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# Congener specific transfer model for dioxins (PCDD/Fs and dI-PCBs) in laying hens, version 1.4 - model documentation.

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# Colophon

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# Summary

The fundamentals of a congener specific feed-food transfer model for PCDD/F and dI-PCB concentrations in body fat and egg yolk fat in laying hens are presented. The model, which is available as a webtool application (https://feedfoodtransfer.nl/), can be used to compare simulated concentrations with regulatory limits for these food matrices.

## Introduction

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Polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs) and dioxin-like polychlorinated biphenyls (dI-PCBs) are persistent environmental pollutants (POPs) that may accumulate in fatty tissues and the liver ("hepatic sequestration") of animals and humans. One of the main sources of human exposure to PCDD/Fs and dI-PCBs is the consumption of animal products, such as meat, milk and eggs. In turn, animal feed is an important contributor to the accumulation of PCDD/Fs and dI-PCBs in animal products used for human consumption.

This report presents the congener-specific transfer model that estimates PCDD/F and dI-PCB concentrations in body fat and egg yolk fat of laying hens exposed to these compounds via feed.

The concentration of the sum of PCDD/Fs and dl-PCBs is expressed in total toxic equivalents of 2,3,7,8-TCDD (total TEQ) using Toxic Equivalence Factors (TEFs) for the different PCDD/F and dl-PCB congeners (van den Berg et al. 2006). The estimated concentrations can be compared to the regulatory limits that have been defined by regulatory agencies in various countries.

For all congeners the same model structure was used, but parameter values were calibrated separately for each congener. The model is available as a webtool application (<u>https://feedfoodtransfer.nl/</u>).

For simulations based on total TEQ levels in feed, a total TEQ transfer model is also available as a webtool application. The calibration of this latter model is based on the total TEQ concentration, i.e. the concentration of PCDD/Fs and dl-PCBs expressed in terms of equivalents of 2,3,7,8-TCDD.

# 2 Model description

#### 2.1 General overview

The transfer model used to estimate PCDD/Fs and dI-PCBs concentrations in egg yolk comprises two compartments representing a central compartment and a fat compartment (Fig 1). Intake of PCDD/Fs and dI-PCBs is modelled as a constant intake amount,  $A_i$ , of which a fraction ( $F_{abs}$ ) is absorbed over the gut wall into the central compartment on a daily basis. PCDD/Fs and dI-PCBs that have been absorbed by the central compartment can migrate to the fat compartment ( $q_c$ ), and vice versa ( $q_f$ ). PCDD/Fs and dI-PCBs can leave the laying hen's body through two processes. The first is excretion to egg yolk fat ( $\varepsilon y$ ), with  $\varepsilon$  being the laying efficiency, and y being the excretion rate constant. The second is hepatic clearance (k).



Figure 1. Two compartments comprised kinetic model for the PCDD/F and dI-PCB congeners in the laying hen (Figure taken from Notenboom et al. 2023).

#### 2.2 Model equations

The transfer model described in this report consists of a set of coupled ordinary differential equations (ODEs). These ODEs describe the distribution of PCDD/Fs and dl-PCBs between the central compartment and the fat compartment over time. For both compartments of the models, an ODE was formulated. Specifically, equations 1 and 2 describe the change in the amount of PCDD/Fs and dl-PCBs in the central compartment and the fat compartment, respectively.

$$\frac{dA_c(t)}{dt} = F_{abs}A_i - (q_c + \varepsilon y + k)A_c(t) + q_f A_f(t)$$
(1)

$$\frac{dA_f(t)}{dt} = q_c A_c(t) - q_f A_f(t)$$
(2)

 $A_c(t)$  [pg]: Amount of substance in the central compartment at time t $A_f(t)$  [pg]: Amount of substance in the fat compartment at time t $F_{abs}$  [-]: Absorption fraction

 $A_i$  [pg day<sup>-1</sup>]: Daily intake amount of substance

 $q_c$ [day<sup>-1</sup>]: Transfer rate constant from central compartment to fat compartment

 $q_f$ [day<sup>-1</sup>]: Transfer rate constant from fat compartment to central compartment

