

## **Supplementary Information 2: ExpoKids Version 1.0 Code**

This file contains the ExpoKids Version 1.0 code used to generate graphs for visualizing aggregate exposure for children compared to adults.

```
# -----
# title: "Expokids v1.0"
# author: "MD"
# date: "May 2020"
# output:
#   png_imgs, pdf_document of ADD, LADD, and cumulative percent graphs
# purpose: This is the Expokids v1.0 code used to generate graphs for
#   visualizing aggregate exposure for children compared to adults.
# -----

## Clear environment
remove(list = ls())

#####
#####
## User Input Section
# =====
# Required:
# -----
# Path to Excel spreadsheet on your computer.
chempath <- "insert_path_here/chemname.xlsx"
# Chemical name
chemname <- "chemical_name"

# =====
# Optional: - To run, uncomment saved variables below and adjust
accordingly.
# -----
# Adjust y-axis scale
# y_lims <- c(0, 1e-3)
#####
#####
#####
#####
##### RUN ALL CODE BELOW THIS ###
#####
#####
# =====
# I. Prepare Environment.
# -----
# Install packages (if not already installed)
install.packages("tidyverse")
install.packages("reshape2")
install.packages("dplyr")
install.packages("scales")
devtools::install_github("tidyverse/readxl")

# Load packages
library(tidyverse)
library(reshape2)
library(dplyr)
library(readxl)
library(scales)
```

```

theme_set(theme_bw(base_size=15))

# =====
# II. Load data
# -----
# A. Load Excel file.
datafile <- read_xlsx(chempath)

# -----
# B. Create lifestage data.
# Copy in data
chemfile <- data.frame(matrix(nrow=nrow(datafile),ncol=3))
chemfile[,1] <- datafile[,1]

# Calculate small infant lifestage (0-1 year)
for (i in 2:nrow(datafile)){
  chemfile[i,2] <- ((datafile[1,2]*datafile[i,2])+
                  (datafile[1,3]*datafile[i,3])+
                  (datafile[1,4]*datafile[i,4])+
                  (datafile[1,5]*datafile[i,5]))/1 # small infant =
1 yr
}
# Calculate infant lifestage (1-3 years)
for (i in 1:nrow(datafile)){
  chemfile[i,3] <- (datafile[1,6]*datafile[i,6]+
                  datafile[1,7]*datafile[i,7])/2
}
# Copy remaining lifestages
for (i in 8:ncol(datafile)){
  chemfile[,i-4] <- datafile[,i]
}

## Rename column headers
chemfile <- chemfile[2:nrow(chemfile),]
names(chemfile) <- c("Media", "Young Infant", "Infant", "Young Child",
                  "Child", "Young Youth", "Youth", "Adult")

# -----
# C. Reorganize data files.
## Prepare file for graphing ADD
meltchemfile <- melt(chemfile,
                    id.vars="Media",
                    measure.var=c("Young Infant","Infant","Young
Child","Child",
                                "Young Youth","Youth","Adult"),
                    na.rm=FALSE,
                    variable.name="Lifestage",value.name="ADD")

## Prepare file for graphing LADD
# Calculate time within each lifestage (tmeweight ADDs)
age <- 70 # assumed lifespan = 70 yrs
lifeyr <- c(0, 1/age, 2/age, 3/age, 5/age, 5/age, 49/age)

# Create new weighted lifestages

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wtchemfile <- chemfile[,1:8]
for (i in 2:ncol(wtchemfile)) {
  wtchemfile[,i] <- Filter(is.numeric,(chemfile[,i]))*lifeyr[i]
}
mwt <- melt(wtchemfile,
            id.vars="Media",
            measure.var=c("Young Infant","Infant","Young
child","child",
                        "Young Youth","Youth","Adult"),
            na.rm=FALSE,
            variable.name="Lifestage",value.name="LADD")

# =====
# III. Plot graphs by media
# -----
# A. Prepare plotting function.
# Create color palette for graphs
colortab <- c("Dust"="#FF6600",
              "Soil"="#660000",
              "Water"="#000033",
              "Breast Milk"="#330033",
              "Dairy"="#CC0066",
              "Meat"="#FF0000",
              "Fish"="#33CCCC",
              "Vegetables"="#006600",
              "Fruit"="#66CC33",
              "Grains"="#FFCC00")

# Create function for plotting individual graphs by media
mediaplot <- function(infile, chem_name){
  outplot <- ggplot(data = lifex, aes(x =
Lifestage,y=get(colnames(infile[3])),
  fill = factor(Lifestage))) +
  geom_bar(stat = "identity", show.legend = FALSE, fill =
colortab[i], alpha = 1) +
  labs(title = paste(tostring(chem_name),
paste(colnames(infile[3]),"for",infile[i, 1])),
  x = "Lifestage", y=paste(colnames(infile[3]),"(mg/kg-
day)"))+
  theme(plot.title = element_text(hjust = 0.5),
  axis.text.x = element_text(angle = 45, hjust = 1))
  # Adjust y-axis
  if (exists('y_lims') == TRUE){
    outplot <- outplot + scale_y_continuous(limits = y_lims,
labels=scientific)}
  return(outplot)
}

# -----
# B. Create & save 10 ADD and LADD graphs by media.
# Create plotList
rm(plotList)
```

