Electronic supplementary information
Children's exposure to perfluoroalkyl acids - a modelling approach

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Abbreviations

diPAP	fluorotelomer phosphate diester
EFSA	European Food Safety Authority
EtFOSAA	*n*-ethyl-perfluorooctane sulfonamidoacetic acid
EtFOSE	*n*-ethyl-perfluorooctane sulfonamidoethanol
FTOH	fluorotelomer alcohol
MeFOSE	*n*-methyl-perfluorooctane sulfonamidoethanol
PAP	polyfluoroalkyl phosphoric acid ester
PFAA	perfluoroalkyl acid
PFAS	per- and polyfluoroalkyl substance
PFCA	perfluoroalkyl carboxylic acid
PFHxS	perfluorohexane sulfonic acid
PFOA	perfluorooctanoic acid
PFOS	perfluorooctane sulfonic acid
PFSA	perfluoroalkane sulfonic acid
PFOSA	perfluorooctane sulfonamide

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1. Methods

1.1. Estimation of dietary intakes

Similarly to Equation 1 from the main text, the following equations quantify the intakes of PFOA, PFOS and PFHxS from air and diet. Note that for precursor molecules (Table 1) biotransformation factors had to be applied.

$$EDI_{air}\left[\frac{ng}{kg\ bw\ d}\right] = \frac{air\ concentration\ [ng/m^3] \times inhalation\ rate\ [m^3/d]}{body\ weight\ [kg]} \qquad \text{Equation A1}$$

$$EDI_{diet}\left[\frac{ng}{kg\ bw\ d}\right] = \frac{dietary\ concentration\ [ng/g] \times ingested\ dietary\ amount\ [g/d]}{body\ weight\ [kg]} \qquad \text{Equation A2}$$

1.2. Dataset on dietary concentrations

A food frequency questionnaire (FFQ) on the children's diet covering the ages from 1 to 10.5 years was available for the studied child cohort (1). However, the FFQ was not sufficient for the quantification of dietary intake for the dynamic modelling. For this reason, a suitable dataset was selected from the literature. The dataset compiled in Papadopoulou et al. (2017) fulfilled the required high analytical data quality and was used to derive PFOA, PFOS and PFHxS concentrations for a wide range of food classes (2). Due to relatively high limits of quantification (LOQ), the authors presented two sets of PFAA concentration data for each food item in their dataset in case the concentration was below the LOQ. In one set (lower bound approach), the PFAA concentration of the respective food was set to zero if the measured concentration was < LOQ; while in the second set (upper bound approach), the PFAA concentration of the respective food was set equal to the LOQ. Thus, the concentrations in the upper bound approach were elevated up to

~70-times (for PFHxS) compared to the lower bound approach. Therefore, the upper bound approach was only applied in the high exposure scenario to represent the worst case.

Table S1: Estimated median dietary PFAS intakes based on Papadopoulou et al. (2017) and the European food consumption database (2, 14). Consumption rates were taken from <10-year-olds from Finnish studies within the database. LB = lower bound approach; UB = upper bound approach; NA = not available.

Food category	**median PFAS intake (ng/kg bw/d)**							
	PFOA		**PFOS**		**PFHxS**		**PFOSA**	
	LB	**UB**	**LB**	**UB**	**LB**	**UB**	**LB**	UB
Vegetables and Grain based products	0.069	0.13	0	0.11	0	0.073	0	0.060
Fruit	0.044	0.041	0.068	0.068	0	0.047	NA	NA
Meat	0.025	0.047	0.051	0.062	0	0.0083	0.0010	0.0041
Fish and Seafood	0	0.029	0	0.039	0	0.029	0	0.059
Animals products	0.074	0.28	0.11	0.19	0	0.042	0	0.031
Sugar, Honey, Snacks and Confectionary	0.0027	0.016	0	0.0049	0	0.0079	0	0.020
Vegetable oils	0.0032	0.013	0.00061	0.0054	0.00035	0.0023	0	0.13
Beverages (excl. Water)	0	0	0	0	0	0	0	NA
Drinking Water*	0.0028	NA	0.0019	NA	0.0019	NA	NA	NA
Infant food	0	0	0	0	0	0	0	0

**tap water sampled from the children's homes, lower and upper bound approach not applicable*

1.3. Model uncertainty analysis

As part of good modelling practice, a sensitivity and uncertainty analysis was conducted on the model (3). The applied uncertainty analysis is termed the *first order error propagation method*, which is a computational less demanding method for uncertainty analysis than a Monte-Carlo analysis (4). However the results of the methods are comparable to each other (4). The first order error propagation method assumes linear sensitivities of each input parameter independent of the change in the parameter value (i.e. the value was changed by 1 or 10 % compared to the default value). Moreover, the method assumes that the variance of each input parameter can be described by a log-normal distribution.

