$z1,
                             x2 = temp$x1, y2 = temp$y1, z2 = temp$z1,
                             radius = temp$radius,
                             length = sqrt((first$x1-temp$x1)^2 +
                                           (first$y1-temp$y1)^2 +
                                           (first$z1-temp$z1)^2 ),
                             R = 0, G = 0, B = 0,
                             time = temp$time,
                             type = temp$type,
                             age = temp$age,
                             rep = temp$rep)
  new_table = rbind(temp_root, connection)
  temp_root = new_table
}
temp_root <- temp_root[order(temp_root$node2ID, decreasing = F),]

# Merge output of MARSHAL on specific root segment
temp_root$suf <- as.vector(hydraulics$suf)
temp_root$suf1 <- as.vector(hydraulics$suf1)
temp_root$kx <- as.vector(hydraulics$kx)
temp_root$kr <- as.vector(hydraulics$kr)
temp_root$jr <- as.vector(hydraulics$jr)
temp_root$psi <- as.vector(hydraulics$psi)
temp_root$jxl <- as.vector(hydraulics$jxl)

```

```

temp_root$psi_soil <- as.vector(hydraulics$psi_soil)
# Add the simulation specificity to the dataset
temp_root$scenario <- sen
temp_root$ex <- exa
temp_root$humid <- hum
temp_root$rep <- re
new_all_roots <- rbind(new_all_roots, temp_root)
}
k <- k + 1
}
}
}
}

# Save the results
# write_csv(new_all_roots, "new_all_roots.csv")
# Load the saved results
# new_all_roots <- read.csv("new_all_roots.csv")
new_all_roots <- new_all_roots%>%
  mutate(age = as.numeric(age)*10)

```

Results :

Once the simulation are computed, it is possible to visualize the output on a various form

Standard uptake fraction (SUF)

The Standard uptake fraction is the relative distribution of root water uptake between root segments when water is equally available in space (units: %) (V. Couvreur, Vanderborght, and Javaux 2012).

Where are the segment with the highest contribution for the SUF.

One of the major advantage of the SUF is to estimate where should be the segments which contribute to the water uptake of the plant. Here we focuses on the smallest regions on which 50% of the water uptake occurs in a soil where the water potential is homogenous along the profile.

```

fif <- NULL
for (exa in 1:length(param_choise)) {
  fi <- new_all_roots%>%
    filter(age == 60,
      rep == nrep,
      scenario == "Doussan et al.",
      humid == min(humid),
      ex == param_choise[exa])%>%
    mutate(or_suf = sort(sufi, decreasing = T))

  # Distribution of the suf value
  # fi%>%
  #   ggplot(aes(x=1:nrow(fi), y = or_suf))+
  #   geom_line(color="#69b3a2")+
  #   geom_area(fill="#69b3a2", alpha=0.5)

  i <- 1
}

```

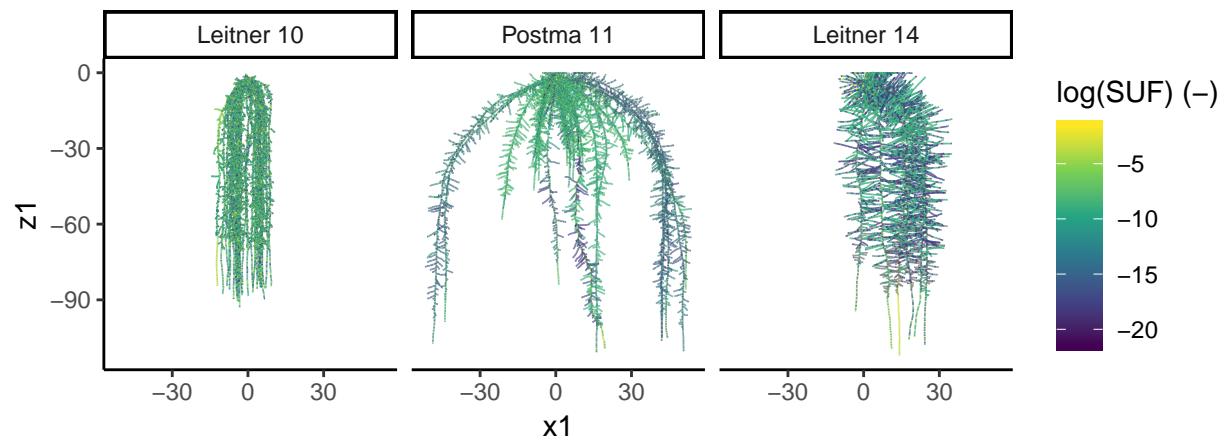


Figure 8: Standard uptake fraction of the different root systsem architecture

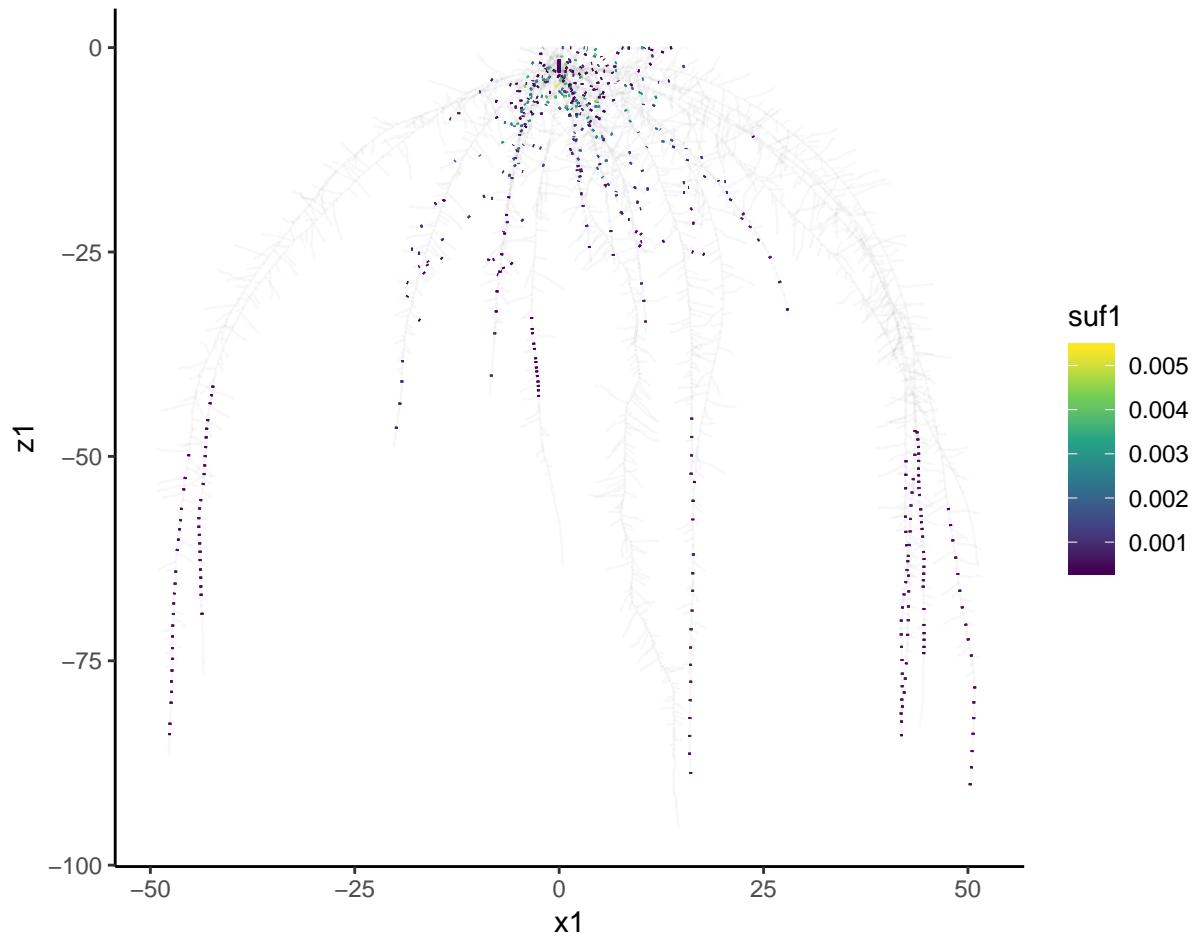


Figure 9: The smallest region on one Postma 2011 RSA example which contains 50 % of the SUF

