```
###########  Impacts of microplastics on the soil biophysical environment  ##################
################################################################################
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############################## Read me: Script guide  ##############################
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# Section 1: Libraries
# Section 2: Data importing
# Section 3: Figure plots
# Section 4: Additional plots for blogs
# Section 5: Statistical inference


############################## Section 1: Libraries  ################################
###############################################################################

library(PMCMRplus) #for Tukey post-hot on kruskal-wallis
library(PMCMR) #for Tukey post-hot on kruskal-wallis
library(plotly) # for fancy 3D plots online
```

```
library(ggplot2) #needed for some graphs
library(sfsmisc) #for proper y axis on base 10
library(scales) #for proper y axis on base 10 in ggplots
library(scatterplot3d) # for simple 3D plots
library(dplyr) # for dataframe manipulation
library(ggthemes) # for changing the themes of ggplot2
library(wesanderson) # for colour palletes
library(RColorBrewer)# for colour palletes
library(cowplot) # for multiple ggplot pannels
library(nlme) # for gls and lme function
library(lme4) # for lmer function
library(MuMIn) # for linear model inference
# library(shiny) # sometimes need to load shiny to plotly proper work

# If not all packages are installed, run the following commands
#install.packages("shiny")  # it seems that shiny is not working at IGB pc
#install.packages("dplyr")
#install.packages("RPostgreSQL")
#install.packages("lubridate")
#install.packages("RColorBrewer")
#install.packages("PMCMRplus") #for Tukey post-hot on kruskal-wallis
#install.packages("ggplot2") #needed for some graphs
#install.packages("sfsmisc") #for proper y axis on base 10
#install.packages("scatterplot3d") # for simple 3D plots
#install.packages("plotly")
#install.packages("ggthemes")
#install.packages("cowplot")
#install.packages("scales")
#install.packages("wesanderson")
#install.packages("nlme")
#install.packages("lme4")
```

```
#install.packages("MuMIn")


#try to get the right version of plotly and ggplot but it did not work
#install.packages("devtools")
#library("devtools")
#install_github("ropensci/plotly")  # plotly is part of ropensci
#install.packages("tidyverse", dependencies=TRUE, type="source")
#packageVersion("plotly")
#packageVersion("ggplot2")



########################### Section 2:  Getting all data ###########################
##############################################################################
experiment=read.table("Supporting_information_S2.txt", header=T, dec= ",", na.strings=NA)
attach(experiment)
summary(experiment)
View(experiment)
detach(experiment)


#The data imported includes
# Sample label (1 to 180);
# Treatment (Control, PAB= Polyamide beads, PAF= Polyacrylic fibres, PEB= Polyethylene high
# density beads, PEF= Polyester fibres); Concentration (% os dry soil weight);
# Concretion (fractions Large and Smaller than 630?m)
# IMPORTANT: FDA was modified so that its current form is 1000* µM FDA/min/g soil


####### Creating another object with the mean, standard deviation, and standard error of each relevant variable


se = function(x) { sd(x, na.rm=T) / sqrt(length(na.omit(x)))} # Creating a function for computing standard error
```

```
resume= experiment %>% group_by(Treatment, Material, Type) %>%
  summarise_all(funs(mean(., na.rm=T),sd(., na.rm=T), se)) %>%
  ungroup() %>% as.data.frame

View(resume)


#################################################################################

# REMEMBER TO CREATE AN DATA FRAME WITH NUMERICAL VARIABLES CENTERED
center_scale <- function(x) {scale(x, scale = FALSE)}

test= center_scale(experiment) #doesn't work because of NAs and categorical

#################################################################################
#creating a vector with colour by plastic type
attach(experiment)
MP=factor(Material)
levels(MP)
colors=MP
levels(colors)=c("gray30","gray65", "gray70","gray100","gray0")
colors=as.character(colors)
detach(experiment)

#trying the colours
par(mfrow=c(1,1), mar=c(4,5,3,1), oma=c(1,1,1,1))
attach(experiment)
options(scipen="10") # avoids scientific notation
plot(FDA~WSA,log="y", pch=21, bg=colors, col="black", ylab=expression("Microbial activity (FDA abs. min"^-1~".g soil"^-1~")"), xlab="Water Stable Aggregates (%)", axes=F)
axis(2,las=1)
```

```
axis(1)
title(main="A", outer=F, adj=0)
detach(experiment)

########################## Section 3:  First figure explorations #####################
###########################################################################

attach(experiment)

plot(experiment)
plot(WSA~FDA)
plot(FDA~D_L_630microm)
plot(FDA~D_L_1mm)
plot(FDA~WHC)
plot(WSA~Bulk_D)
plot(WHC~Bulk_D)
plot(FDA~Bulk_D)
plot(FDA~DosePartNumber, log="x")
boxplot(FDA~DosePartNumber, log="x")
boxplot(WHC~Concentration, notch=T, xlab=" Material", ylab="WHC", col=(c("gray100","gray80",
"gray60","gray30","gray0")), axes=T)
boxplot(WSA~Material, notch=T, xlab=" Material", ylab="WSA", col=(c("gray100","gray80",
"gray60","gray30","gray0")), axes=T)
boxplot(FDA~Material, notch=T, xlab=" Material", ylab="FDA", col=(c("gray100","gray80",
"gray60","gray30","gray0")), axes=T)
detach(experiment)

# With ggplot

ggplot(experiment, aes(x=Concentration, WHC)) +
  geom_smooth(method = "loess", se = TRUE, colour = "grey10")+
  geom_point(size=3.5, aes(colour = Material)) +
```

```
  theme(text=element_text(size=16))+
  facet_wrap(~Material, scales="free_x")

ggplot(resume, aes(x=Concentration_mean, y=WHC_mean, colour=Material)) +
  geom_errorbar(aes(ymin=WHC_mean-WHC_sd, ymax=WHC_mean+WHC_sd), width=.0) +
  geom_line() +
  geom_point()+
  facet_wrap(~Material, scales="free_x")

ggplot(resume, aes(x=Concentration_mean, y=WHC_mean, colour=Material)) +
  geom_errorbar(aes(ymin=WHC_mean-WHC_se, ymax=WHC_mean+WHC_se), width=.0, size=0.8) +
  geom_line(size=0.7) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_few()+
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.8, linetype =
"solid"))+
  facet_wrap(~Material, scales="free_x")

ggplot(experiment, aes(x=Concentration, WSA)) +