Table S2: Argumentation for assigned confidence factors for each input parameter in the model. Confidence factors were assigned based on the relation in Equation 4 from the main script. Conc= concentration, CfI = confidence factor of parameter I, SD = standard deviation, bw = body weight.

Input parameter *I* used in model	**Argumentation for assignment of confidence factor**	**Assigned confidence factor (Cf_I)**
Body weight adjustment factor	SD of log-normal distribution used to estimate Cf_I (5)	1.2
Volume of distribution (mL/kg), PFOA	Assumption that parameter varied by 15 % (6)	1.1
Volume of distribution (mL/kg), PFOS		1.1
Volume of distribution (mL/kg), PFHxS		1.1
Half-life (years), PFOA	Same Cf_I assumed as in (7)	1.1
Half-life (years), PFOS	Same Cf_I assumed as for PFOA in (7)	1.1
Half-life (years), PFHxS	Expert judgement based on 8.5 ±5.2 (mean ± SD) from (8)	2.0
Initial serum conc (ng/mL), PFOA	SD from log normal transformed serum measurements from (9) used to estimate Cf_I	1.7
Initial serum conc (ng/mL), PFOS		2.0
Initial serum conc (ng/mL), PFHxS		3.0
Dietary conc (ng/g), PFOA	SD and mean of lower bound concentrations from (2) used for Cf_I assignment	1.1
Dietary conc (ng/g), PFOS		1.2
Dietary conc (ng/g), PFOSA		1.3
Dietary conc (ng/g), PFHxS		1.2
Dust conc (ng/g), PFOA	SD from log normal transformed conc measurements from (10) and (11)	2
Dust precursor conc (ng/g), PFOA		2.7
Dust conc (ng/g), PFOS		2.2
Dust precursor conc (ng/g), PFOS		3
Dust conc (ng/g), PFHxS		3
Air conc (ng/m^3), PFOA		1.8
Air precursor conc (ng/m^3), PFOA		1.6
Air conc (ng/m^3), PFOS		1.7
Air precursor conc (ng/m^3), PFOS		2.2
Air conc (ng/m^3), PFHxS		1.4
Absorption efficiency, dust and diet, excluding FTOH	0.66 and 0.91 of absorption efficiencies assumed to be 5th and 95th percentile (12)	1.1
Absorption efficiency, dust and diet, only for FTOH	0.27 and 0.56 of absorption efficiencies assumed to be 5th and 95th percentile (12)	2
Absorption efficiency from air	Cf_I taken from (7), assumed to pertain to all PFAAs and precursors	1.3

Biotransformation rate, air, dust and diet to PFOA	margin of error 0.0006 and 0.01 from (7) as 5th and 95th percentile to estimate Cf_I	4
Biotransformation rate, air, dust and diet to PFOS	0.095 and 0.32 taken as 5th and 95th percentile for estimation of Cf_I (12)	2
Air inhalation rate (m^3/d) of 10.5 year olds	18.7 and 12.4 taken (13) as 5th and 9th percentile for Cf_I assignment	1.5
Amount of dust ingested (mg/d)	100 and 60 mg (13) taken as 5th and 95th percentile for Cf_I assignment	1
Dietary consumption rate (g/kg bw/d)	24 and 192 assumed (14) as 5th and 95th percentile and 79 as mean to estimate Cf_I	2

2. Results

2.1. Sensitivities

One parameter, the half-life, displayed non-linear sensitivities with relative changes of 1 and 10 % in its value compared to the default value (results not shown). This violated the assumption of linear sensitivities of input parameters for this type of analysis (4). However, the share of the half-life to the model uncertainty was less important, compared to the contribution of most other parameters (Figure S1-S3, Figure 3). Thus, the non-linear behavior of the half-life parameter was considered negligible.