```

k <- 0
while(k <= 0.5){
  k <- k + fi$or_suf[i]
  i <- i + 1
}
fif <- rbind(fif, c(ex = param_choise[exa], suf = fi$or_suf[i]))%>%
  as.tibble()%>%
  mutate(suf = as.numeric(suf))
}

```

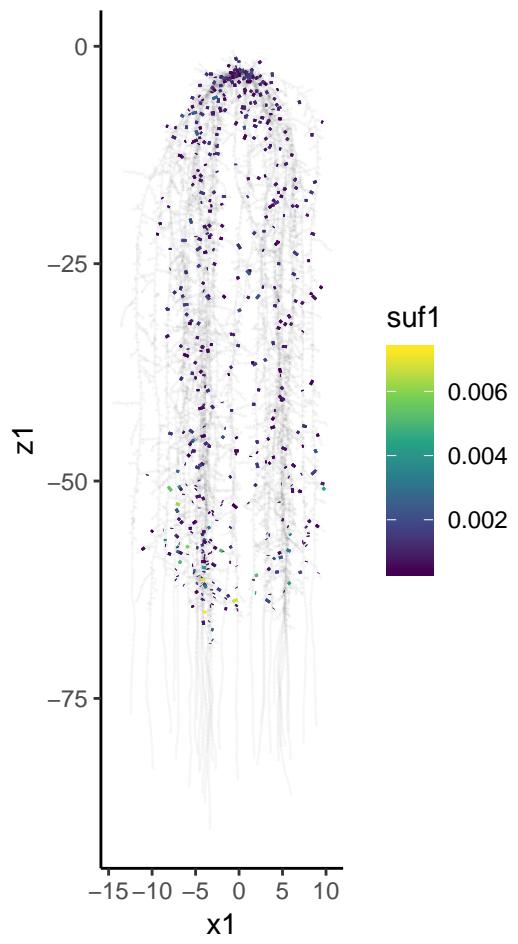


Figure 10: The smallest region on one Leitner 2010 RSA example which contains 50 % of the SUF

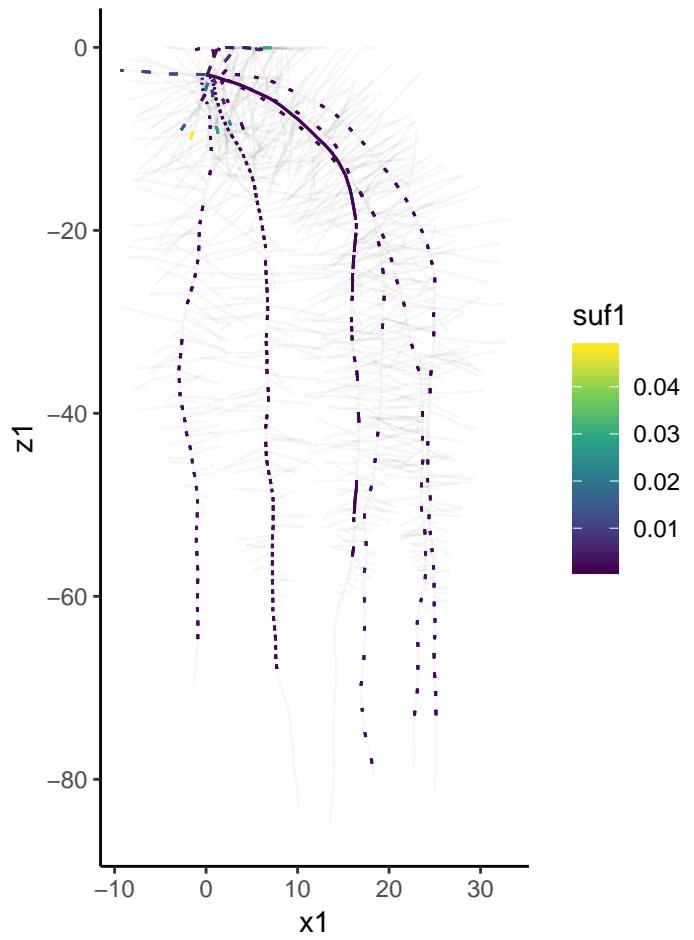


Figure 11: The smallest region on one Leitner 2014 RSA example which contains 50 % of the SUF

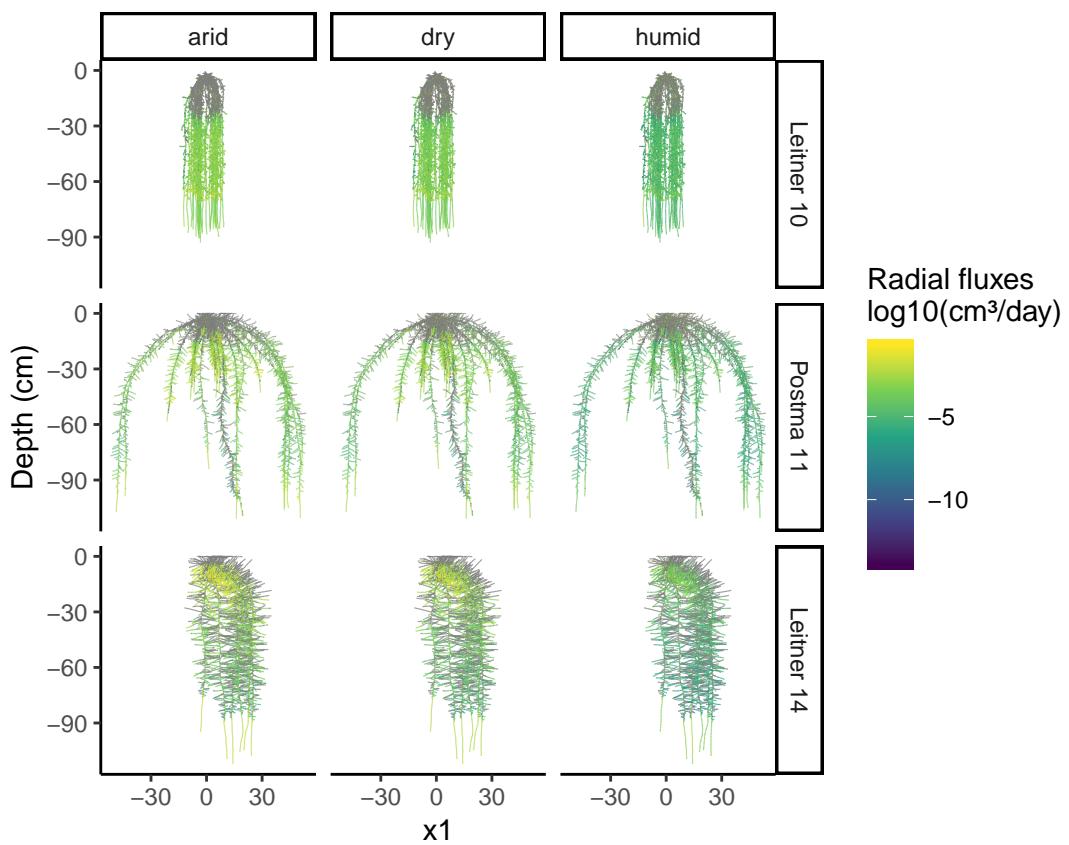