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plotList <- list()

# Create & save 'By Media' ADD Plots
for (i in 1:nrow(chemfile)) {
  # Create plots
  lifex <- subset(meltchemfile,meltchemfile$Media==meltchemfile[i,1])
  ADDmedia <- mediaplot(meltchemfile, chemname)
  ADD <- paste("p_ADD",sep = "_", chemfile[i, 1])
  assign(ADD, ADDmedia)
  # Save plots
  plotList[[i]] <- print(ADDmedia)
  plotList[[i]]
  dev.copy(png, filename=paste(chemname, chemfile[i, 1],
"ADD_bylife.png", sep = '_'))
  dev.off()
}

# Create & save 'By Media' LADD Plots
for (i in 1:nrow(chemfile)) {
  # Create plots
  lifex <- subset(mwt,mwt$Media==mwt[i,1])
  LADDmedia <- mediaplot(mwt, chemname)
  LADD <- paste("p_LADD", sep = "_", chemfile[i, 1])
  assign(LADD, LADDmedia)
  # Save plots
  plotList[[i+nrow(chemfile)]] <- print(LADDmedia)
  plotList[[i+nrow(chemfile)]]
  dev.copy(png, filename=paste(chemname, chemfile[i, 1],
"LADD_bylife.png", sep = '_'))
  dev.off()
}

# =====
# IV. Plot graphs by lifestages
# -----
# A. Prepare plotting function.
lifeplot <- function(infile, chem_name){
  outplot <- ggplot(data=infile,
                    aes(x=Lifestage,
                        y=get(colnames(infile[3])),
                        fill=factor(Media))) +
    geom_bar(stat="identity", alpha = 1) +
    scale_fill_manual(name="Media",values=colortab,drop=drop(TRUE)) +
    labs(title=paste(toString(chem_name), colnames(infile[3]),"by
Lifestage"),
         x="Lifestage",y=paste(colnames(infile[3]),"(mg/kg-day)")) +
    theme(plot.title = element_text(hjust = 0.5),
          axis.text.x = element_text(angle = 45, hjust = 1))
  # Adjust y-axis
  if (exists('y_lims') == TRUE){
    outplot <- outplot + scale_y_continuous(limits = y_lims,
labels=scientific)}
  return(outplot)
}

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    return(outplot)
  }

# -----
# B. Plot ADD & LADD graphs by lifestage.
p_ADDlife <- lifeplot(meltchemfile, chemname)
p_LADDlife <- lifeplot(mwt, chemname)

# -----
# C. Save plots as png
p_ADDlife
dev.copy(png, filename=paste(chemname,"ADD_bylife.png", sep = '_'))
dev.off()

p_LADDlife
dev.copy(png, filename=paste(chemname,"LADD_bylife.png", sep = '_'))
dev.off()

# =====
# V. Plot graphs by cumulative percent.
# -----
# A. Prepare plotting function.
pctplot <- function(infile, chem_name){
  outplot <-
  ggplot(data=infile,aes(x=Lifestage,y=get(colnames(infile[3])),
                        fill=factor(Media)))+
    geom_bar(stat="identity",position="fill", alpha = 1) +
    scale_y_continuous(labels=scales::percent) + # percent label axis
    scale_fill_manual(name="Media",values=colortab,drop=drop(TRUE)) +
    labs(title=paste(toString(chem_name),
                    "Percent",colnames(infile[3]),"by Lifestage"),
         x="Lifestage",y="Percent (%)")+
    theme(plot.title = element_text(hjust = 0.5),
          axis.text.x = element_text(angle = 45, hjust = 1))
  return(outplot)
}

