Well-Mixed Room Box Model—ATSDR

File name: formaldehyde_model.R (sha1sum: cbfec5c671f7809165a599d8dbc037c792544dbc)

```
#Purpose: To model indoor air concentrations for formaldehyde emissions from laminate flooring
#Output generated by this script can be found in the report "Possible Health Implications from
Exposure to Formaldehyde Emitted from Laminate Flooring Samples Tested by the Consumer Product
Safety Commission"---ATSDR 2016

#Load required libraries
library(ggplot2)
library(reshape)
library(lattice)
library(plyr); library(dplyr)

#Well-mixed room box model with a constant emmision rate. Equations definitions are found in
https://www.aiha.org/get-involved/VolunteerGroups/Documents/IHMOD_Korean-AIHA-MathModel209.xls and
in Keil et al. 2009
#IH_Ct is the formaldehyde indoor air concentration at time t; G is the generation rate; Cin is
the background formaldehyde concentration; Q is the ventilation rate; KL is the loss mechanism
value; V is the room volume; t is time; and C0 is the initial concentration.
IH_Ct<-function (G,Cin,Q,KL,V,t,C0){
  A<-(G+Cin*Q)/(Q+KL*V); B<--(Q+KL*V)/V*t
  A*(1-exp(B))+C0*exp(B)
}

#Steady state concentration as a function of Air Change Ratio. This equation was modified from CB
Keil et al. 2009. Equation 4-14 was modified using the definition for generation rate (G=EF*A),
air change ratio (AC=Q/V) and V=A*h where EF is the emission factor, A is area, Q is flow rate, V
is volume, and h is ceiling height.
C_AC <- function (EF,AC,h) {EF/(AC*h)}

#Generate input parameters for small chamber dataset
set.seed(5)
n=100000  #Set number of realizations for Monte Carlo simulation
EF=rlnorm(n,meanlog=3.73242,sdlog=0.8469912)
AC=runif(n,0.1,1.21)
h=2.44

#Perform Monte Carlo simulation
MCsmall<-data.frame(indoorC=C_AC(EF,AC,h))
MCsmall$EF<-EF
MCsmall$AC<-AC
MCsmall<-arrange(MCsmall,indoorC)
MCsmall$pexc=1-(1:n*(1/n))
MCsmall$pcum=(1:n*(1/n))

summary(MCsmall$indoorC)

quantile(MCsmall$indoorC,probs = seq(0.05,0.95,0.05))
```

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```
#Generate input parameters for large chamber dataset
set.seed(5)
n=100000  #Set number of realizations for Monte Carlo simulation
EF=rlnorm(n,meanlog=5.620327,sdlog=0.587986)
AC=runif(n,0.1,1.21)
h=2.44

#Perform Monte Carlo simulation
MClarge<-data.frame(indoorC=C_AC(EF,AC,h))
MClarge$EF<-EF
MClarge$AC<-AC
MClarge<-arrange(MClarge,indoorC)
MClarge$pexc=1-(1:n*(1/n))
MClarge$pcum=(1:n*(1/n))
mean(MClarge$indoorC)

summary(MClarge$indoorC)

quantile(MClarge$indoorC,probs = seq(0.05,0.95,0.05))

#Plot probability of exceedance for small chamber
xat<-seq(0,300,50)
xatL<-as.character(format(xat,big.mark=",",scientific=F,drop0trailing=T))
yat <- qnorm(c(0.001,0.01, 0.05, 0.10,0.20,0.30,0.40, 0.50, 0.60, 0.70,0.80,0.90,0.95,0.99,0.999))
yatL<-c("0.1","1","5","10","20","30","40","50","60","70","80","90","95","99","99.9")

xyplot(qnorm(pexc)~indoorC,MCsmall,type=c("l","g"),
       xlab="Simulated formaldehyde indoor concentration, in micrograms per cubic meter",
       ylab="Probability of exceedance",
       scales=list(x = list(log = F,at=xat,labels=xatL),y = list(at = yat, labels = yatL)),
       xlim=c(0,300),
       ylim=c(qnorm(0.001),qnorm(.999)))

#Plot probability of exceedance for large chamber
xat<-seq(0,1000,100)
xatL<-as.character(format(xat,big.mark=",",scientific=F,drop0trailing=T))
xyplot(qnorm(pexc)~indoorC,MClarge,type=c("l","g"),
       xlab="Simulated formaldehyde indoor concentration, in micrograms per cubic meter",
       ylab="Probability of exceedance",
       scales=list(x = list(log = F,at=xat,labels=xatL),y = list(at = yat, labels = yatL)),
       xlim=c(0,1000),
       ylim=c(qnorm(0.001),qnorm(.999)))

#Plot concentration vs ACH (dimensionless or percent)
ACvalues<-seq(0.1,2,0.05)
conc<-C_AC(EF = quantile(100,probs = 0.5),AC=ACvalues,h = 2.44)
conc_normalized<-data.frame(AC=ACvalues,indoorC=conc)
conc_normalized$indoorC<-conc_normalized$indoorC/max(conc_normalized$indoorC)*100
ggplot(conc_normalized,aes(AC,indoorC))+geom_line()+theme_bw()+scale_y_continuous(limits=c(0,100),
breaks=seq(0,100,10))+scale_x_continuous(limits=c(0,2))
```

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```
#Example plot for transient model
G=100*250 #EF=100 micrograms per square meter per hour ; A=250 meter square
Cin=0
V=250*2.44 #250 meter square times 2.44 meter (8 feet) ceiling
Q=0.35*V
KL=0
C0=0
example<-data.frame(tmin = 1:1440/60,C=IH_Ct(G = G,Cin = Cin,Q = Q,KL = KL,V = V,t = 1:1440/60,C0
= C0))
ggplot(example,aes(tmin,C))+geom_line()+xlab("Time, in hours")+
  ylab("Inoor air formaldehyde concentration, in micrograms per cubic meter")+
  scale_x_continuous(limits=c(0,24),breaks=seq(0,24,4))+
  theme_bw()

#Calculate various percentiles
quantile(MCsmall$indoorC,probs = c(0.05,0.25,0.5,0.75,0.90,0.95,0.99))

quantile(MClarge$indoorC,probs = c(0.05,0.25,0.5,0.75,0.90,0.95,0.99))
```

```
> sessionInfo()
R version 3.2.3 (2015-12-10)
Platform: x86_64-w64-mingw32/x64 (64-bit)
Running under: Windows 7 x64 (build 7601) Service Pack 1

locale:
[1] LC_COLLATE=English_United States.1252  LC_CTYPE=English_United States.1252
LC_MONETARY=English_United States.1252
[4] LC_NUMERIC=C                           LC_TIME=English_United States.1252

attached base packages:
[1] stats     graphics  grDevices utils     datasets  methods   base

other attached packages:
[1] dplyr_0.4.3     plyr_1.8.3      lattice_0.20-33 reshape_0.8.5   ggplot2_2.0.0

loaded via a namespace (and not attached):
 [1] Rcpp_0.12.3       digest_0.6.9      assertthat_0.1    grid_3.2.3        R6_2.1.2
gtable_0.1.2
 [7] DBI_0.3.1         magrittr_1.5      scales_0.3.0      lazyeval_0.1.10   fortunes_1.5-2
rmarkdown_0.9.2
[13] labeling_0.3      tools_3.2.3       munsell_0.4.2     parallel_3.2.3    rsconnect_0.4.1.4
colorspace_1.2-6
[19] htmltools_0.3     knitr_1.12.3
```