  geom_smooth(method = "loess", se = TRUE, colour = "grey10")+
  geom_point(size=3.5, aes(colour = Material)) +
  theme(text=element_text(size=16))+
  facet_wrap(~Material, scales="free_x")

ggplot(experiment, aes(x=Concentration, FDA)) +
  geom_smooth(method = "loess", se = TRUE, colour = "grey10")+
  geom_point(size=3.5, aes(colour = Material)) +
  theme(text=element_text(size=16))+
  facet_wrap(~Material, scales="free_x")

ggplot(experiment, aes(x=Concentration, Hyd_cond)) +
```

```
  geom_smooth(method = "loess", se = TRUE, colour = "grey10")+
  geom_point(size=3.5, aes(colour = Material)) +
  theme(text=element_text(size=16))+
  facet_wrap(~Material, scales="free_x")


####################### GRAPHS FOR THE MANUSCRIPT ###########################
##########################################################################################


cbPalette= c("gray20", "#E69F00", "#009E73", "#D55E00",  "#0072B2") # to use in plots with control treatment in black
cPalette= c("#E69F00", "#009E73", "#D55E00",  "#0072B2") # to use in plots without control treatments (log scale of microplastic levels)
pd= position_dodge(0.06) # The errorbars overlapped move them .06 to the left and right

# Figure: Water holding capacity

ggplot(resume, aes(x=Concentration_mean, y=WHC_mean, colour=Material)) +
  geom_errorbar(aes(ymin=WHC_mean-WHC_se, ymax=WHC_mean+WHC_se), width=.0, size=0.8) +
  geom_line(size=0.7) +
  geom_point(size=3.5, aes(colour = Material)) +
  geom_rangeframe() +
  theme_tufte() +
  theme(text=element_text(size=16))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Material, scales="free_x")



F1A=ggplot(resume, aes(x=Concentration_mean, y=WHC_mean, colour=Material)) +
  geom_errorbar(aes(ymin=WHC_mean-WHC_se, ymax=WHC_mean+WHC_se),position = pd, width=.0, size=0.8) +
  geom_point(size=3.5, aes(colour = Material), position=pd) +
```

```
  theme_tufte() +
  theme(text=element_text(size=16), legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)



F1B=ggplot(experiment, aes(x=Material, y=WHC, fill = Material, alpha= 0.1)) +
  geom_violin(trim= F) +
  theme_tufte() +
  scale_fill_manual(values=cbPalette)+
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  geom_boxplot(width=0.1)


F1C=ggplot(experiment, aes(x=DosePartNumber, WHC)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')


F1D=ggplot(experiment, aes(x=Dose_Area, WHC)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')
```

```
F1E=ggplot(experiment, aes(x=Dose_Vol, WHC)) +

  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in%
c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +

  theme_tufte() +

  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour =
"grey10", size = 0.3, linetype = "solid"))+

  scale_colour_manual(values=cPalette)+

  scale_x_continuous(trans='log10')


plot_grid(F1A, F1B, cols = 2, rows = 1, labels = "AUTO")

plot_grid(F1C, F1D, F1E, cols = 3, rows = 1, labels = "AUTO")


# plot_grid(F1A, F1B, F1C, F1D, F1E, cols = 3, rows = 2, labels = "AUTO")


#check this figures for control variance

ggplot(experiment, aes(x=DosePartNumber, WHC)) +

  geom_point(size=3.5, aes(colour = Material)) +

  theme_tufte() +

  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype =
"solid"))+

  scale_colour_manual(values=cbPalette)+

  scale_x_continuous(trans='log10')


ggplot(experiment, aes(x=Dose_Area, WHC)) +

  geom_point(size=3.5, aes(colour = Material)) +

  theme_tufte() +

  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype =
"solid"))+

  scale_colour_manual(values=cbPalette)+

  scale_x_continuous(trans='log10')


ggplot(experiment, aes(x=Dose_Vol, WHC)) +
```

```
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')
```

```
#### Figure: Water stable aggregates
```

```
ggplot(resume, aes(x=Concentration_mean, y=WSA_mean, colour=Material)) +
  geom_errorbar(aes(ymin=WSA_mean-WSA_se, ymax=WSA_mean+WSA_se), width=.0, size=0.8) +
  geom_line(size=0.7) +
  geom_point(size=3.5, aes(colour = Material)) +
  geom_rangeframe() +
  theme_tufte() +
  theme(text=element_text(size=16))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Material, scales="free_x")
```

```
F2A=ggplot(resume, aes(x=Concentration_mean, y=WSA_mean, colour=Material)) +
  geom_errorbar(aes(ymin=WSA_mean-WSA_se, ymax=WSA_mean+WSA_se),position = pd, width=.0, size=0.8) +
  geom_point(size=3.5, aes(colour = Material), position=pd) +
  theme_tufte() +
  theme(text=element_text(size=16), legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)
```

```
F2B=ggplot(experiment, aes(x=Material, y=WSA, fill = Material, alpha= 0.1)) +
  geom_violin(trim= F) +
  theme_tufte() +
  scale_fill_manual(values=cbPalette)+
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  geom_boxplot(width=0.1)


F2C=ggplot(experiment, aes(x=DosePartNumber, WSA)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')


F2D=ggplot(experiment, aes(x=Dose_Area, WSA)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')



F2E=ggplot(experiment, aes(x=Dose_Vol, WSA)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
```

```
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')

plot_grid(F2A, F2B, cols = 2, rows = 1, labels = "AUTO")
plot_grid(F2C, F2D, F2E, cols = 3, rows = 1, labels = "AUTO")

# plot_grid(F2A, F2B, F2C, F2D, F2E, cols = 3, rows = 2, labels = "AUTO")

# Check this for position of control

ggplot(experiment, aes(x=DosePartNumber, WSA)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')

ggplot(experiment, aes(x=Dose_Area, WSA)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')

ggplot(experiment, aes(x=Dose_Vol, WSA)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
```

```
  scale_x_continuous(trans='log10')


### Figure: Microbial activity

ggplot(resume, aes(x=Concentration_mean, y=FDA_mean, colour=Material)) +
  geom_errorbar(aes(ymin=FDA_mean-FDA_se, ymax=FDA_mean+FDA_se), width=.0, size=0.8) +
  geom_line(size=0.7) +
  geom_point(size=3.5, aes(colour = Material)) +
  geom_rangeframe() +
  theme_tufte() +
  theme(text=element_text(size=16))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Material, scales="free_x")


F3A=ggplot(resume, aes(x=Concentration_mean, y=FDA_mean, colour=Material)) +
  geom_errorbar(aes(ymin=FDA_mean-FDA_se, ymax=FDA_mean+FDA_se),position = pd, width=.0, size=0.8) +