# -----
# B. Save cumulative percentage graph by lifestage as png.
# Plot
p_perlife <- pctplot(meltchemfile, chemname)

# Save plot
p_perlife
dev.copy(png, filename=paste(chemname,"Percent.png", sep = '_'))
dev.off()

# =====
# VI. Create tables.
# -----
# A. Create new childhood & lifetime categories.
# Create childhood lifestage.
hood <- NA

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for(i in 1:nrow(chemfile)){
  hood[i]<-(((1*chemfile[i,2])+(2*chemfile[i,3])+(3*chemfile[i,4])+
(5*chemfile[i,5])+(5*chemfile[i,6])+(5*chemfile[i,7]))/21) # childhood
= 21 yrs
}

# Create new table.
finchemfile <- chemfile
finchemfile$Childhood <- hood # Add childhood column
finchemfile$Lifetime<- rowSums(Filter(is.numeric,wtchemfile[,1:8])) #
Add lifetime column

# Reorganize table.
mfin <- melt(finchemfile,
            id.vars="Media",
            measure.var=c("Childhood","Adult","Lifetime"),
            na.rm=FALSE,
            variable.name="Lifestage",value.name="ADD")

# -----
# B. Plot and save childhood, adult, lifetime graphs.
## Plot graphs
# Plot ADD graph
p_ADDfin <- lifeplot(mfin, chemname)
# Plot percent graph
p_perfin <- pctplot(mfin, chemname)

## Save plots
p_ADDfin
dev.copy(png, filename=paste(chemname,"Summary_ADD.png", sep = '_'))
dev.off()

p_perfin
dev.copy(png, filename=paste(chemname,"Summary_Percent.png", sep =
'_'))
dev.off()

# -----
# C. Create finalized tables for display with childhood, lifetime, and
aggregate columns.
## Create ADD table.
add_tab <- finchemfile
aggrow1<-colSums(Filter(is.numeric,add_tab))
# Add aggregate row to table.
add_tab[nrow(add_tab)+1,1]<-"Aggregate"
add_tab[nrow(add_tab),2:ncol(add_tab)]<-aggrow1

## Create LADD table.
ladd_tab <- wtchemfile
# Add childhood column.
ladd_tab$Childhood <- rowSums(Filter(is.numeric,wtchemfile[,1:7]))
```

```
#####  
#####  
# =====  
# VII. Save and View outputs.  
# -----  
# A. View ADD & LADD tables.  
## View ADD table  
print('ADD Table')  
add_tab  
# Save table as CSV file  
write.csv(add_tab, paste(chemname,"ADD_table.csv", sep = '_'))  
  
# View LADD table  
print('LADD Table')  
ladd_tab  
# Save table as CSV file  
write.csv(ladd_tab, paste(chemname,"LADD_table.csv", sep = '_'))  
  
# -----  
# B. View all graphs.  
# ADD by Media Plots  
p_ADD_Dust  
p_ADD_Soil  
p_ADD_Water  
p_ADD_BreastMilk  
p_ADD_Dairy  
p_ADD_Meat  
p_ADD_Fish  
p_ADD_Vegetables  
p_ADD_Fruit  
p_ADD_Grains  
  
# LADD by Media Plots  
p_LADD_Dust  
p_LADD_Soil  
p_LADD_Water  
p_LADD_BreastMilk  
p_LADD_Dairy  
p_LADD_Meat  
p_LADD_Fish  
p_LADD_Vegetables  
p_LADD_Fruit  
p_LADD_Grains  
  
# ADD by Lifestage Plot  
p_ADDlife  
  
# LADD by Lifestage Plot  
p_LADDlife  
  
# Cumulative Percentage Plot  
p_perlife  
  
# Childhood, Lifetime ADD Plot
```



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p\_ADDfin

# Childhood, Lifetime Percent Plot  
p\_perfin

# -----

# C. Save all plots to same PDF.

## Add to plotList

# By Life Plots

plotList[[length(plotList)+1]] <- lifeplot(meltchemfile, chemname)

plotList[[length(plotList)+1]] <- lifeplot(mwt, chemname)

# Remainder Plots

plotList[[length(plotList)+1]] <- pctplot(meltchemfile, chemname)

plotList[[length(plotList)+1]] <- lifeplot(mfin, chemname)

plotList[[length(plotList)+1]] <- pctplot(mfin, chemname)

## Create PDF

pdf(file=paste(chemname,"plots.pdf", sep = '\_'))

plotList

dev.off()

##### END CODE

#####