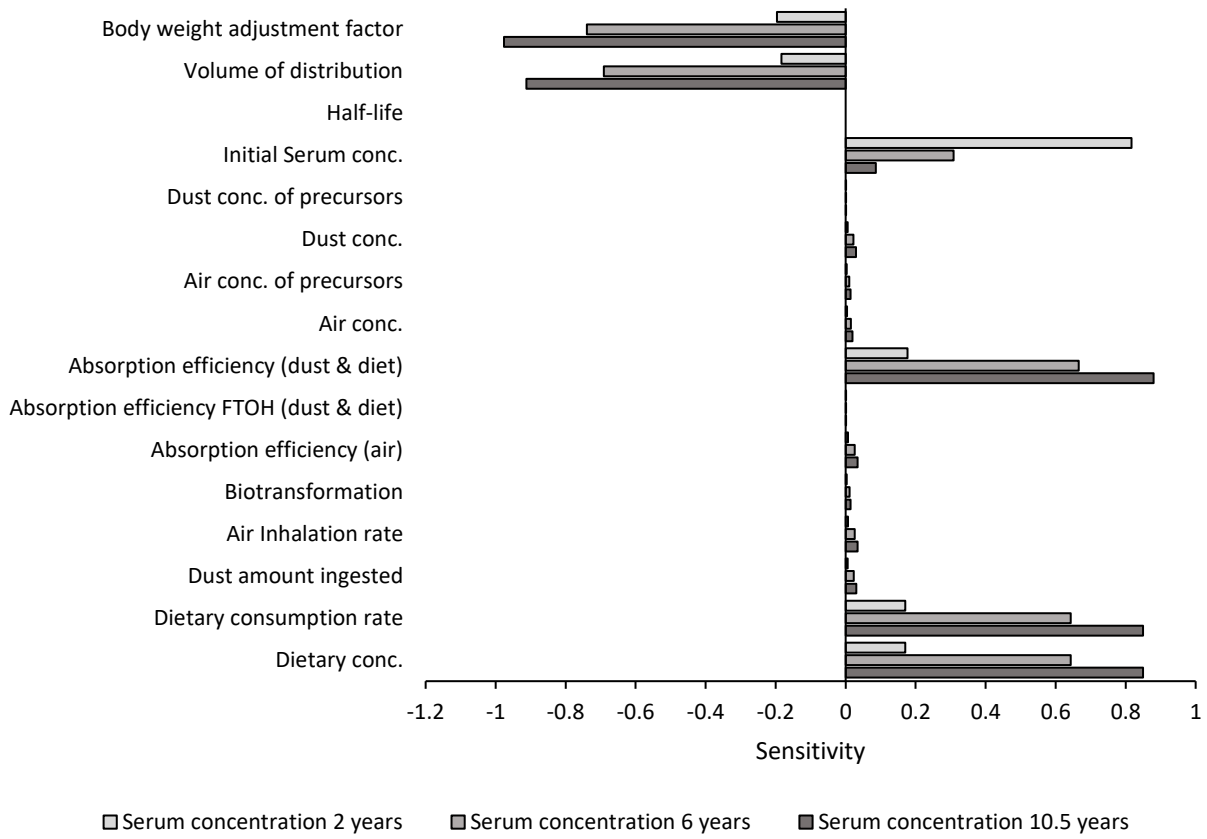

Figure S1: Sensitivity of the model output to input parameters for modelled PFOA serum concentration. Sensitivity is the difference between the default scenario output and the scenario output where the respective input parameter was increased by 0.1 % divided by the relative change of the respective input parameter (see Methods). Conc. = concentration.