Figure 12: Absorption speed, comparison between the RSA and the soil scenario

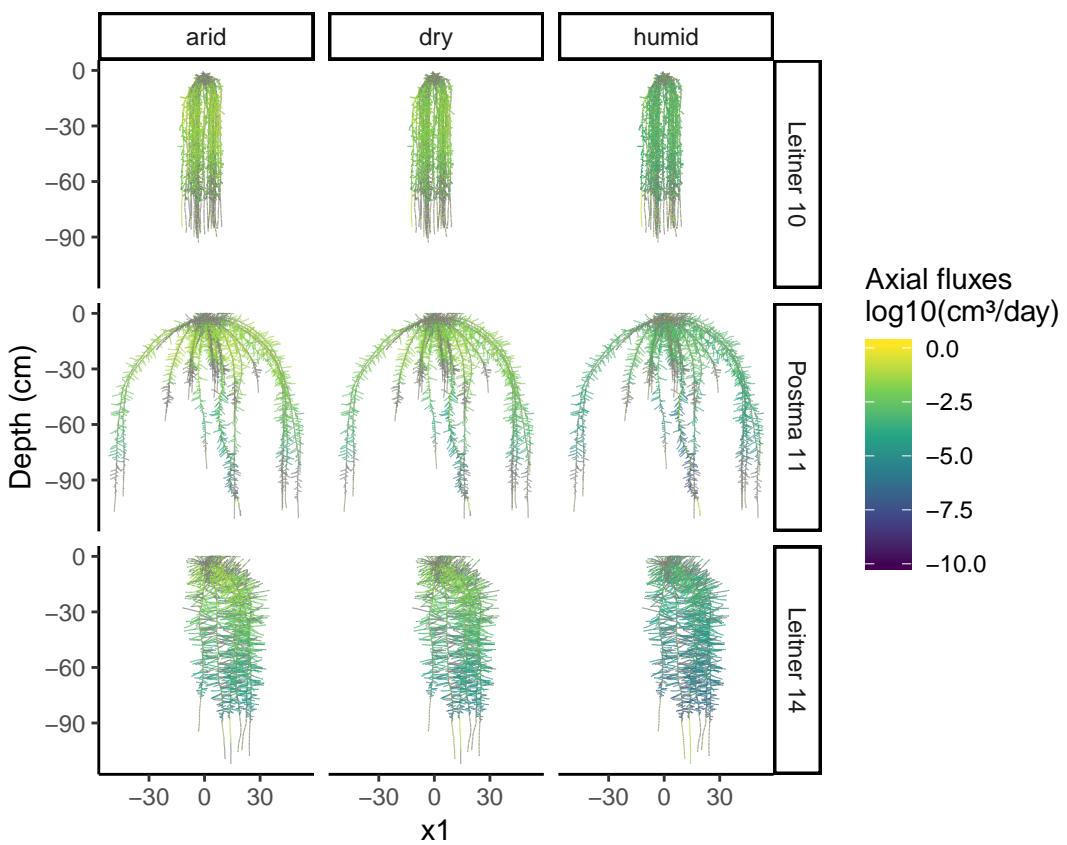


Figure 13: Absorption speed, comparison between the RSA and the soil scenario

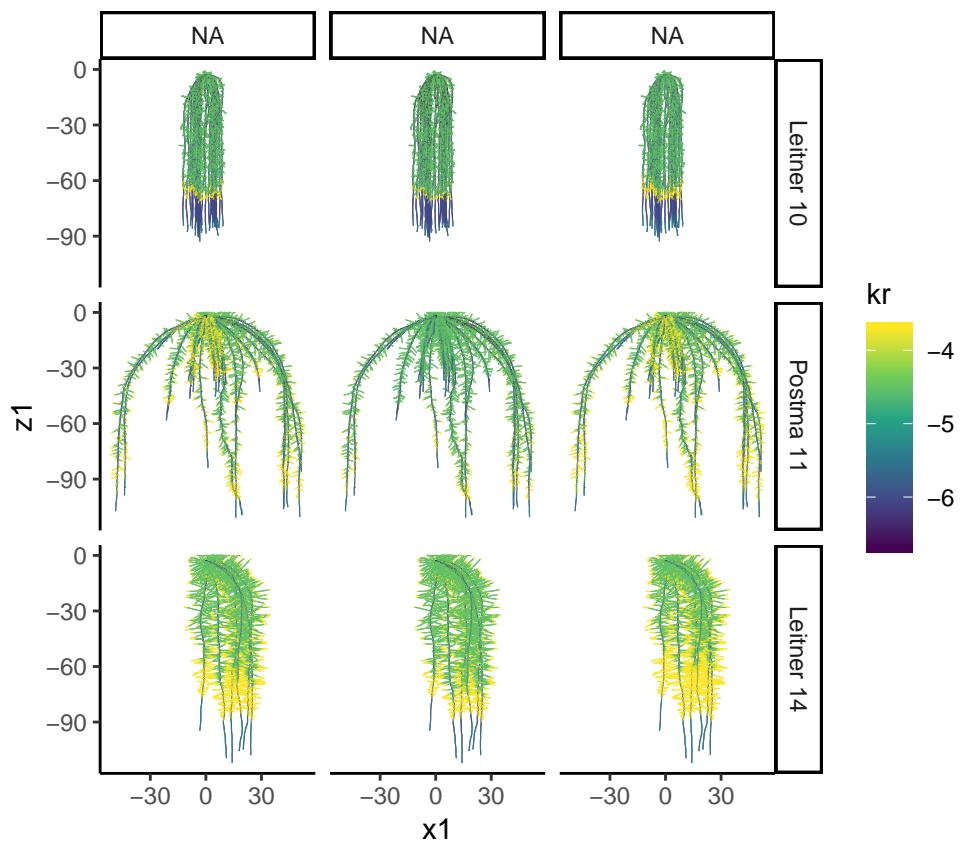


Figure 14: The radial conductivity (Kr) on root segment, comparison between the different conductivity scenario and main root system architecture examples

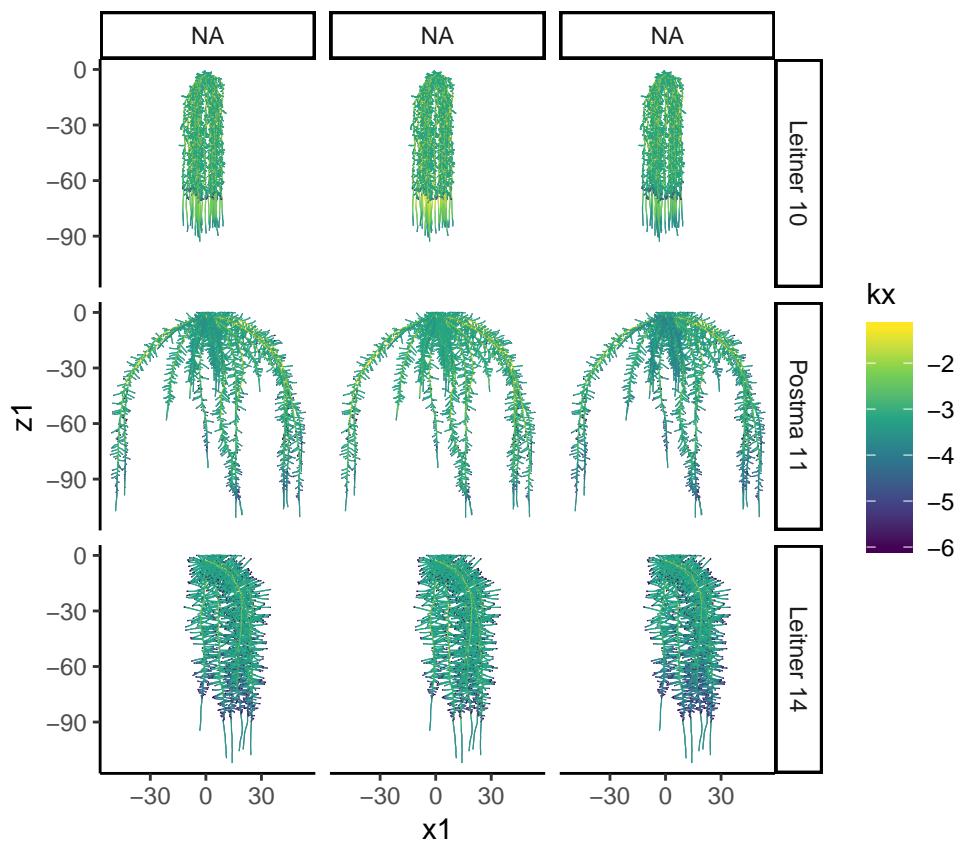


Figure 15: The axial conductance (K_x) on root segment, comparison between the different conductivity scenario and main root system architecture examples