 $\varepsilon$  [-]: Laying efficiency

y [day<sup>-1</sup>]: Excretion rate constant from central compartment to egg yolk fat

k [day<sup>-1</sup>]: Hepatic clearance rate constant

The transfer rate parameters used in equations 1 and 2 can be expressed as unknown model parameters (van Eijkeren et al., 2006):

$$q_c = \frac{Q}{P_c V_c}$$
(3)  
$$q_f = \frac{Q}{P_f V_f}$$
(4)

$$y = \frac{P_{y,f}W_{y,f}}{P_c V_c} \tag{5}$$
$$k = \frac{CL}{CL} \tag{6}$$

$$k = \frac{1}{P_c V_c} \tag{6}$$

Here, *Q* represents the compartment blood flow.  $V_c$  and  $V_f$  represent the volumes of the central and fat compartment, respectively.  $P_c$  and  $P_f$  represent the blood-body partition coefficient and the blood-fat partition coefficients, respectively. *CL* represents the hepatic clearance rate.  $W_{y,f}$  is the amount of fat in the egg yolk and  $P_{y,f}$  is the partition coefficient between the blood and the egg yolk fat.

The amount of PCDD/F and dI-PCB congeners in the body and fat compartment can be converted into concentrations by dividing the amount by the volume of the respective compartments,  $V_c$  and  $V_f$ .

Finally, the change in the amount of PCDD/F and dI-PCB congeners in eggs at a given time,  $A_{yf}(t)$ , can be calculated as follows:

$$\frac{dA_{yf}(t)}{dt} = \epsilon y A_c(t) - A_{yf}(t)$$
(7)

#### 2.3 Model assumptions

The following assumptions were made in the presented model:

- PCDD/Fs and dl-PCBs homogeneously distribute over the fat compartment.
- PCDD/F and dI-PCB concentrations measured in abdominal fat are representative of the PCDD/F and dI-PCB concentrations in the fat compartment.
- Hepatic sequestration was neglected
- The amount of fat in the egg yolk,  $W_{y,f}$  is constant over time and can be measured.
- The laying hens are assumed to weigh 1840 grams ( $V_{total}$ ). The sizes of the two compartments (central and fat) are calibrated.
- It is assumed that the hens get fed once a day with a constant amount of feed per day.
- The volume of the central compartment can be derived by taking the difference between the total volume and the volume of the fat compartment (which was calibrated (see section 2.5)).
- The density of the compartments is 1 g/cm<sup>3</sup>. The volume of the model compartments,  $V_c$  and  $V_f$ , are thus equal to the weights of the compartments ( $W_c$  and  $W_f$ ).
- Limitations of the available experimental data prevented the calibration of 1,2,3,4,6,7,8,9-OCDF, 1,2,3,4,6,7,8-HpCDD, 1,2,3,4,6,7,8,9-OCDD and PCB123. For these congeners the simulation is performed using the parameters for the total TEQ model.

#### 2.4 Generic parameters

The remaining parameters (*Table 1*) are not specific to PCDD/Fs or dl-PCBs and can all be obtained from literature.

Parameter	Value	Unit	Source
ε	0.9	day⁻¹	Mean of exposure groups in Kan and Jonker-Den Rooyen (1978)
Vtotal	1840	cm <sup>3</sup>	expert opinion
$W_{egg}$	60	g	Kan and Jonker-Den Rooyen (1978)
$W_y$	19.2	g	Gilbert (1971)
$W_{v,f}$	5.76	g	Gilbert (1971)

Table 1. Generic parameter values

### 2.5 System-dependent parameters

As explained by van Eijkeren et al. (2006), the presented transfer model contains two parameters,  $q_c$  and  $q_f$ , that can be identified unconditionally from the available experimental data, whereas it contains four parameters, y, k,  $F_{abs}$ , and  $W_f$ , that are conditionally identifiable. The four conditionally identifiable parameters cannot be directly fitted to the data.

However, they can be determined in relation with each other (van Eijkeren et al., 2006):

$c_1 = r = \varepsilon y + k$	(8)
$c_2 = yF_{abs}$	(9)
$c_3 = \frac{F_{abs}}{W_f}$	(10)

Here, parameters  $c_1$ ,  $c_2$ , and  $c_3$  can be fitted to the available experimental data. Although the four conditionally identifiable parameters cannot be directly fitted to the data and it is thus impossible to find a single value they should take on, it is possible to find the possible range of values they might take on. This can be done by defining boundary conditions on the parameter values. More specifically, the hepatic clearance, k, cannot be lower than 0 day<sup>-1</sup>, whereas the absorption fraction,  $F_{abs}$  cannot exceed 1. If the model is fitted with the first boundary condition, i.e.,  $k \ge 0$ , then it follows that  $y \le \frac{c_1}{\varepsilon}$ ,  $F_{abs} \ge \frac{c_2}{y}$ , and  $W_f \ge \frac{F_{abs}}{c_3}$ . Similarly, from the second boundary condition, i.e.,  $F_{abs} \le 1$ , it follows that  $y => c_2$ ,  $k \le c_1 - \varepsilon c_2$  and  $W_f \le \frac{1}{c_1}$ .