  geom_point(size=3.5, aes(colour = Material), position=pd) +
  theme_tufte() +
  theme(text=element_text(size=16), legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)


F3B=ggplot(experiment, aes(x=Material, y=FDA, fill = Material, alpha= 0.1)) +
  geom_violin(trim= F) +
  theme_tufte() +
  scale_fill_manual(values=cbPalette)+
```

```
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = 
"grey10", size = 0.3, linetype = "solid"))+
  geom_boxplot(width=0.1)


F3C=ggplot(experiment, aes(x=DosePartNumber, FDA)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% 
c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = 
"grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')


F3D=ggplot(experiment, aes(x=Dose_Area, FDA)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% 
c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = 
"grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')



F3E=ggplot(experiment, aes(x=Dose_Vol, FDA)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% 
c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = 
"grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')


plot_grid(F3A, F3B, cols = 2, rows = 1, labels = "AUTO")
```

```
plot_grid(F3C, F3D, F3E, cols = 3, rows = 1, labels = "AUTO")

# plot_grid(F3A, F3B, F3C, F3D, F3E, cols = 3, rows = 2, labels = "AUTO")


# Check this for position of control

ggplot(experiment, aes(x=DosePartNumber, FDA)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')

ggplot(experiment, aes(x=Dose_Area, FDA)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')

ggplot(experiment, aes(x=Dose_Vol, FDA)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')
```

```
#### Figures Bulk density


ggplot(resume, aes(x=Concentration_mean, y=Bulk_D_mean, colour=Material)) +
  geom_errorbar(aes(ymin=Bulk_D_mean-Bulk_D_se, ymax=Bulk_D_mean+Bulk_D_se), width=.0, size=0.8) +
  geom_line(size=0.7) +
  geom_point(size=3.5, aes(colour = Material)) +
  geom_rangeframe() +
  theme_tufte() +
  theme(text=element_text(size=16))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Material, scales="free_x")



F4A=ggplot(resume, aes(x=Concentration_mean, y=Bulk_D_mean, colour=Material)) +
  geom_errorbar(aes(ymin=Bulk_D_mean-Bulk_D_se, ymax=Bulk_D_mean+Bulk_D_se),position = pd, width=.0, size=0.8) +
  geom_point(size=3.5, aes(colour = Material), position=pd) +
  theme_tufte() +
  theme(text=element_text(size=16), legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)



F4B=ggplot(experiment, aes(x=Material, y=Bulk_D, fill = Material, alpha= 0.1)) +
  geom_violin(trim= F) +
  theme_tufte() +
  scale_fill_manual(values=cbPalette)+
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  geom_boxplot(width=0.1)
```

```
F4C=ggplot(experiment, aes(x=DosePartNumber, Bulk_D)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')


F4D=ggplot(experiment, aes(x=Dose_Area, Bulk_D)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')



F4E=ggplot(experiment, aes(x=Dose_Vol, Bulk_D)) +
  geom_point(size=2, aes(colour = Material), data = subset(experiment, Material %in% c("Polyacrylic","Polyamide", "Polyester", "PolyethyleneHD"))) +
  theme_tufte() +
  theme(text=element_text(size=16),legend.position="none", axis.line = element_line(colour = "grey10", size = 0.3, linetype = "solid"))+
  scale_colour_manual(values=cPalette)+
  scale_x_continuous(trans='log10')


plot_grid(F4A, F4B, cols = 2, rows = 1, labels = "AUTO")
plot_grid(F4C, F4D, F4E, cols = 3, rows = 1, labels = "AUTO")


# plot_grid(F4A, F4B, F4C, F4D, F4E, cols = 3, rows = 2, labels = "AUTO")
```

```
# Figure: Hydraulic conductivity (Supporting information)

ggplot(resume, aes(x=Concentration_mean, y=Hyd_cond_mean, colour=Material)) +

  geom_errorbar(aes(ymin=Hyd_cond_mean-Hyd_cond_se, ymax=Hyd_cond_mean+Hyd_cond_se), 
width=.0, size=0.8) +

  geom_line(size=0.7) +

  geom_point(size=3.5, aes(colour = Material)) +

  geom_rangeframe() +

  theme_tufte() +

  theme(text=element_text(size=16))+

  scale_colour_manual(values=cbPalette)+

  facet_wrap(~Material, scales="free_x")



ggplot(resume, aes(x=Concentration_mean, y=Hyd_cond_mean, colour=Material)) +

  geom_errorbar(aes(ymin=Hyd_cond_mean-Hyd_cond_se, ymax=Hyd_cond_mean+Hyd_cond_se), 
position=pd, width=.0, size=0.8) +

  geom_point(size=3.5, aes(colour = Material), position=pd) +

  theme_tufte() +

  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = 
"solid"))+

  scale_colour_manual(values=cbPalette)



ggplot(experiment, aes(x=Material, y=Hyd_cond, fill = Material, alpha= 0.1)) +

  geom_violin(trim= F) +

  geom_rangeframe() +

  theme_tufte() +

  scale_fill_manual(values=cbPalette)+

  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = 
"solid"))+
```

```
  geom_boxplot(width=0.1)


ggplot(experiment, aes(x=DosePartNumber, Hyd_cond)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype =
"solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')


ggplot(experiment, aes(x=Dose_Area, Hyd_cond)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype =
"solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')


ggplot(experiment, aes(x=Dose_Vol, Hyd_cond)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype =
"solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')



# Figure: Concretion (Supporting information)


ggplot(resume, aes(x=Concentration_mean, y=Concretion_L_630_mean, colour=Material)) +
  geom_errorbar(aes(ymin=Concretion_L_630_mean-Concretion_L_630_se,
ymax=Concretion_L_630_mean+Concretion_L_630_se), width=.0, size=0.8) +
```

```
  geom_line(size=0.7) +

  geom_point(size=3.5, aes(colour = Material)) +

  geom_rangeframe() +

  theme_tufte() +

  theme(text=element_text(size=16))+

  scale_colour_manual(values=cbPalette)+

  facet_wrap(~Material, scales="free_x")



ggplot(resume, aes(x=Concentration_mean, y=Concretion_L_630_mean, colour=Material)) +

  geom_errorbar(aes(ymin=Concretion_L_630_mean-Concretion_L_630_se,
ymax=Concretion_L_630_mean+Concretion_L_630_se), width=.0, size=0.8) +

  geom_point(size=3.5, aes(colour = Material)) +

  theme_tufte() +

  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype =
"solid"))+

  scale_colour_manual(values=cbPalette)+

  scale_x_continuous(trans='log10')