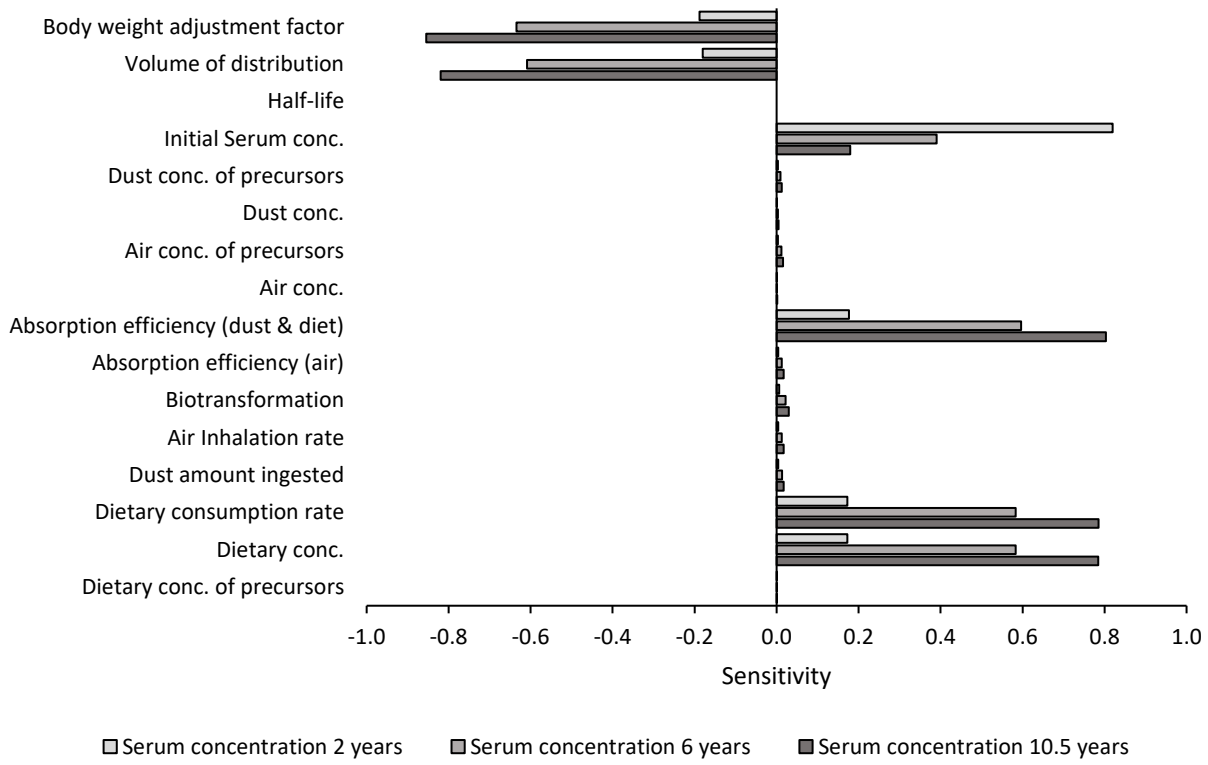

Figure S2: Sensitivity of the model output to input parameters for modelled PFOS serum concentration. Sensitivity is the difference between the default scenario output and the scenario output where the respective input parameter was increased by 0.1 % divided by the relative change of the respective input parameter (see Methods). Conc. = concentration.