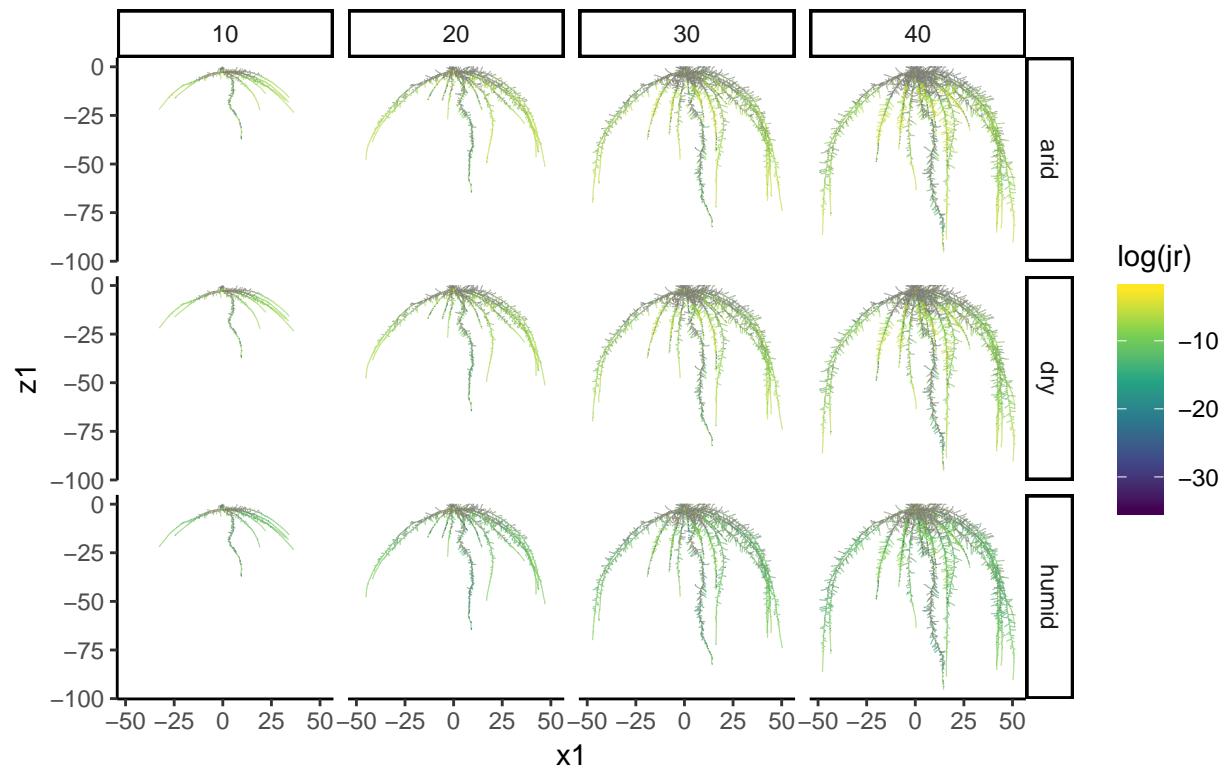


Figure 16: Absorption dynamics due to different soil scenarios on the Postma root system architecture example

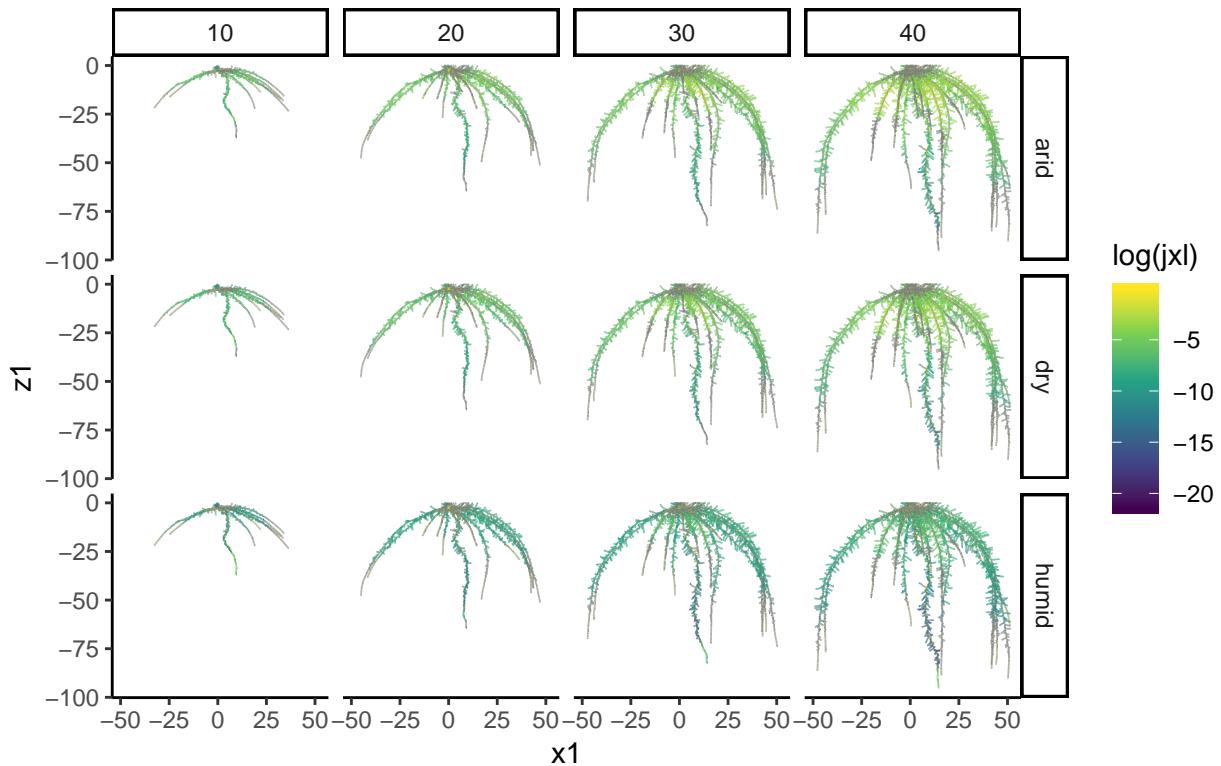
The radial fluxes

The axial fluxes

The radial conductivities

The axial conductance

The evolution of the radial fluxes



To look at the different hydraulic macro-properties along the profile depth, we took the mean values of the variable total on every two centimeters.

