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# Code for aggregating consumer exposures

# Written by CG at ICF in January 2024

# Last updated 03/04/2024 HAF

#User defined fraction absorbed values by pathway

fabs_derm = 1 #fabs_dermal already accounted for in CEM results

fabs_ing = 0.775 #fabs_ing depends on logKow based on Fang and Stapleton (2014)

fabs_inh = 0.5 #fabs_inh assumed to be 0.5 for all chemicals

# Number of people in simulation

n_people <- 100000

# Importing libraries needed

library(readxl)

library(base)

library(data.table)

# Set working directory

setwd(dirname(rstudioapi::getSourceEditorContext()$path)) #This should automatically set the working
directory

# Import input file

cpsc_data <- read_xlsx("10_35656-01-0_Aggregate_Estimate_Inputs_2024-01-20_v2.xlsx")

adjustments <- read_xlsx("Probability_Adjustments_Aggregate_Estimate_Inputs_Tier3_2024-03-
11.xlsx")

# Make copy of data to edit

data1 <- cpsc_data[,c(1,5:13)]

data2 <- copy(adjustments)
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# Variable of unique number of scenarios (18 in current version)
n_cem <- uniqueN(data1$`CPSC Scenario #`)

# Make new column that indexes each scenario and repeats 7 times in same scenario (7 ages)
data1$index <- c(1:nrow(data1))
data_unadj <- copy(data1)

#Create totals. Broken out to easily alter or add adjustments when needed
data1$Total_Derm <- data1$A_DER1 + data1$A_DER2 * data2$DermalAdj + data1$A_DER3
data1$Total_Ing <- data1$A_ING1 + data1$A_ING2 * data2$MouthingAdj + data1$A_ING3
data1$Total_Inh <- data1$A_INH1G + data1$A_INH1P

data_unadj$Total_Derm <- data1$A_DER1 + data1$A_DER2 + data1$A_DER3
data_unadj$Total_Ing <- data1$A_ING1 + data1$A_ING2 + data1$A_ING3
data_unadj$Total_Inh <- data1$A_INH1G + data1$A_INH1P

# Random number generator
RNGkind("Mersenne-Twister")

# Set seed and x1 is matrix with unique number of scenarios
set.seed(100)
x1_temp <- matrix(runif(n_people*n_cem), nrow = n_cem, ncol = n_people)
x1 <- apply(x1_temp, 2, function(x) rep(x, each = 7))

# Probabilities from each scenario
probs1 <- data2$Probability1
probs2 <- data2$Probability2

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# x2 is matrix with unique number of scenarios
x2_temp <- matrix(runif(n_people*n_cem), nrow = n_cem, ncol = n_people)
x2 <- apply(x2_temp, 2, function(x) rep(x, each = 7))

ages <- uniqueN(data2$Receptor)
# Initializing exposure pathway vectors
total_dermal_unadj <- matrix(0,nrow = ages, ncol = n_people)
total_ingestion_unadj <- matrix(0,nrow = ages, ncol = n_people)
total_inhalation_unadj <- matrix(0,nrow = ages, ncol = n_people)

total_dermal_adj <- matrix(0,nrow = ages, ncol = n_people)
total_ingestion_adj <- matrix(0,nrow = ages, ncol = n_people)
total_inhalation_adj <- matrix(0,nrow = ages, ncol = n_people)

total_dermal_prob <- matrix(0,nrow = ages, ncol = n_people)
total_ingestion_prob <- matrix(0,nrow = ages, ncol = n_people)
total_inhalation_prob <- matrix(0,nrow = ages, ncol = n_people)

total_dermal <- matrix(0,nrow = ages, ncol = n_people)
total_ingestion <- matrix(0,nrow = ages, ncol = n_people)
total_inhalation <- matrix(0,nrow = ages, ncol = n_people)

# For loop to go over every person, for total exposure via dermal, ingestion, inhalation
for (i in 1:n_people){

#Select relevant scenarios based on p1 (p2 below). 0 = not selected , otherwise 1.
y1 <- as.integer(x1[, i] <= probs1)
y2 <- as.integer(x2[, i] <= probs2)

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intersect = y1*y2 #All scenarios that are selected from both probabilities