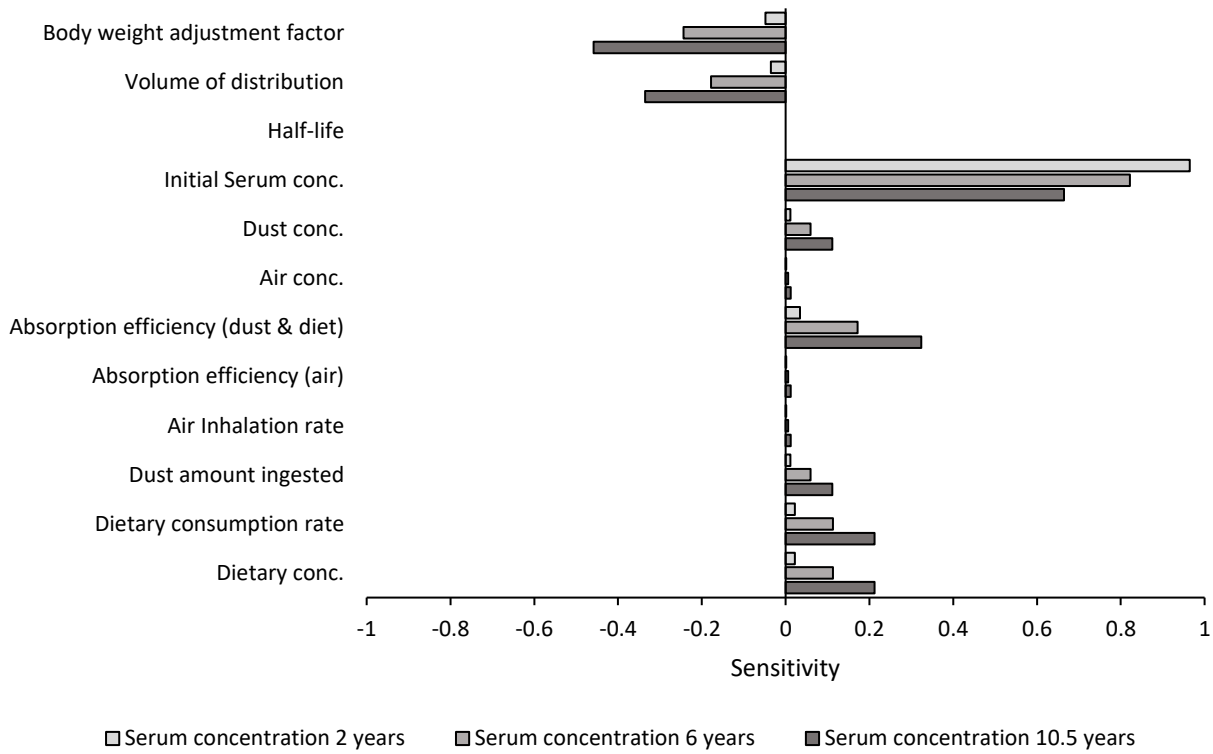

Figure S3: Sensitivity of the model output to input parameters for modelled PFHxS serum concentration. Sensitivity is the difference between the default scenario output and the scenario output where the respective parameter was increased by 0.1 % divided by the relative change of the respective input parameter. Conc. = concentration.

2.2. Confidence factors

Table S3: Confidence factors (CF_0) and margin of error for the modelled serum PFOA, PFOS and PFHxS concentrations at 6 and 10.5 years of age. Margin of error calculated from confidence factor (CF_0), see Equation 6 and Equation 4.

PFAA	**PFOA**		**PFOS**		**PFHxS**	
Child age (years)	**6**	**10.5**	**6**	**10.5**	**6**	**10.5**
Modelled serum conc. (intermediate scenario, median, ng/mL)	2.1	1.2	3.0	1.8	0.19	0.093
Confidence factor of the model (CF_0)	1.7	1.9	1.7	1.8	2.5	2.1
Margin of error of modelled serum conc. (5th - 95th percentile, ng/mL)	1.3 - 3.6	0.62 - 2.2	1.8 - 5.1	1.0 - 3.4	0.076 - 0.47	0.044 - 0.20
Measured serum conc. (5th - 95th percentile, ng/mL) taken from (9)	1.9 - 4.1	1.0 -2.1	1.2 - 4.1	0.84 - 2.8	0.13 - 0.82	0.080 - 0.42
Measured serum conc. (median ± standard deviation, ng/mL) taken from (9)	2.80 ±0.78	1.5 ±0.38	2.1 ±0.82	1.6 ±0.62	0.43 ±0.19	0.21 ±0.11

2.3. Methods of EDI derivation from different studies

Table S4: EDI derivation methods of each study used for comparison in Figure 4. Note that the studies use either a modelling approach or an EDI derivation, which considers different ways of handling method detection limits. For chemical acronyms, see list of Abbreviations.