ggplot(experiment, aes(x=Material, y=Concretion_L_630, fill = Material, alpha= 0.1)) +

  geom_violin(trim= F) +

  geom_rangeframe() +

  theme_tufte() +

  scale_fill_manual(values=cbPalette)+

  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype =
"solid"))+

  geom_boxplot(width=0.1)


ggplot(experiment, aes(x=DosePartNumber, Concretion_L_630)) +

  geom_point(size=3.5, aes(colour = Material)) +

  theme_tufte() +
```

```
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')


ggplot(experiment, aes(x=Dose_Area, Concretion_L_630)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')


ggplot(experiment, aes(x=Dose_Vol, Concretion_L_630)) +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  scale_x_continuous(trans='log10')




# Figure: Microbial function and soil aggregation


ggplot(experiment, aes (FDA, WSA))+
  geom_smooth(method = "lm", se = TRUE, colour = "grey20")+
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  geom_point(size=4, aes(colour = Material))
```

```r
ggplot(experiment, aes(FDA, WSA)) +
  geom_point(size=3, data = transform(experiment, Material = NULL), colour = "grey85") +
  geom_smooth(method = "lm", se = TRUE, colour = "grey10")+
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Material)



#############################  Supporting information ################################
###################################################################################



# Figure clumps


ggplot(resume, aes(x=Concentration_mean, colour = Material)) +
  geom_errorbar(aes(ymin=Concretion_L_630_mean-Concretion_L_630_se, ymax=Concretion_L_630_mean+Concretion_L_630_se), width=.0, size=0.8) +
  geom_errorbar(aes(ymin=Concretion_S_630_mean-Concretion_S_630_se, ymax=Concretion_S_630_mean+Concretion_S_630_se), width=.0, size=0.8) +
  geom_line(aes(y = Concretion_L_630_mean)) +
  geom_point(size=3.5, shape=17, aes(y= Concretion_L_630_mean)) +
  geom_line(aes(y = Concretion_S_630_mean))+
  geom_point(size=3.5, aes(y= Concretion_S_630_mean)) +
  geom_rangeframe() +
  theme_tufte() +
  theme(text=element_text(size=16))+
  scale_colour_manual(values=cbPalette)+
```

```
  facet_wrap(~Material, scales="free_x")



# Figure Dry Aggregates


ggplot(resume, aes(x=Concentration_mean, colour = Material)) +
  geom_errorbar(aes(ymin=(D_S_630microm_mean-D_S_630microm_se)*100/Total_D_mean,
ymax=(D_S_630microm_mean+D_S_630microm_se)*100/Total_D_mean), width=.0, size=0.8) +
  geom_errorbar(aes(ymin=(D_S_630microm_mean+D_L_630microm_mean-
D_L_630microm_se)*100/Total_D_mean,
ymax=(D_S_630microm_mean+D_L_630microm_mean+D_L_630microm_se)*100/Total_D_mean),
width=.0, size=0.8) +
  geom_errorbar(aes(ymin=(D_S_630microm_mean+D_L_630microm_mean+D_L_1mm_mean-
D_L_1mm_se)*100/Total_D_mean,
ymax=(D_S_630microm_mean+D_L_630microm_mean+D_L_1mm_mean+D_L_1mm_se)*100/Total
_D_mean), width=.0, size=0.8) +

geom_errorbar(aes(ymin=(D_S_630microm_mean+D_L_630microm_mean+D_L_1mm_mean+D_L_2
mm_mean-D_L_2mm_se)*100/Total_D_mean,
ymax=(D_S_630microm_mean+D_L_630microm_mean+D_L_1mm_mean+D_L_2mm_mean+D_L_2
mm_se)*100/Total_D_mean), width=.0, size=0.8) +
  geom_line(aes(y = D_S_630microm_mean*100/Total_D_mean)) +
  geom_point(size=3, shape=18, aes(y= D_S_630microm_mean*100/Total_D_mean)) +
  geom_line(aes(y = (D_S_630microm_mean+D_L_630microm_mean)*100/Total_D_mean)) +
  geom_point(size=2.5, shape=16, aes(y=
(D_S_630microm_mean+D_L_630microm_mean)*100/Total_D_mean)) +
  geom_line(aes(y =
(D_S_630microm_mean+D_L_630microm_mean+D_L_1mm_mean)*100/Total_D_mean)) +
  geom_point(size=2.5, shape=17, aes(y=
(D_S_630microm_mean+D_L_630microm_mean+D_L_1mm_mean)*100/Total_D_mean)) +
  geom_line(aes(y =
(D_S_630microm_mean+D_L_630microm_mean+D_L_1mm_mean+D_L_2mm_mean)*100/Total_D
_mean)) +
  geom_point(size=2.5, shape=15, aes(y=
(D_S_630microm_mean+D_L_630microm_mean+D_L_1mm_mean+D_L_2mm_mean)*100/Total_D
_mean))+
  geom_rangeframe() +
```

```
  theme_tufte() +
  theme(text=element_text(size=16))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Material, scales="free_x")

ggplot(resume, aes(x=Concentration_mean, y=D_S_630microm_mean*100/Total_D_mean, colour=Material)) +
  geom_errorbar(aes(ymin=(D_S_630microm_mean-D_S_630microm_se)*100/Total_D_mean, ymax=(D_S_630microm_mean+D_S_630microm_se)*100/Total_D_mean), width=.0, size=0.8) +
  geom_point(size=3.5,shape=18, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)


#geom_area(aes(y = D_S_630microm_mean*100/Total_D_mean, fill="darkolivegreen1")) +
#geom_area(aes(y = (D_S_630microm_mean+D_L_630microm_mean)*100/Total_D_mean, fill="yellow4")) +
#geom_area(aes(y = (D_S_630microm_mean+D_L_630microm_mean+D_L_1mm_mean)*100/Total_D_mean, fill="orange3")) +
#geom_area(aes(y = (D_S_630microm_mean+D_L_630microm_mean+D_L_1mm_mean+D_L_2mm_mean)*100/Total_D_mean, fill="darkred")) +


# Water holding capacity and dry stable aggregates
ggplot(experiment, aes(WHC, D_L_1mm)) +
  geom_point(size=3, data = transform(experiment, Material = NULL), colour = "grey85") +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
```

```
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)

ggplot(experiment, aes(Bulk_D, WHC)) +
  geom_point(size=3, data = transform(experiment, Material = NULL), colour = "grey85") +
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Material, scales="free_x")


# Figure: Dry and wet stable soil aggregation

ggplot(experiment, aes (D_L_1mm, WSA))+
  geom_smooth(method = "lm", se = TRUE, colour = "grey20")+
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  geom_point(size=3, aes(colour = Material))

ggplot(experiment, aes(D_L_1mm, WSA)) +
  geom_point(size=3, data = transform(experiment, Material = NULL), colour = "grey85") +
  geom_smooth(method = "lm", se = TRUE, colour = "grey10")+
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
```

```
  facet_wrap(~Material)




ggplot(experiment, aes(FDA, WSA)) +
  geom_point(size=3, data = transform(experiment, Type = NULL), colour = "grey85") +
  geom_smooth(method = "lm", se = TRUE, colour = "grey10")+
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype =
"solid"))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Type)


ggplot(experiment, aes (FDA, WSA))+
  geom_smooth(method = "lm", se = TRUE, colour = "grey20")+
  geom_point(size=3.5, aes(colour = DosePartNumber))+
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype =
"solid"))+
  scale_color_gradient(low = "darkgreen", high = "orange")


ggplot(experiment, aes (FDA, WSA))+
  geom_smooth(method = "lm", se = TRUE, colour = "grey20")+
  geom_point(size=3.5, aes(colour = Dose_Area))+
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype =
"solid"))+
  scale_color_gradient(low = "darkgreen", high = "orange")


ggplot(experiment, aes (FDA, WSA))+
  geom_smooth(method = "lm", se = TRUE, colour = "grey20")+
```

```
  geom_point(size=3.5, aes(colour = Dose_Vol))+
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_color_gradient(low = "darkgreen", high = "orange")


ggplot(experiment, aes(D_L_1mm, WSA)) +
  geom_point(data = transform(experiment, Type = NULL), colour = "grey85") +
  geom_smooth(method = "lm", se = TRUE, colour = "grey10")+
  geom_point(aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Type)

### Not used in the supplementary material

ggplot(experiment, aes (FDA, D_L_1mm))+
  geom_smooth(method = "lm", se = TRUE, colour = "grey20")+
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  geom_point(size=4, aes(colour = Material))

ggplot(experiment, aes(FDA, D_L_1mm)) +
  geom_point(size=3, data = transform(experiment, Material = NULL), colour = "grey85") +
  geom_smooth(method = "lm", se = TRUE, colour = "grey10")+
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
```

```
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Material)


ggplot(experiment, aes (WSA, D_L_1mm))+
  geom_smooth(method = "lm", se = TRUE, colour = "grey20")+
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  geom_point(size=4, aes(colour = Material))


ggplot(experiment, aes(WSA, D_L_1mm)) +
  geom_point(size=3, data = transform(experiment, Material = NULL), colour = "grey85") +
  geom_smooth(method = "lm", se = TRUE, colour = "grey10")+
  geom_point(size=3.5, aes(colour = Material)) +
  theme_tufte() +
  theme(text=element_text(size=16), axis.line = element_line(colour = "grey10", size = 0.5, linetype = "solid"))+
  scale_colour_manual(values=cbPalette)+
  facet_wrap(~Material)



######## Section 4:  Additional graphs for blogs, presentations, and my future website ##########
###################################################################################
plot_ly(experiment, x = ~WSA, color = ~Material, type = "box")


plot_ly(experiment, x = ~FDA, y = ~WSA, color = ~Material) %>%
  slice(which.max(FDA)) %>%
  add_annotations(text = "Maximum slope")
```

```
plot_ly(experiment, x = ~FDA, y = ~WSA, z = ~DosePartNumber, color = ~Material) %>%
  add_markers() %>%
  layout(scene = list(xaxis = list(title = 'FDA'),
                     yaxis = list(title = 'WSA'),
                     zaxis = list(title = 'DosePartNumber')))



plot_ly(experiment, x = ~FDA, y = ~WSA, z = ~D_L_1mm, color = ~Material) %>%
  add_markers() %>%
  layout(scene = list(xaxis = list(title = 'FDA'),
                     yaxis = list(title = 'WSA'),
                     zaxis = list(title = '1mm')))


attach(experiment)
scatterplot3d(FDA,Material,WSA,pch=16, highlight.3d=TRUE, type="h", main="Trial") #concentration (y) is not so relevant as there are beads- high concentration*Low effec
scatterplot3d(D_L_1mm,FDA,WSA,pch=16, highlight.3d=TRUE, type="h", main="Trial")
detach(experiment)




######################## Section 5:  Statistical Inference  ################################
########################################################################################


## Note: lm for traditional linear regression, normal errors, constant variance
# example: lm (y~x, data) means y= a+ bx + error
## Note: glm for linear models, possible non-normal errors, possible non-constant variance
# example: glm (y~x, data, family=poisson) means y= e^(a+bx)+ error
## Note: gls for least square models, possible non-normal & correlated errors, possible non-constant variance with spatial temporal treds
```

```r
### That is why I prefer to use the gls function generally, with simple structures gls is pretty much equivalent to lm

# Making selection of particle types

PA=experiment[129:168,]
summary(PA)

PAN=experiment[49:88,]
summary(PAN)

PES=experiment[9:48,]
summary(PES)

PEHD=experiment[89:128,]
summary(PEHD)

control=filter(experiment, Treatment=="Control")
summary(control)



### Bulk density

# Exploratory

kruskal.test(Bulk_D~Treatment, experiment) #it is not significant per individual treatment
kruskal.test(Bulk_D~Type, experiment) #it is significant per type (control, linear, volumetric; p=0.0265)
attach(experiment)
posthoc.kruskal.nemenyi.test(x=Bulk_D,g=Type, method="Tukey") #control and fibers may differ (p=0.019) but ties are present: check with linear models
```

```
detach(experiment)
kruskal.test(Bulk_D~Material, experiment) # quasi significant per material, check linear model because low power

# Testing effects of particle type
bulk_type=glm(Bulk_D~Type, family=poisson, experiment, na.action=na.exclude)
qqnorm(resid(bulk_type)) # it has few points with considerable error, but generally fine
summary(bulk_type)# Linear model confirm kruskal results: significant effects of fibers (p=0.02)
plot(bulk_type)
anova(bulk_type)

bulk_material=glm(Bulk_D~Material, family=poisson, experiment, na.action=na.exclude)
qqnorm(resid(bulk_material)) # it has few points with considerable error, but generally fine
summary(bulk_material)# Linear model confirms all materials had an effec (p<0.0026)
plot(bulk_material)
bulk_material0=glm(Bulk_D~1, family=poisson, experiment, na.action=na.exclude)
anova(bulk_material,bulk_material0, test="F") # F test with poisson is tricky!

# Testing the effects of concentration per particle

bulk_PAN=gls(Bulk_D~Concentration, PAN, na.action=na.exclude)
summary(bulk_PAN)# not Significant
summary(lm(Bulk_D~Concentration, PAN, na.action=na.exclude))
anova(bulk_PAN)

bulk_PEHD=gls(Bulk_D~Concentration, PEHD, na.action=na.exclude)
summary(bulk_PEHD)# not Significant
anova(bulk_PEHD)

bulk_PA=gls(Bulk_D~Concentration, PA, na.action=na.exclude)
summary(bulk_PA)# not Significant
```

```
anova(bulk_PA)


bulk_PES=gls(Bulk_D~Concentration, PES, na.action=na.exclude)

summary(bulk_PES)# Significant effects of polyester fibres (p= 0.0217)

plot(bulk_PES)

qqnorm(resid(bulk_PES)) #fit of the model does not seem too problematic so I believe it.