The true parameter values are thus mathematically bound to be within the boundaries described above. However, in order to find definitive parameter values for the transfer model, assumptions were necessary. Therefore, as a conservative estimate for the substance concentrations in egg yolk fat, an hepatic clearance of 0 was assumed, i.e., k = 0. From this assumption, it follows that  $y = \frac{c_1}{\varepsilon}$ ,  $F_{abs} = \frac{\varepsilon c_2}{c_1}$  and  $W_f = \frac{\varepsilon c_2}{c_1 c_3}$ . Based on these assumptions, Notenboom et al. (2023) calibrated these model parameters using the experimental data reported by Hoogenboom et al. (2006) and Traag et al. (2006) for the PCDD/F and dl-PCB toxic equivalent (TEQ) as well as for each of the individual congeners. The calibrated parameters used in the transfer model are shown in Table 2. Note that calibration of the parameters was not possible for 1,2,3,4,6,7,8,9-OCDF, 1,2,3,4,6,7,8-HpCDD, 1,2,3,4,6,7,8,9-OCDD and PCB 123. For these compounds, a web tool user can either choose to use the parameter values calibrated for PCDD/F and dl-PCB TEQ, or to exclude these compounds from the analyses.

Compound	<i>q<sub>c</sub></i> [day <sup>-1</sup> ] Mass transfer rate from central compartment to fat compartment.*	<i>q<sub>f</sub></i> [day <sup>-1</sup> ] Mass transfer rate from fat compartment to central compartment.*	F <sub>abs</sub> [-] Absorption fraction. Calibrated.*	y [day <sup>-1</sup> ] Excretion rate constant to egg yolk fat	k [day <sup>-1</sup> ] Hepatic clearance rate	<i>V<sub>f</sub></i> [g]
PCDD/F and dI-PCB TEQ	0.14	0.06	0.78	0.057	0	230
2,3,7,8-TCDF	0.31	0.205	0.70	0.040	0	200
1,2,3,7,8-PeCDF	0.19	0.073	0.71	0.078	0	210
2,3,4,7,8-PeCDF	0.10	0.057	0.71	0.055	0	190
1,2,3,4,7,8-HxCDF	0.08	0.029	0.60	0.110	0	180
1,2,3,6,7,8-HxCDF	0.08	0.031	0.55	0.109	0	180
2,3,4,6,7,8-HxCDF	0.10	0.034	0.45	0.131	0	200
1,2,3,7,8,9-HxCDF	0.10	0.040	0.54	0.103	0	180
1,2,3,4,6,7,8-HpCDF	0.06	0.034	0.18	0.182	0	140
1,2,3,4,7,8,9-HpCDF	0.04	0.018	0.24	0.167	0	150
1,2,3,4,6,7,8,9-OCDF**	-	-	-	-	-	-
2,3,7,8-TCDD	0.35	0.230	0.78	0.042	0	210
1,2,3,7,8-PeCDD	0.14	0.070	0.75	0.055	0	220
1,2,3,4,7,8-HxCDD	0.09	0.030	0.61	0.101	0	190
1,2,3,6,7,8-HxCDD	0.09	0.036	0.59	0.106	0	170
1,2,3,7,8,9-HxCDD	0.07	0.032	0.42	0.118	0	150
1,2,3,4,6,7,8-HpCDD**	-	-	-	-	-	-
1,2,3,4,6,7,8,9-OCDD**	-	-	-	-	-	-
PCB 81	0.11	0.121	0.92	0.024	0	190
PCB 77	0.25	0.136	0.89	0.044	0	240
PCB 126	0.13	0.067	1.00	0.038	0	270

Table 2. Calibrated parameter values used in the transfer model for each of the 29 congeners