Study	EDI derivation method	Subjects	Pathways	Biotransformation considered?	Absorption efficiency
Gebbink et al. 2015 (12)	one-compartment PK model (based on (15) considering 3 input parameters: Intake, elimination rate, volume of distribution; For comparison in Figure 3: Median, 5th and 95th percentile of each input parameter used for low, intermediate and high exposure scenario	general Western adult population	diet, drinking water, dust, air	Yes, MeFOSE, EtFOSE, EtFOSAA, PFOSA to PFOS: 0.095, 0.20, 0.32; FTOH to PFOA: 0.0002, 0.005, 0.017 / diPAPs to PFOA: 0.01, 0.1, 1	PFOS, PFOA and all other except FTOH in diet, dust and water: 0.66, 0.80, 0.91; for FTOH; 0.27, 0.38,0.56; air absorption efficiency 1
Haug et al. 2011 (16)	one-compartment PK model (based on (17)) considering 3 input parameters: Intake, elimination rate, volume of distribution; For comparison in Figure 3: median of low, intermediate and high scenario based on air inhalation and dust ingestion rates	Norwegian women	diet, drinking water, dust, air	Yes, from air inhalation of FOSA/FOSE to PFOS: 0.01, 0.2, 1; FTOH to PFOA: 0.0002, 0.005, 0.017	1 for all
Noorlander et al. 2011 (18)	EDI derivation from databases; Scenarios base on handling method detection limit, no modelling approach used	average Dutch 10-year-olds	diet and drinking water	No	1 for all
Vestergren et al. 2012 (19)	Lower bound and upper bound scenario for handling method detection limit, no modelling approach used	general Swedish population	diet	No	1 for all

2.4. Dynamic modelling results

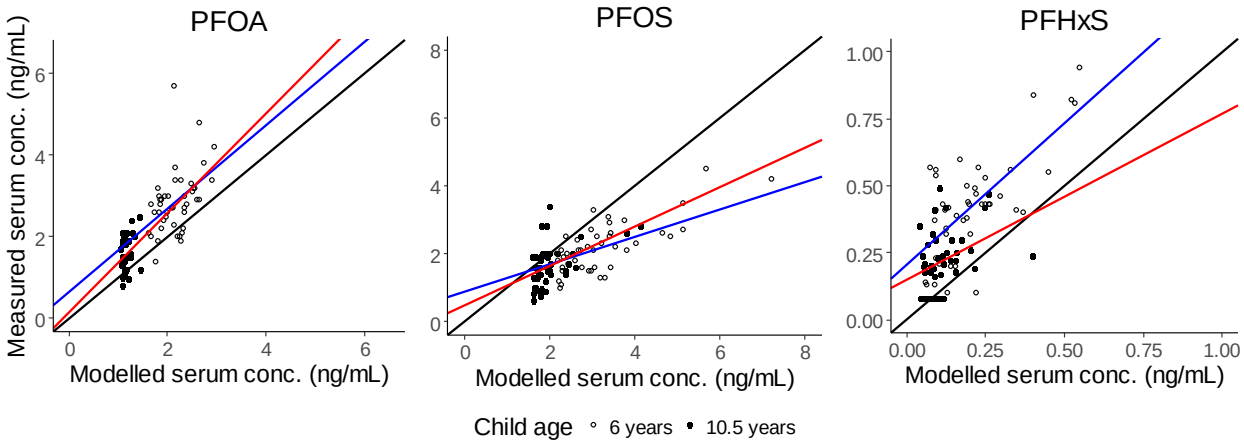

Figure S4: Measured against modelled PFAA serum concentrations of the intermediate scenario of 44 individuals at 6 and 10.5 years of age from the LUKAS2 study. The diagonal black line represents the perfect-fit-1:1-line. Corresponding R^2 values presented in Table 4. Blue line = regression through serum concentrations of 6-year-olds; Red line = regression through serum concentrations. of 10.5-year-olds. Additional statistical values from the Student's t-test in Table S7.