anova(bulk_PES)



# Testing effects of contamination level disconsidering particle properties

bulk_c0=gls(Bulk_D~Concentration+Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)

qqnorm(resid(bulk_c0)) # it has few points with considerable error, but generally fine

summary(bulk_c0) ### Significant negative effect of concentration (p=0.0338)



bulk_c1=gls(Bulk_D~Concentration, experiment, na.action=na.exclude)

qqnorm(resid(bulk_c1)) # it has few points with considerable error, but generally fine

summary(bulk_c1) ### Not significant effect of concentration (p=0.64)

anova(bulk_c1)


bulk_c2=gls(Bulk_D~Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)

qqnorm(resid(bulk_c2)) # it has few points with considerable error, but generally fine

summary(bulk_c2) ### Significant negative effect of volume (p=0.0403) and area (p=0.0204)


AICc(bulk_c0, bulk_c1, bulk_c2) # model whc_c1 has smaller AICc (AIC corrected by sample sizeswithin library MuMIn less AICc means better model)


# CONCLUSIONS: all particles had significant effects on bulk density, with PES showing strongest dose response

# trust model c1= effects of concentration or other dose metrics ignoring particle properties might be not significant
```

```
##################################################################################
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### Water holding capacity


# Exploratory


kruskal.test(WHC~Treatment, experiment) #it is not significant per individual treatment
kruskal.test(WHC~Type, experiment) #it is not significant per type (linear vs volumetric)
kruskal.test(WHC~Material, experiment) #it is not significant per polymer


# Testing the effects of concentration per particle


whc_PAN=gls(WHC~Concentration, PAN, na.action=na.exclude)
summary(whc_PAN)# not Significant


whc_PEHD=gls(WHC~Concentration, PEHD, na.action=na.exclude)
summary(whc_PEHD)# not Significant


whc_PA=gls(WHC~Concentration, PA, na.action=na.exclude)
summary(whc_PA)# not Significant


whc_PES=gls(WHC~Concentration, PES, na.action=na.exclude)
summary(whc_PES)# Significant effects of polyester fibres (p= 0.016)
summary(lm(WHC~Concentration, PES, na.action=na.exclude))
anova(whc_PES)
plot(whc_PES)
qqnorm(resid(whc_PES)) #fit of the model does not seem too problematic so I believe it.
```

```
# Testing effects of contamination level disconsidering particle properties

whc_c0=gls(WHC~Concentration+Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)

qqnorm(resid(whc_c0)) # it has one point with big error, but generally fine

summary(whc_c0) ### Significant positive effect of concentration (p=0.0419)

whc_test=lm(WHC~Concentration+Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)

summary(whc_test)


whc_c1=gls(WHC~Concentration, experiment, na.action=na.exclude)

qqnorm(resid(whc_c1)) # error might be problematic in the higher quantiles

summary(whc_c1) ### Not significant effect of concentration (p=0.14)


whc_c2=gls(WHC~Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)

qqnorm(resid(whc_c2)) # it has one point with big error, but generally fine

summary(whc_c2) ### no significant effect of concentration


AICc(whc_c0, whc_c1, whc_c2) # model whc_c1 has smaller AICc (AIC corrected by sample sizeswithin library MuMIn less AICc means better model)

anova(whc_c0, whc_c1) # anova is not the best to compare because they have different fixed effects, but it gives same AICc result


# CONCLUSIONS: only PES seem to have dose-response effect

# trust model whc_c1= effects of concentration or other dose metrics ignoring particle properties might be not significant

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### Hydraulic conductivity


# Exploratory
```

```
kruskal.test(Hyd_cond~Treatment, experiment) #it is not significant per individual treatment

kruskal.test(Hyd_cond~Type, experiment) #it is not significant per type

kruskal.test(Hyd_cond~Material, experiment) # quasi significant per material, check linear model because low power


# Testing the effects of concentration per particle


hyd_PAN=gls(Hyd_cond~Concentration, PAN, na.action=na.exclude)

summary(hyd_PAN)# not Significant


hyd_PEHD=gls(Hyd_cond~Concentration, PEHD, na.action=na.exclude)

summary(hyd_PEHD)# not Significant


hyd_PA=gls(Hyd_cond~Concentration, PA, na.action=na.exclude)

summary(hyd_PA)# not Significant


hyd_PES=gls(Hyd_cond~Concentration, PES, na.action=na.exclude)

summary(hyd_PES)# Not significant



# Testing effects of contamination level disconsidering particle properties

hyd_c0=gls(Hyd_cond~Concentration+Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)

qqnorm(resid(hyd_c0)) # it has few points with considerable error, but generally fine

summary(hyd_c0) ### Concentration and Dose_volume almost significant, but not really (p 0.054 and 0.08, respectively)


hyd_c1=gls(Hyd_cond~Concentration, experiment, na.action=na.exclude)

qqnorm(resid(hyd_c1)) # it has few points with considerable error, but generally fine

summary(hyd_c1) ### Not significant effect of concentration (p=0.78)
```

```
hyd_c2=gls(Hyd_cond~Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)

qqnorm(resid(hyd_c2)) # it has few points with considerable error, but generally fine

summary(hyd_c2) ### Significant negative effect of volume (p=0.0403) and area (p=0.0204)


AICc(hyd_c0, hyd_c1, hyd_c2) # model whc_c1 has smaller AICc (AIC corrected by sample sizeswithin library MuMIn less AICc means better model)


# CONCLUSIONS: effects of concentration or other dose metrics might be not significant

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### Water Stable Aggregates


# Exploratory


attach(experiment)

kruskal.test(WSA~Treatment, experiment) #it is significant per individual treatment (p=0.002252)

posthoc.kruskal.nemenyi.test(x=WSA,g=Treatment, method="Tukey") #but it cannot find which treatments, i.e. low power in replication for that


kruskal.test(WSA~Type, experiment) #it is significant per type (control, linear, volumetric; p=0.00089)

posthoc.kruskal.nemenyi.test(x=WSA,g=Type, method="Tukey") # linear and volumetric MPs may differ (p=0.00007)


kruskal.test(WSA~Material, experiment) #it is significant per polymer (p=0.002957)

posthoc.kruskal.nemenyi.test(x=WSA,g=Material, method="Tukey") # the difference in type seems to be because polyacrylic fibers differ from polyamid (p=0.0051) and polyethylene (p=0.0182)

detach(experiment)



# Testing effects of particle type
```

```
wsa_type=glm(WSA~Type, family=poisson, experiment, na.action=na.exclude)
qqnorm(resid(wsa_type)) # generally fine
summary(wsa_type)# Linear model confirm kruskal results: significant effects of linear MPs (p=0.00019)


wsa_material=glm(WSA~Material, family=poisson, experiment, na.action=na.exclude)
qqnorm(resid(wsa_material)) # generally fine
summary(wsa_material)# Linear model confirm kruskal results: polyacrylic fibers differ from the rest (p=0.0294)
wsa_material0=glm(WSA~1, family=poisson, experiment, na.action=na.exclude)
anova(wsa_material, wsa_material0, test="F")



# Testing the effects of concentration per particle


wsa_PAN=gls(WSA~Concentration, PAN, na.action=na.exclude)
summary(wsa_PAN)# not Significant


wsa_PEHD=gls(WSA~Concentration, PEHD, na.action=na.exclude)
summary(wsa_PEHD)# not Significant


wsa_PA=gls(WSA~Concentration, PA, na.action=na.exclude)
summary(wsa_PA)# not Significant


wsa_PES=gls(WSA~Concentration, PES, na.action=na.exclude)
summary(wsa_PES)# Significant effects of polyester fibres (p= 0.0027)
plot(wsa_PES)
qqnorm(resid(wsa_PES)) #fit of the model does not seem too problematic so I believe it.