```
# For the two repetitions on which we have values on each segment,  
# we take the mean values of the sum of each variables.  
dens <- new_all_roots %>%  
  mutate(age = as.numeric(age)) %>%  
  group_by(type, age, rz1 = round(z1/2)*2, # on every two cm of the profile  
           scenario, ex, humid) %>%  
  summarise(root = sum(length)/2, # The mean of the sum on the two repetitions  
            su = sum(suf)/2,  
            sud = sum(suf/length)/2,  
            su1 = sum(suf1)/2,  
            j = sum(jr)/2,  
            jx = sum(jxl)/2,  
            p = sum(psi)/2,  
            kr = sum(kr)/2)
```

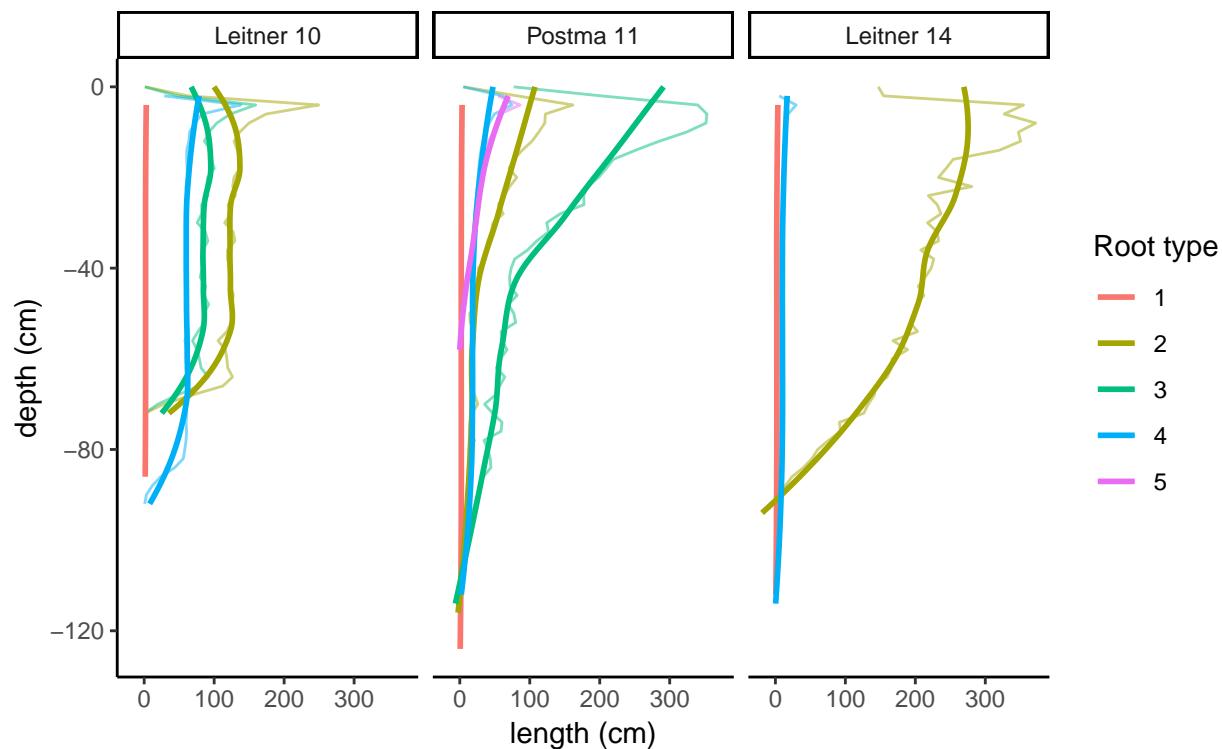