Compound	<i>q<sub>c</sub></i> [day <sup>-1</sup> ] Mass transfer rate from central compartment to fat compartment.*	<i>q<sub>f</sub></i> [day <sup>-1</sup> ] Mass transfer rate from fat compartment to central compartment.*	F <sub>abs</sub> [-] Absorption fraction. Calibrated.*	y [day <sup>-1</sup> ] Excretion rate constant to egg yolk fat	k [day <sup>-1</sup> ] Hepatic clearance rate	<i>V<sub>f</sub></i> [g]
PCB 169	0.11	0.029	0.85	0.081	0	220
PCB 123**	-	-	-	-	-	-
PCB 118	0.12	0.063	0.98	0.041	0	230
PCB 114	0.20	0.090	0.89	0.061	0	180
PCB 105	0.12	0.084	0.92	0.037	0	200
PCB 167	0.10	0.095	1.00	0.062	0	70
PCB 156	0.11	0.039	0.92	0.063	0	220
PCB 157	0.16	0.051	0.86	0.094	0	190
PCB 189	0.06	0.017	0.80	0.102	0	190

\* Notenboom et al., 2023 \*\* No calibration possible. For these congeners the simulation is performed using the parameters for the total TEQ model (PCDD/F and dl-PCB TEQ).

## Software details

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The transfer model simulations were developed and run using the R modelling language and using the deSolve package. Specifications on the programming packages are listed below:

Name software: R (tested with version 4.0.5) Manufacturer: The R Foundation for Statistical Computing Place of manufacture: online Year of manufacture: 2021 Description: A programming language for statistical computing

Name software: DeSolve (tested with version 1.30) Manufacturer: Karline Soetaert, Thomas Petzoldt and R. Woodrow Setzer Place of manufacture: online Year of manufacture: 2023 Description: Package to solve systems of differential equations url: https://cran.r-project.org/web/packages/deSolve/index.html

Name software: dplyr (tested with version 1.1.4) Manufacturer: Hadley Wickham, Romain François, Lionel Henry, Kirill Müller, Davis Vaughan, Ryan Dickerson, Posit Software, PBC Place of manufacture: online Year of manufacture: 2023 Description: A fast, consistent tool for working with data frame like objects, both in memory and out of memory. url: https://cran.r-project.org/web/packages/dplyr/index.html

### Model applicability

The transfer model presented in this report can be used to simulate the carry-over of PCDD/Fs and dI-PCBs from feed to body fat and egg yolk fat of laying hens. As such, the model enables comparison of the estimated concentration to regulatory limits of these food matrices. Similarly the model can be used to estimate the wash-out period needed to comply with regulatory limits in case the concentrations exceeded such regulatory limits.

An example of a model application is given in Figure 2. The grey line depicts the dioxin concentration in egg yolk fat based on the sum of the transfer of the individual congeners.

In addition, the black line shows the model calculations based on the total TEQ model, i.e. based on the total TEQ concentration in feed. This total TEQ model is also available as a separate model on the website feedfoodtransfer.nl.

Exposure to various congeners was simulated for an exposure duration of 56 days. Concentrations of congeners in the contaminated feed are given in Table 3. Feed intake was 0.113 kg per day. After the 56 days of exposure to contaminated feed, an additional 200 days were simulated in which only clean feed was provided (i.e. feed not containing any PCDD/F and dI-PCB congeners).



Figure 2 Simulated total TEQ concentration in egg yolk of laying hens fed contaminated feed during 56 days followed by clean feed for 200 days. Laying hens were fed 0.113 kg dry feed per day.

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Table 3 Congener concentrations in feed used to illustrate the simulation of the total TEQ concentration in egg yolk.

Congener	Concentration (ng kg <sup>-1</sup> dry feed)
2,3,7,8-TCDF	0.12
2,3,4,7,8-PeCDF	0.34
1,2,3,6,7,8-HxCDF	0.21
1,2,3,7,8,9-HxCDF	0.10
1,2,3,4,6,7,8-HpCDF	0.22
1,2,3,6,7,8-HxCDD	0.51

#### References

Gilbert, A. (1971) The egg: its physical and chemical aspects. In "Physiology and Biochemistry of the Domestic Fowl" Vol. 3, eds. Bell, DJ, and Freeman, BM. Academic, New York.

Hoogenboom, LAP, Kan CA, Zeilmaker MJ, van Eijkeren JCH, Traag WA. (2006). Carry-over of dioxins and PCBs from feed and soil to eggs at low contamination levels. Food Additives and Contaminants 23:518–527. <u>https://doi.org/10.1080/02652030500512037</u>.

Kan, CA and JC. Jonker-Den Rooyen, JC. (1978) Accumulation and depletion of some organochlorine pesticides in high-producing laying hens. Journal of Agricultural and Food Chemistry. 26(4): 935-940. <u>https://doi.org/10.1021/jf60218a007</u>.