anova(wsa_PES)


# Testing effects of contamination level disconsidering particle properties
```

```
wsa_c0=gls(WSA~Concentration+Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)
qqnorm(resid(wsa_c0)) # generally fine
summary(wsa_c0) ### Significant effect of particle number (p=0.0029)

wsa_c1=gls(WSA~Concentration, experiment, na.action=na.exclude)
qqnorm(resid(wsa_c1)) # it has few points with considerable error, but generally fine
summary(wsa_c1) ### Not significant effect of concentration (p=0.0992)

wsa_c2=gls(WSA~Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)
qqnorm(resid(wsa_c2)) # it has few points with considerable error, but generally fine
summary(wsa_c2) ### Significant particle number (p=0.0023)

AICc(wsa_c0, wsa_c1, wsa_c2) # model whc_c1 has smaller AICc (AIC corrected by sample sizeswithin library MuMIn less AICc means better model)

# CONCLUSIONS: Linear MPS had significant effects on WSA, with polyacrylic fiber with strong average impact and PES steepest dose response
# trust model c1= effects of concentration or other dose metrics ignoring particle properties might be not significant
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### Dry Aggregates & Soil structure

# Exploratory

attach(experiment)
kruskal.test(D_S_630microm~Treatment, experiment) #it is significant per individual treatment (p=0.004939)
posthoc.kruskal.nemenyi.test(x=D_S_630microm,g=Treatment, method="Tukey") #but it cannot find which treatments, i.e. low power in replication for that
```

```r
kruskal.test(D_S_630microm~Type, experiment) #it is significant per type (control, linear, volumetric; p=0.0002329)

posthoc.kruskal.nemenyi.test(x=D_S_630microm,g=Type, method="Tukey") # linear MPs may differ from other (p=0.0017)


kruskal.test(D_S_630microm~Material, experiment) #it is significant per polymer (p=0.0004125)

posthoc.kruskal.nemenyi.test(x=D_S_630microm,g=Material, method="Tukey") # the difference in type seems to be because polyester fibers differ from control and volumetric (p< 0.05)

detach(experiment)



# Testing effects of particle type

ds630_type=gls(D_S_630microm~Type, experiment, na.action=na.exclude)

qqnorm(resid(ds630_type)) # generally fine PS: only GLM with poisson would give AIC infinite!

summary(ds630_type)# Linear model confirm kruskal results: significant effects of linear MPs to controls and volumetric (p=0.00019)

anova(ds630_type)


ds630_material=gls(D_S_630microm~Material, experiment, na.action=na.exclude)

qqnorm(resid(ds630_material)) # generally fine

summary(ds630_material)# Linear model confirm kruskal results: polyester fibers differ from the controls (p=0.0029, F= 5.25)

anova(ds630_material)



# Testing the effects of concentration per particle


ds630_PAN=gls(D_S_630microm~Concentration, PAN, na.action=na.exclude)

summary(ds630_PAN)# not Significant


ds630_PEHD=gls(D_S_630microm~Concentration, PEHD, na.action=na.exclude)

summary(ds630_PEHD)# not Significant
```

```
ds630_PA=gls(D_S_630microm~Concentration, PA, na.action=na.exclude)
summary(ds630_PA)# not Significant

ds630_PES=gls(D_S_630microm~Concentration, PES, na.action=na.exclude)
summary(ds630_PES)# not Significant



# Testing effects of contamination level disconsidering particle properties
ds630_c0=gls(D_S_630microm~Concentration+Dose_Vol*Dose_Area*DosePartNumber,
experiment, na.action=na.exclude)
qqnorm(resid(ds630_c0)) # generally fine
summary(ds630_c0) ### Significant effect of concentration (p=0.0279), particle volume (p=0.0387)

ds630_c1=gls(D_S_630microm~Concentration, experiment, na.action=na.exclude)
qqnorm(resid(ds630_c1)) # it has few points with considerable error, but generally fine
summary(ds630_c1) ### Significant effect of concentration (p=0.0097)
anova(ds630_c1)
plot(D_S_630microm~Concentration, experiment)

ds630_c2=gls(D_S_630microm~Dose_Vol*Dose_Area*DosePartNumber, experiment,
na.action=na.exclude)
qqnorm(resid(ds630_c2)) # it has few points with considerable error, but generally fine
summary(ds630_c2) ### Significant particle area (p=0.0434)

AICc(ds630_c0, ds630_c1, ds630_c2) # model whc_c1 has smaller AICc (AIC corrected by sample
sizeswithin library MuMIn less AICc means better model)

# CONCLUSIONS: Linear MPS had significant effects on WSA, with polyacrylic fiber with strong
average impact and PES steepest dose response
# trust model c1= effects of concentration  might be significant
```

```
### Microbial activity


# Exploratory


attach(experiment)
kruskal.test(FDA~Treatment, experiment) #it is significant per individual treatment (p=0.01952)
posthoc.kruskal.nemenyi.test(x=FDA,g=Treatment, method="Tukey") #but it cannot find which treatments, i.e. low power in replication for that


kruskal.test(FDA~Type, experiment) #it is significant per type (control, linear, volumetric; p=0.0002496)
posthoc.kruskal.nemenyi.test(x=FDA,g=Type, method="Tukey") # linear MPs may differ from volumetric and controls (p<0.01507)


kruskal.test(FDA~Material, experiment) #it is significant per polymer (p=0.001835)
posthoc.kruskal.nemenyi.test(x=FDA,g=Material, method="Tukey") # the difference in type seems to be because polyacrylic fibers differ from polyamid (p<0.041) and polyethylene (p=0.0182) polyester quasi significant
detach(experiment)



# Testing effects of particle type
fda_type=gls(FDA~Type, experiment, na.action=na.exclude)