Figure 17: Root length density

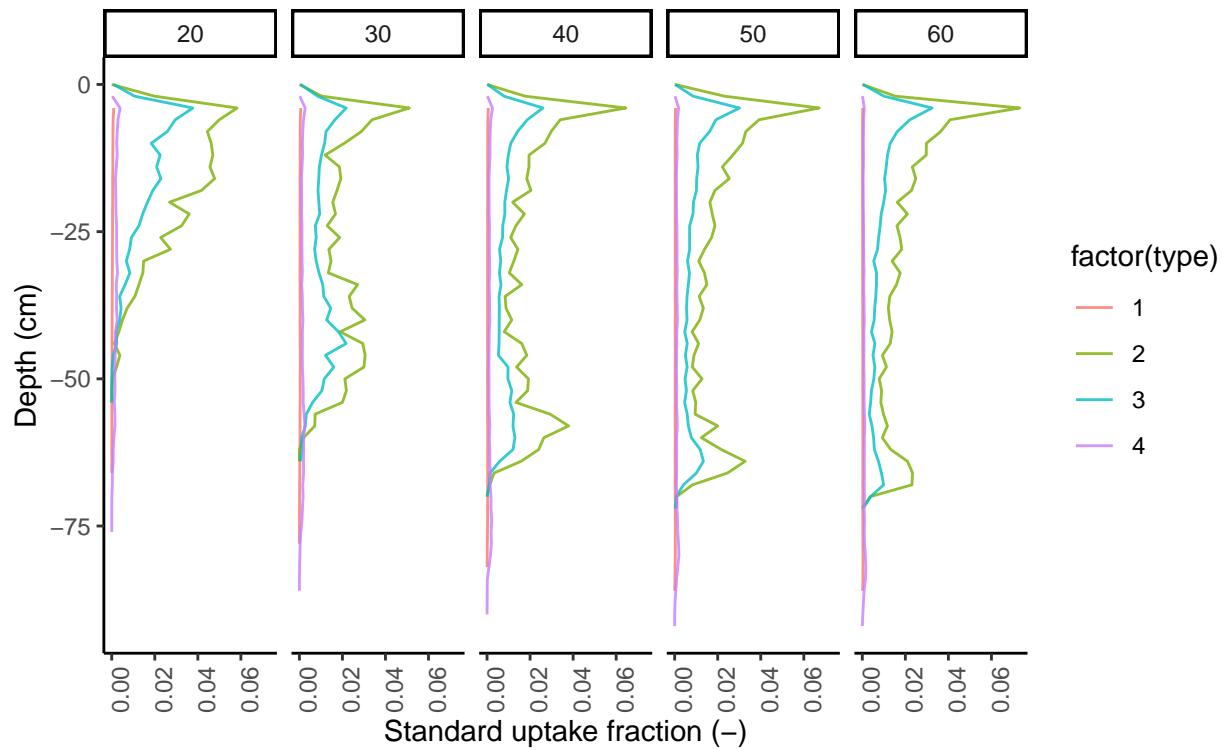


Figure 18: Evolution of the SUF with Leitner 2010 RSA parameter

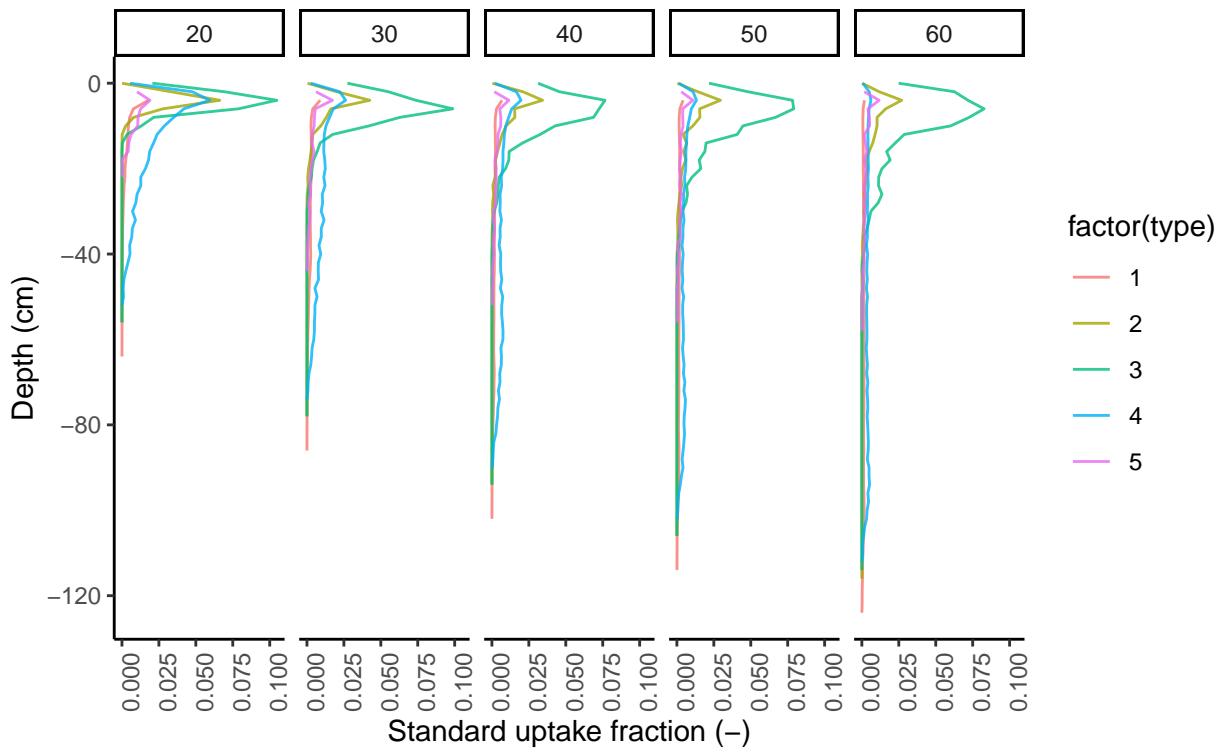


Figure 19: Evolution of the SUF with Postma 2011 RSA parameter

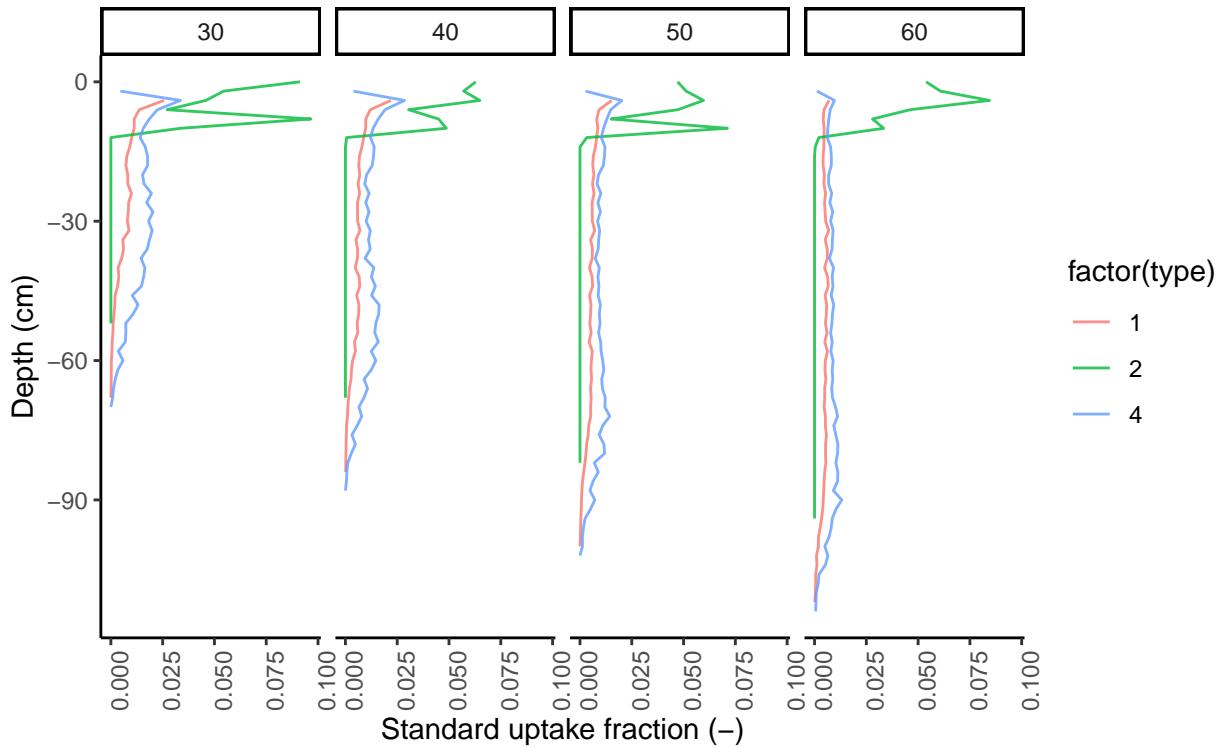


Figure 20: Evolution of the SUF with Leitner 2014 RSA parameter

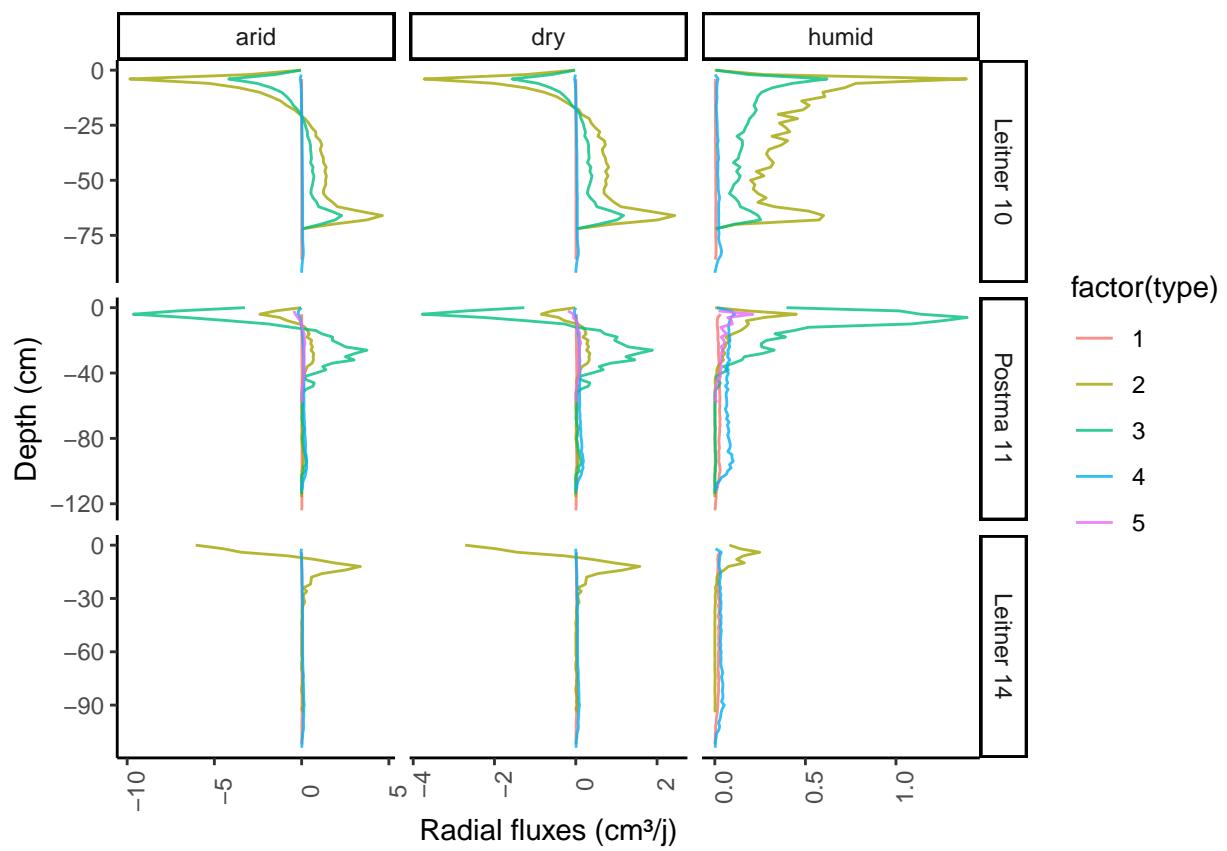


Figure 21: Comparison of the radial fluxes between the different soil scenarios and the root system architectures

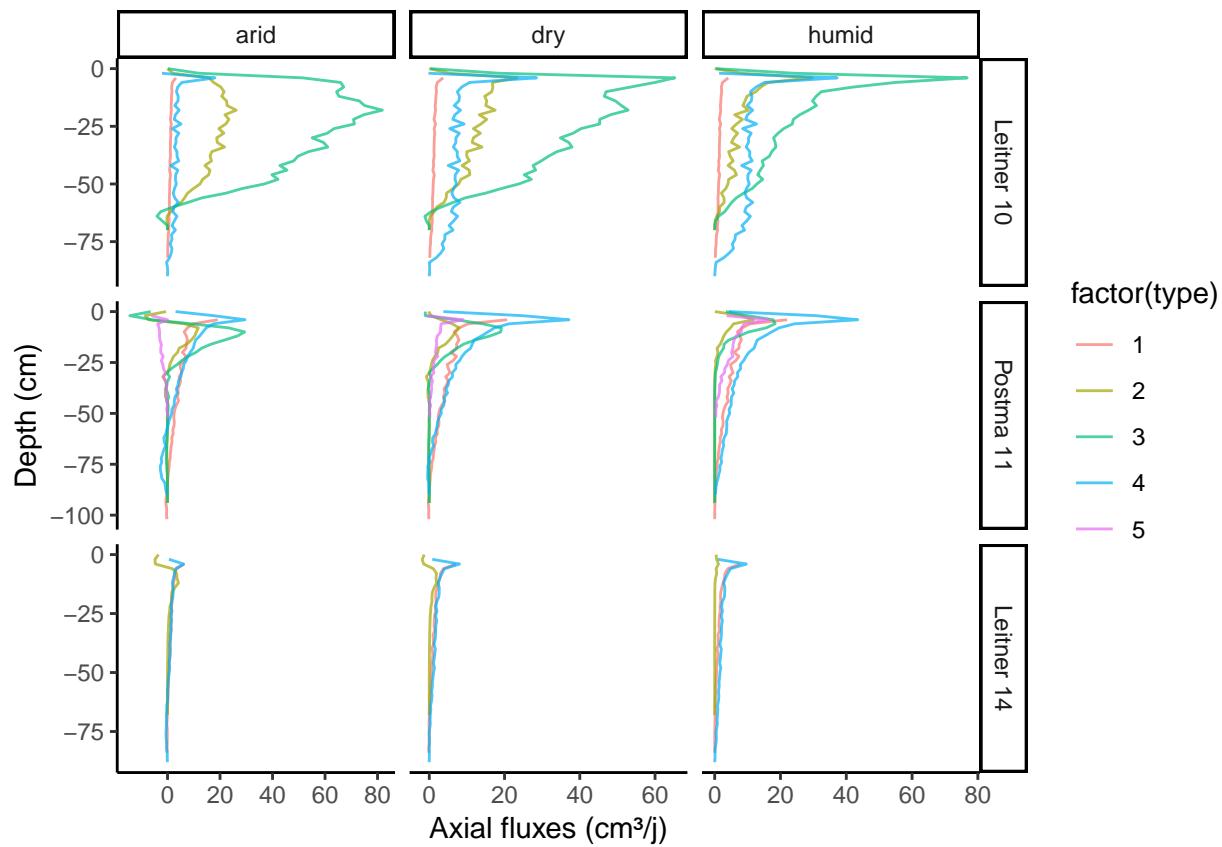


Figure 22: Comparison of the axial fluxes between the different soil scenarios and the root system architectures