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Annex I: R-Code

The code below illustrates the basic implementation of the congener specific transfer model for dioxins (PCDD/Fs and dI-PCBs) in laying hens, v1.3. This code can be used freely and is provided "as is" without warranty of any kind. The National Institute of Public Health and the Environment (RIVM) expressly rejects all liability for the accuracy, completeness, or suitability of the information provided. Use of the information is entirely at your own risk.

#### Model code (dioxin-congener-laying-hen.R):

library(deSolve)

```
assign_parameters <- function(cpd) {</pre>
 #' Assign default parameters for the model
 #'
 #' @param cpd name of the compound for which the parameters are
needed
 #'
 #' @return parameter vector
 inputParameters <- modelParameters |>
  mutate(
   contaminationLevel = input$contaminationLevel,
   dose = Fabs * contaminationLevel * 1000 * input$feedIntake * tef
  )
 inputParameters[30, "dose"] <- sum(inputParameters$dose, na.rm =
TRUE)
 # return all variables in this function's environment
 as.list(inputParameters |> filter(compound == cpd))
}
calculate_variables <- function(parameters) {
 #' Calculate derived parameters from the input parameters, e.g.
scaling.
 #'
 #' @param parameters vector containing the model parameters
 #'
 #' @return parameter vector updated with derived parameters
 # calculate derived parameters from the input parameters, e.g.
scaling.
 with(parameters, {
  # return all variables in this function's environment
  as.list(sys.frame(sys.nframe()))
 }) # end with
}
```

# END!INITIAL

```
# DYNAMIC
```

```
# DERIVATIVE
```

```
derivative <- function(t, y, parameters, ...) {
 #' ODEs defining the model
 #'
 #' @param current time step
 #' @param y current state in a named list: `y <- c(D=dose, Ac=0,
Af=0, AEgg=0)`
 #' @param parameters vector containing the model parameters
 #'
 #' @return derivative of each variable
 # define the derivatives of the model
 with(as.list(c(y, parameters)), {
  dD <- -D
  dAc <- D - (qcentral + k + e * yy) * Ac + qfat * Af
  dAf <- qcentral * Ac - qfat * Af
  dAEgg <- (e * yy) * Ac - AEgg
  return(list(c(dD, dAc, dAf, dAEgg),
    Cf = Af / Vf_{,}
    Cegg = AEgg / 5.76
  ))
 })
}
run_model <- function(parameters) {</pre>
 #' Run model
 #'
 #' @param parameters vector containing the model parameters
 #'
 #' @return simulation results
 parameters <- calculate_variables(parameters)</pre>
 with(parameters, {
  tout <- seq(0, input$tdoseoff + input$tstop, by = 1)
  y0 < -c(D = dose, Ac = 0, Af = 0, AEgg = 0)
  dosing <- data.frame(
    var = c("D"),
    time = c(seq(0, input \\to seoff, by = 1)), #
   value = c(dose),
   method = c("add")
  )
  solution <- ode(
   y = y0, times = tout, events = list(data = dosing),
   func = derivative, parms = parameters, method = "rk4"
  )
```

```
return(as.matrix(unclass(solution)))
})
```

#### Running the model (example)

```
library(dplyr)
library(ggplot2)
source("dioxin-congener-laying-hen.R")
modelParameters <<- read.csv("modelInputParameters.csv", header =
TRUE)
### User input ###
compounds <- c("C1", "C3", "C5", "C7", "C8", "C14")
contaminationLevel <- c("C1"=0.12, "C3"=0.34, "C5"=0.21, "C7"=0.10,
"C8"=0.22, "C14"=0.51) # ng / kg
feedIntake <- 0.113 # kg
tstop <- 200 # days
tdoseoff <- 56 # days
### Run model ###
result <- list()
for (c in 1:length(compounds)){
 cpd <- compounds[c]</pre>
 input <- c(feedIntake = feedIntake, tstop = tstop, tdoseoff = tdoseoff,
contaminationLevel = list(contaminationLevel[[cpd]]))
 p <- assign_parameters(cpd)</pre>
 p <- calculate_variables(p)</pre>
 result[[c]] <- as.data.frame(run_model(p))</pre>
}
### Visualizing sum of individual models ###
total_teq_egg <- data.frame(result[[1]]["time"], Reduce(` + `,</pre>
lapply(result, `[`, 'Cegg')))
total_teq_fat <- data.frame(result[[1]]["time"], Reduce(`+`,
lapply(result, `[`, 'Cf')))
total_teq_egg %>% ggplot(aes(time,Cegg)) +
geom_line()
```