qqnorm(resid(fda_type)) # generally fine
summary(fda_type)# Linear model confirm kruskal results: significant effects of linear MPs (p=0.00019)
anova(fda_type)


fda_material=gls(FDA~Material, experiment, na.action=na.exclude)
qqnorm(resid(fda_material)) # generally fine
```

```
summary(fda_material)# Linear model confirm kruskal results: polyacrylic and polyester fibers differ from the rest (p=0.0036 and 0.0213, respectively)

anova(fda_material)



# Testing the effects of concentration per particle


fda_PAN=gls(FDA~Concentration, PAN, na.action=na.exclude)

summary(fda_PAN)# not Significant


fda_PEHD=gls(FDA~Concentration, PEHD, na.action=na.exclude)

summary(fda_PEHD)# not Significant


fda_PA=gls(FDA~Concentration, PA, na.action=na.exclude)

summary(fda_PA)# not Significant


fda_PES=gls(FDA~Concentration, PES, na.action=na.exclude)

summary(fda_PES)# not significant



# Testing effects of contamination level disconsidering particle properties

fda_c0=gls(FDA~Concentration+Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)

qqnorm(resid(fda_c0)) # generally fine

summary(fda_c0) ### no significant effect


fda_c1=gls(FDA~Concentration, experiment, na.action=na.exclude)

qqnorm(resid(fda_c1)) # generally fine

summary(fda_c1) ### Significant effect of concentration (p=0.0152)

anova(fda_c1)


fda_c2=gls(FDA~Dose_Vol*Dose_Area*DosePartNumber, experiment, na.action=na.exclude)
```

```
qqnorm(resid(fda_c2)) # generally fine

summary(fda_c2) ###  no significant effect


AICc(fda_c0, fda_c1, fda_c2) # model whc_c1 has smaller AICc (AIC corrected by sample sizeswithin
library MuMIn less AICc means better model)


# CONCLUSIONS: Linear MPS had significant effects on FDA, with polyacrylic fiber with strong
average impact and PES steepest dose response

# trust model c1= effects of concentration are significant (p=0152) but other dose metrics ignoring
particle properties might be not significant

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#### Functional change



# Exploratory phase


summary(lm(WSA~FDA, experiment)) # significant (p=0.0005352)

summary(lm(WSA~FDA, PA)) # not significant

summary(lm(WSA~FDA, PAN)) # not significant

summary(lm(WSA~FDA, PES)) # not significant

summary(lm(WSA~FDA, PEHD)) # significant (p=0.0003279)

summary(lm(WSA~FDA, control)) # not significant


summary(lm(FDA~D_L_1mm, experiment)) # significant (p=0.003735)

summary(lm(FDA~D_L_1mm, PA)) # not significant

summary(lm(FDA~D_L_1mm, PAN)) # not significant

summary(lm(FDA~D_L_1mm, PES)) # not significant

summary(lm(FDA~D_L_1mm, PEHD)) # not significant

summary(lm(FDA~D_L_1mm, control)) # not significant
```

```
# The most comprehensive model for this could be a generalized mixed effects model with random slopes and intercept

f_change= lmer(WSA ~ FDA + (1+FDA|Material), data = experiment)

plot(f_change) # generally fine

qqnorm(resid(f_change)) # quite good

summary(f_change)

anova(f_change)


# alternative model with random intercept only

functional=lme(WSA~FDA, experiment, random=~1|Material, na.action=na.exclude)

plot(functional)

qqnorm(resid(functional)) # generally fine

summary(functional)

anova(functional)

anova.lme(functional)


# traditional model

wsa_fda=lm(WSA~FDA, experiment, na.action=na.exclude)

plot(wsa_fda)

summary(wsa_fda)


AICc(f_change,functional, wsa_fda) # The model that disregards material as random factor scores poorly compared to others




# Further explorations that do not add much information but confirm that including the random factor material is better & there were no significant effects of concentration

m1=gls(WSA~FDA*Material, experiment, na.action=na.exclude)

summary(m1)
```

```
plot(m1)

a1=lmer(WSA~FDA+ (1|Material) , data=experiment, na.action = na.exclude) # same as 'functional'model but the another library
plot(a1)
summary(a1)

f1=lme(WSA~FDA+Concentration, experiment, random=~1|Material, na.action=na.exclude)
plot(f1)
qqnorm(resid(f1)) # generally fine
summary(f1)

f2=lme(WSA~FDA+Material, experiment, random=~1|Type, na.action=na.exclude)
plot(f2)
qqnorm(resid(f2)) # generally fine
summary(f2)



### Clumps

# Exploratory

kruskal.test(Concretion_L_630~Treatment, experiment) #it is not significant per individual treatment
kruskal.test(Concretion_L_630~Type, experiment) #it is significant per type (p < 0.05)
kruskal.test(Concretion_L_630~Material, experiment) #it is not significant per polymer


# Testing effects of particle type
L630_type=gls(Concretion_L_630~Type, experiment, na.action=na.exclude)
qqnorm(resid(L630_type)) # generally fine
```

```
summary(L630_type)# Linear model confirm kruskal results: significant difference between linear and volumetric MPs (p=0.0176)



# Testing the effects of concentration per particle


L630_PAN=gls(Concretion_L_630~Concentration, PAN, na.action=na.exclude)

summary(L630_PAN)# not Significant


L630_PEHD=gls(Concretion_L_630~Concentration, PEHD, na.action=na.exclude)

summary(L630_PEHD)# not Significant


L630_PA=gls(Concretion_L_630~Concentration, PA, na.action=na.exclude)

summary(L630_PA)# not Significant


L630_PES=gls(WHC~Concentration, PES, na.action=na.exclude)

summary(L630_PES)# Significant effects of polyester fibres (p= 0.016)

plot(L630_PES)

qqnorm(resid(L630_PES)) #fit of the model does not seem too problematic so I believe it.
```