```

dens%>%
  filter(age == 40,
        scenario == "Doussan et al.")%>%
  ggplot(aes(rz1, jx, colour=factor(type))) +
  geom_line(alpha = 0.7) +
  #geom_smooth(se=F) +
  coord_flip() +
  theme_classic() +
  xlab("Depth (cm)") +
  ylab("Axial fluxes (cm³/j)")+
  facet_grid(ex~humid, scales = "free", labeller = as_labeller(babbel))

```

```

Transpiration<- results%>%
  mutate(humid = as.character(humid))%>%
  group_by(age, rep, scenario, humid, ex)%>%
  summarise(Tpot = max(tpot, tact),
            Tact = min(tpot, tact))

```

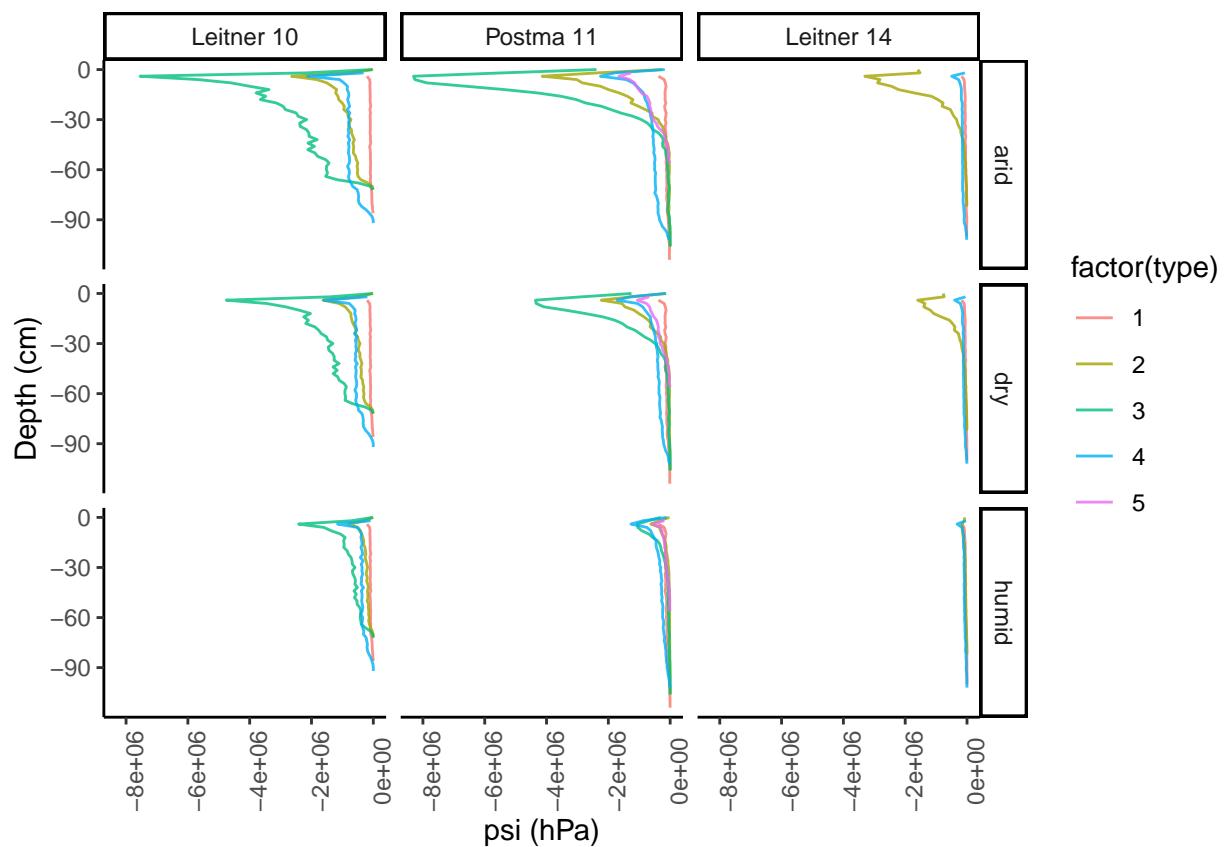


Figure 23: Water pressure head at the soil-root interface

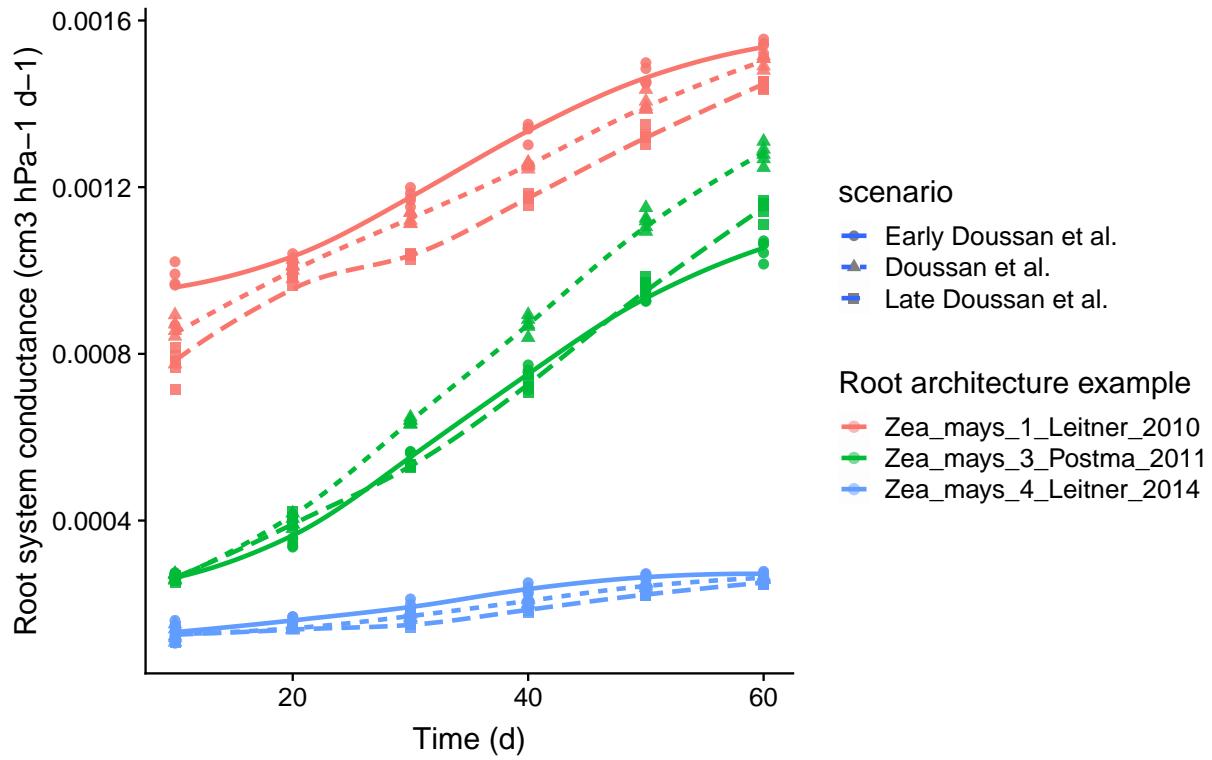
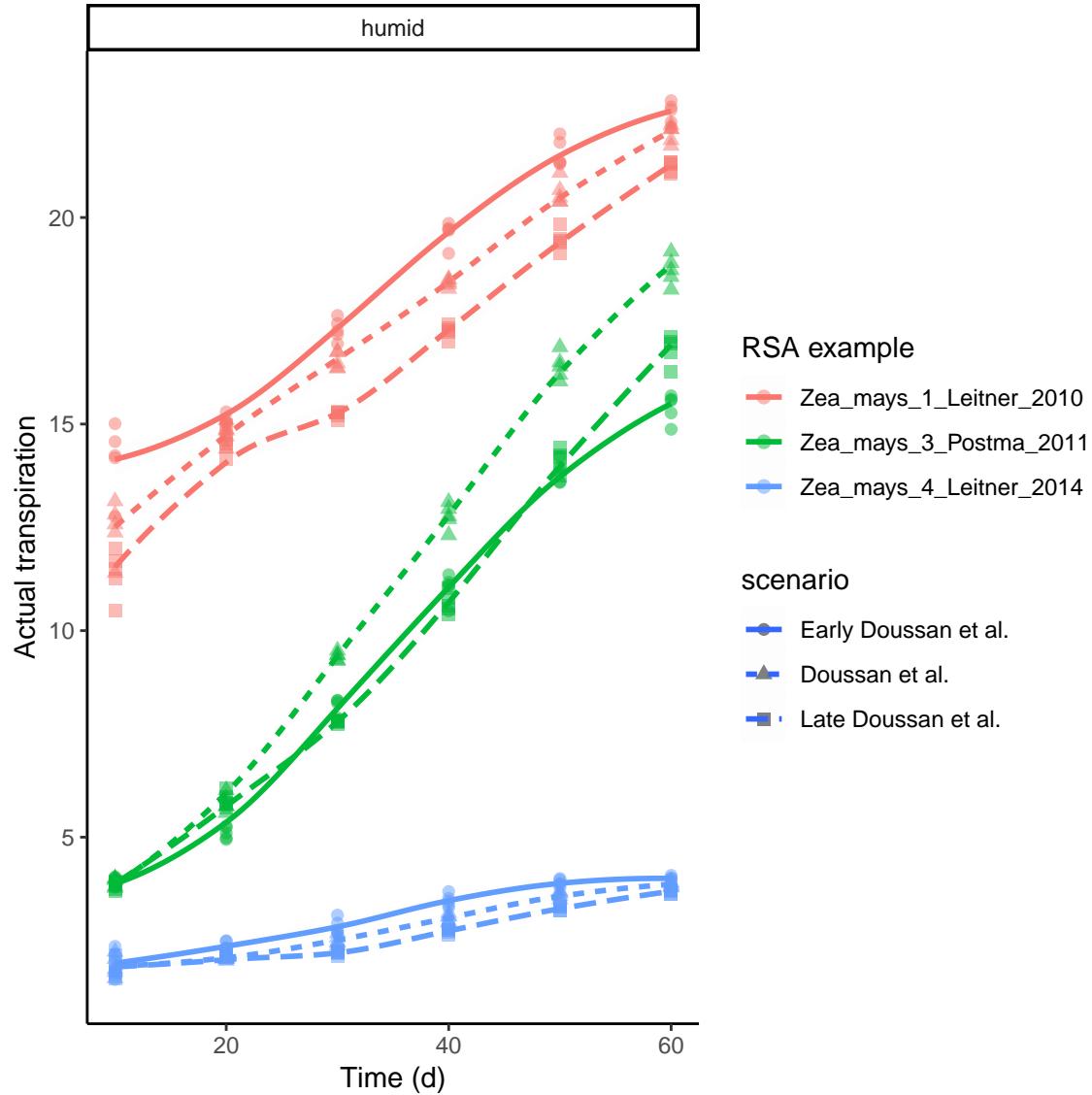
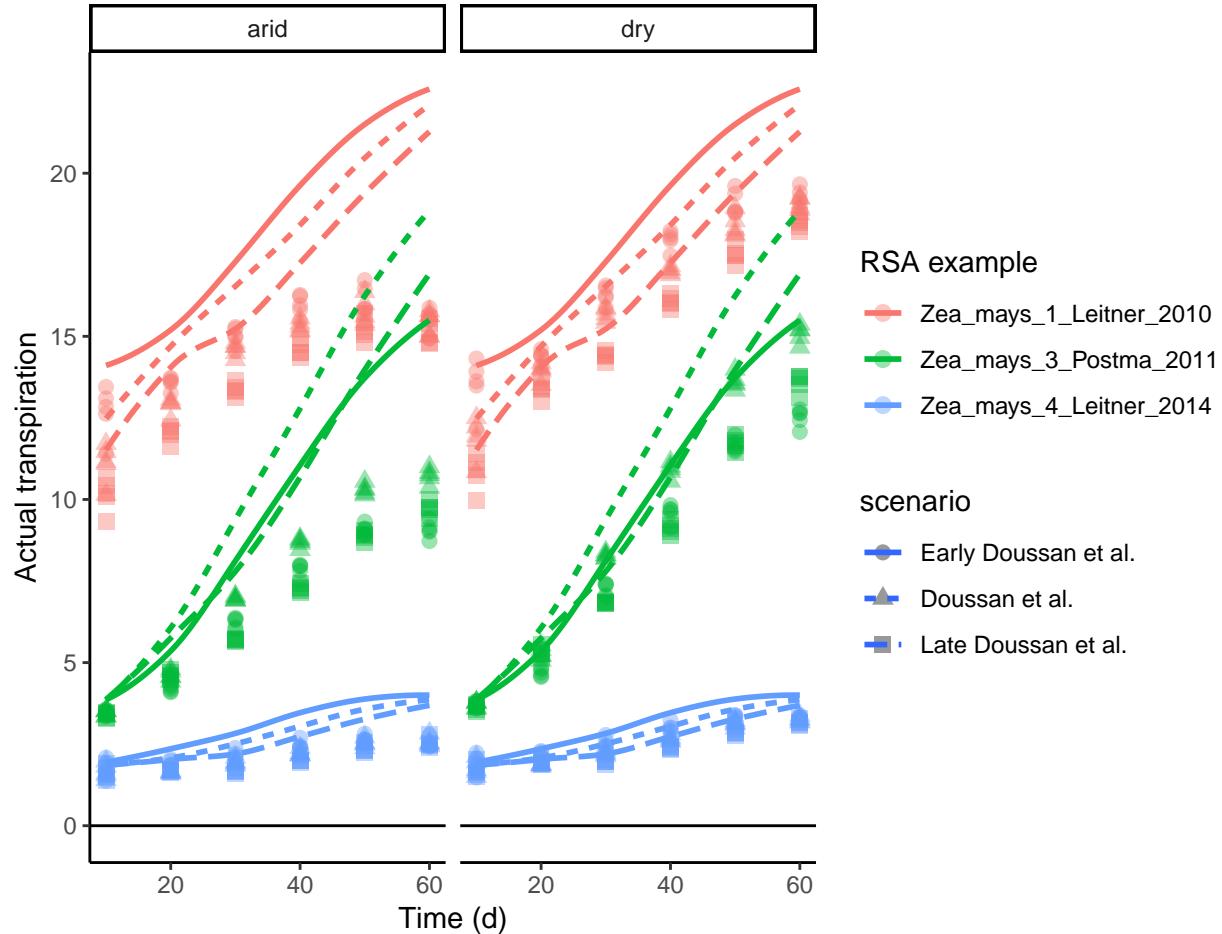


Figure 24: Evolution of the whole root system conductance. Effect comparison between root system architecture and root conductivity modification.



The actual transpiration under drought whith two scenarion of conductivities



The different line represent a potential transpiration.

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