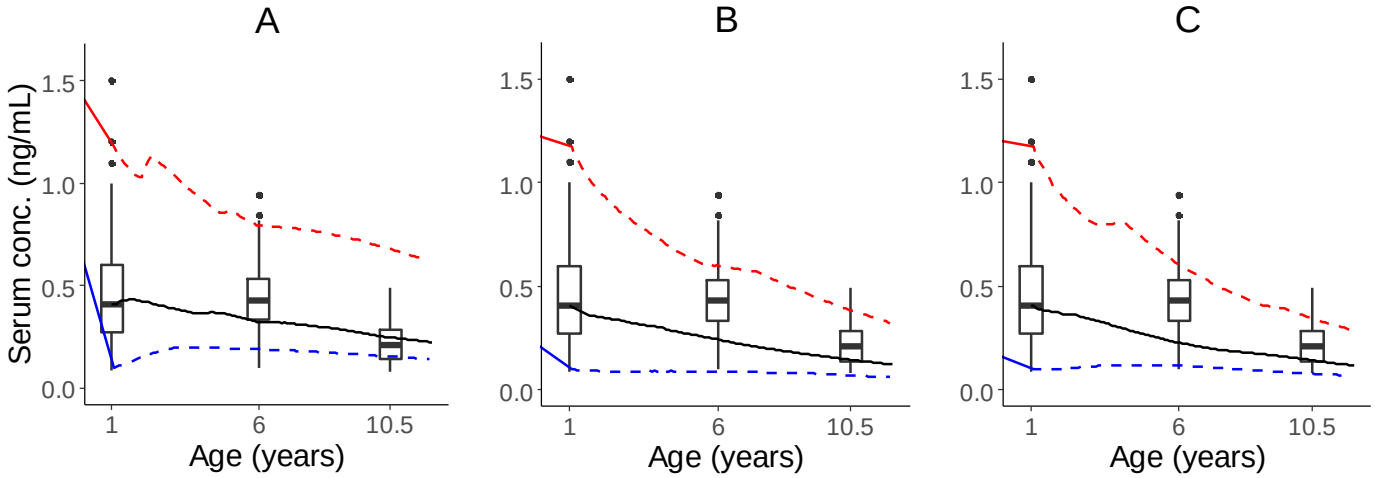

Figure S5: Manipulation of the different PK parameters of PFHxS in the intermediate exposure scenario. Aim was to reach a better curve fit between the modelled and the measured serum concentrations. A = intake changed by a factor 5, B = Half-life increased to 17 years, C = Volume of distribution halved to 117.5 mL/kg, black solid line = median, blue dashed line = 5th percentile, red dashed line = 95th percentile.

Table S5: Statistical metrics for model evaluation of the intermediate exposure scenario to PFHxS at 6 and 10.5 years of age. PFHxS intake was increased by a factor of 5. R^2 = coefficient of determination, RMSD = root mean square deviation, Significantly different from 1:1 line = significant deviation of the linear regression to the 1:1 line in Student's-test with $\alpha = 0.05$ (see Methods).

PFAA	Age (years)	R^2	RMSD (± ng/mL)	Slope significantly different from 1:1 line
PFHxS	6	0.32	0.23	yes
	10.5	0.044	0.27	yes

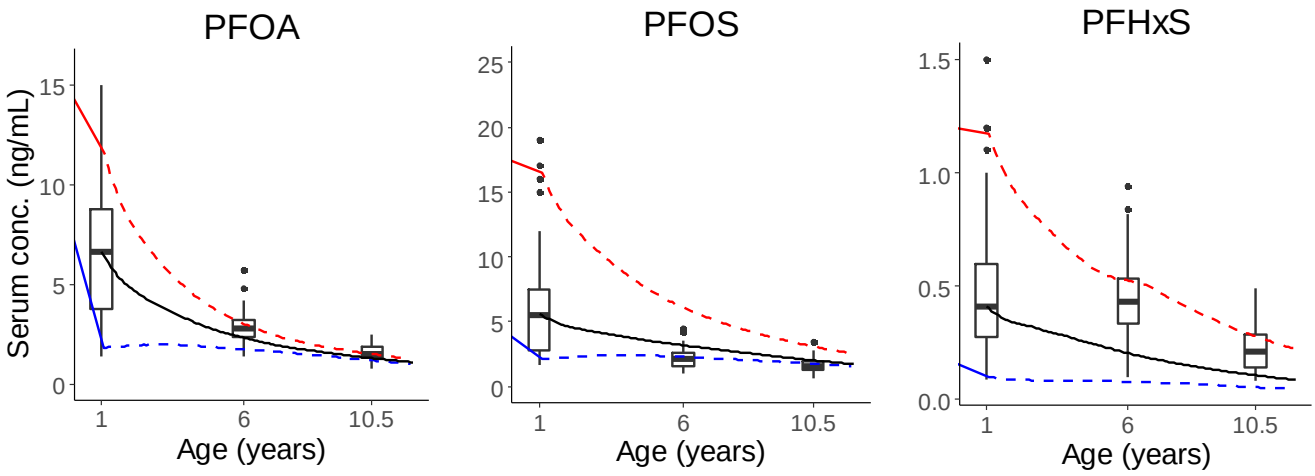

Figure S6: Median of the intermediate exposure scenario of PFOA, PFOS and PFHxS including the 5th and the 95th percentile. Blue dashed line = 5th percentile. Red dashed line = 95th percentile, black solid line =median.