# Total route exposure is sum of the intersection of when total route is less than the prob

# UnAdj (the original CEM output)
total_dermal_unadj[, i] <- rowSums(matrix(data_unadj$Total_Derm, nrow = ages))

total_ingestion_unadj[, i] <- rowSums(matrix(data_unadj$Total_Ing, nrow = ages))

total_inhalation_unadj[, i] <- rowSums(matrix(data_unadj$Total_Inh, nrow = ages))

# Adj (CEM output with adjustments)
total_dermal_adj[, i] <- rowSums(matrix(data1$Total_Derm, nrow = ages))

total_ingestion_adj[, i] <- rowSums(matrix(data1$Total_Ing, nrow = ages))

total_inhalation_adj[, i] <- rowSums(matrix(data1$Total_Inh, nrow = ages))

# Prob (averages across population including non-users, uses adjusted CEM output)
total_dermal_prob[, i] <- rowSums(matrix(data1$Total_Derm*intersect, nrow = ages))

total_ingestion_prob[, i] <- rowSums(matrix(data1$Total_Ing*intersect, nrow = ages))

total_inhalation_prob[, i] <- rowSums(matrix(data1$Total_Inh*intersect, nrow = ages))

# Fabs (population average of absorbed dose, now with fraction absorbed values)
total_dermal[, i] <- rowSums(matrix(data1$Total_Derm*intersect, nrow = ages)) * fabs_derm

total_ingestion[, i] <- rowSums(matrix(data1$Total_Ing*intersect, nrow = ages)) * fabs_ing

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total_inhalation[, i] <- rowSums(matrix(data1$Total_Inh*intersect, nrow = ages)) * fabs_inh
}

#Output

#Make tables

table1 = cbind(rowMeans(total_dermal_unadj),
rowMeans(total_ingestion_unadj),rowMeans(total_inhalation_unadj),
              rowMeans(total_dermal_unadj) + rowMeans(total_ingestion_unadj) +
rowMeans(total_inhalation_unadj))

rownames(table1) <- unique(data2$Receptor)

colnames(table1) <- c('DermalUnadj',      'IngestionUnadj',      'InhalationUnadj',
                    'TotalUnadj')

table2= cbind(rowMeans(total_dermal_adj),
rowMeans(total_ingestion_adj),rowMeans(total_inhalation_adj),
            rowMeans(total_dermal_adj) + rowMeans(total_ingestion_adj) +
rowMeans(total_inhalation_adj))

rownames(table2) <- unique(data2$Receptor)

colnames(table2) <- c('DermalAdj',  'IngestionAdj',  'InhalationAdj', 'TotalAdj')

table3= cbind(rowMeans(total_dermal_prob),
rowMeans(total_ingestion_prob),rowMeans(total_inhalation_prob),
            rowMeans(total_dermal_prob) + rowMeans(total_ingestion_prob) +
rowMeans(total_inhalation_prob))

rownames(table3) <- unique(data2$Receptor)

colnames(table3) <- c('DermalProbs','IngestionProbs',      'InhalationProbs',      'TotalProbs')

table4= cbind(rowMeans(total_dermal), rowMeans(total_ingestion),rowMeans(total_inhalation),
              rowMeans(total_dermal) + rowMeans(total_ingestion) + rowMeans(total_inhalation))

rownames(table4) <- unique(data2$Receptor)

colnames(table4) <- c('DermalFabs', 'IngestionFabs', 'InhalationFabs',      'TotalFabs')

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#Combine tables
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Table <- cbind(table1,table2,table3,table4)
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#Write to csv
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write.csv(Table, "10_35656-01-0_Consumer_Aggregate_Results_2024-01-20_v2_ReverseOrder.csv")
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#Reorder Rows and write to csv
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Table2 = Table[c("Infant1", "Infant2", "Child1", "Child2", "Youth1", "Youth2", "Adult"), ]
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write.csv(Table2, "10_35656-01-0_Consumer_Aggregate_Results_2024-01-20_v2.csv")
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#Write to csv the individual scenarios adjusted for mouthing and dermal
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write.csv(data1, "10_35656-01-0_Individual_Scenarios_Adjusted_2024-01-20_v2.csv")
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