#### modelInputParameters.csv

compound,name,tef, gcentral, gfat,e,yy,k,Fabs,Vf,Vc,Vtotal C1,"1: 2,3,7,8-TCDF",0.1,0.31,0.205,0.9,0.04,0,0.7,200,1640,1840 C2,"2: 1,2,3,7,8-PeCDF", 0.03, 0.19, 0.073, 0.9, 0.078, 0, 0.71, 210, 1630, 1840 C3,"3: 2,3,4,7,8-PeCDF",0.3,0.1,0.057,0.9,0.055,0,0.71,190,1650,1840 C4,"4: 1,2,3,4,7,8-HxCDF", 0.1, 0.08, 0.029, 0.9, 0.11, 0, 0.6, 180, 1660, 1840 C5, "5: 1, 2, 3, 6, 7, 8-HxCDF", 0.1, 0.08, 0.031, 0.9, 0.109, 0, 0.55, 180, 1660, 1840 C6,"6: 2,3,4,6,7,8-HxCDF", 0.1, 0.1, 0.034, 0.9, 0.131, 0, 0.45, 200, 1640, 1840 C7, "7: 1, 2, 3, 7, 8, 9-HxCDF", 0.1, 0.1, 0.04, 0.9, 0.103, 0, 0.54, 180, 1660, 1840 C8, "8: 1, 2, 3, 4, 6, 7, 8-HpCDF", 0.01, 0.06, 0.034, 0.9, 0.182, 0, 0.18, 140, 1700, 1840 C9, "9: 1, 2, 3, 4, 7, 8, 9-HpCDF", 0.01, 0.04, 0.018, 0.9, 0.167, 0, 0.24, 150, 1690, 1840 C10, "10: 1, 2, 3, 4, 6, 7, 8, 9-OCDF",0.0003,0.14,0.06,0.9,0.057,0,0.78,230,1610,1840 C11,"11: 2,3,7,8-TCDD",1,0.35,0.23,0.9,0.042,0,0.78,210,1630,1840 C12,"12: 1,2,3,7,8-PeCDD",1,0.14,0.07,0.9,0.055,0,0.75,220,1620,1840 C13,"13: 1,2,3,4,7,8-HxCDD", 0.1, 0.09, 0.03, 0.9, 0.101, 0, 0.61, 190, 1650, 1840 C14,"14: 1,2,3,6,7,8-HxCDD", 0.1, 0.09, 0.036, 0.9, 0.106, 0, 0.59, 170, 1670, 1840 C15,"15: 1,2,3,7,8,9-HxCDD", 0.1, 0.07, 0.032, 0.9, 0.118, 0, 0.42, 150, 1690, 1840 C16, "16: 1, 2, 3, 4, 6, 7, 8-HpCDD", 0.01, 0.14, 0.06, 0.9, 0.057, 0, 0.78, 230, 1610, 1840 C17,"17: 1,2,3,4,6,7,8,9-OCDD",0.0003,0.14,0.06,0.9,0.057,0,0.78,230,1610,1840 C18,18: PCB 81,0.0003,0.11,0.121,0.9,0.024,0,0.92,190,1650,1840 C19,19: PCB 77,0.0001,0.25,0.136,0.9,0.044,0,0.89,240,1600,1840 C20,20: PCB 126 ,0.1,0.13,0.067,0.9,0.038,0,1,270,1570,1840 C21,21: PCB 169,0.03,0.11,0.029,0.9,0.081,0,0.85,220,1620,1840 C22,22: PCB 123,0.00003,0.14,0.06,0.9,0.057,0,0.78,230,1610,1840 C23,23: PCB 118,0.00003,0.12,0.063,0.9,0.041,0,0.98,230,1610,1840 C24,24: PCB 114,0.00003,0.2,0.09,0.9,0.061,0,0.89,180,1660,1840 C25,25: PCB 105,0.00003,0.12,0.084,0.9,0.037,0,0.92,200,1640,1840 C26,26: PCB 167,0.00003,0.1,0.095,0.9,0.062,0,1,70,1770,1840 C27,27: PCB 156,0.00003,0.11,0.039,0.9,0.063,0,0.92,220,1620,1840 C28,28: PCB 157,0.00003,0.16,0.051,0.9,0.094,0,0.86,190,1650,1840 C29,29: PCB 189,0.00003,0.06,0.017,0.9,0.102,0,0.8,190,1650,1840 totalTeq,Total TEQ model,1,0.14,0.06,0.9,0.057,0,0.78,230,1640,1840