Table S6: Bodyweight normalized intakes of PFOA, PFOS and PFHxS for different child ages. The intakes were calculated for 10.5-year-olds and kept at steady-state (ng/d) in PK model. To derive body weight normalized intakes (ng/ kg bw/ d), the constant intake was divided by median body weight at the respective child age. Top-down estimates were derived from respective serum samples.

PFAA	**Exposure scenario**	**EDI (ng/ kg bw /d)**		
		1 year	**6 years**	**10.5 years**
PFOA	low	0.59	0.27	0.16
	intermediate	0.70	0.32	0.19
	high	2.0	0.93	0.55
PFOS	low	0.59	0.26	0.16
	intermediate	0.74	0.32	0.20
	high	2.1	0.91	0.56
PFHxS	low	0.0093	0.0043	0.0026
	intermediate	0.011	0.0051	0.0032
	high	0.71	0.32	0.19
PFOA	Top-down estimate	1.14	0.48	0.26
PFOS		0.57	0.22	0.16
PFHxS		0.011	0.02	0.011

Table S7: Additional statistical information on results from Student's t-test on regression slopes. Probabilities and according t-statistics presented.

PFAA	Scenario	Probability	t-statistic
PFOA	intermediate at 6 years	0.96	0.055
	intermediate at 10.5 years	0.74	0.34
PFOS	intermediate at 6 years	5.1E-14	-11
	intermediate at 10.5 years	0.012	-2.6
PFHxS	intermediate at 6 years	0.73	0.34
	intermediate at 10.5 years	0.11	-1.6

3. Model code

To run the code, the open source software R is needed, which can be downloaded at https://cran.r-project.org/mirrors.html. After download and installation of R, ensure that the ggplot2 package is installed in R. To run the code, copy the code sections below, paste it into the R console or into a new R script and execute. To obtain the figure, which is coded in the bottom, run this section separately from the remaining code.

```
# Model code of Balk et al's "Children's exposure to perfluoroalkyl acids - a
modelling approach", 2019

# INSTRUCTIONS
# You can play with the parameters and exposure settings in the following lin
es: 8-10, 70-72, 79-81 and line 87 or with any other code if you are familiar
with R (line indices will be shown if you copy the code into an R script)
# There are some clarifying comments throughout the script.

######## Set the conditions for model run ########
Compound         <- 3 # PFAS compound (1: PFOS, 2: PFOA, 3: PFHxS)
Exposure         <- 3  # Exposure scenario for dust, air and dietary EDIs (1:
low, 2: intermediate, 3: high)
biotrans         <- 1  # 1 = include precursor biotransformation, 0 = exclude
precursor biotransformation

# Important time points
model_run_length <- 11*365*24 # translates the set model run length from year
s into hours & starts when the child is 1 year old
child_6yrs       <- 5*365*24
child_10.5yrs    <- 10.5*365*24

######## Relevant data ########

# Median and mean weights (kg) of the Finnish child cohort at different ages
weights_df <- data.frame(3.6, 3.6 , 0.45 , 9.95 , 9.9 , 1.02 , 22.41 , 21.5 ,
4.67 , 37.79 , 36.65 , 9.62)
colnames(weights_df) <- c("Mean weight at birth", "Median weight at birth", "
Standard deviation",
                          "Mean weight at one year", "Median weight at one ye
ar", "Standard deviation",
```

```
                           "Mean weight at six years", "Median weight at six y
ears", "Standard deviation",
                           "Mean weight at ten years", "Median weight at ten y
ears", "Standard deviation")

# Serum concentrations
serum_df <- signif(data.frame(c(6.429545, 6.600000, 3.327586),
                              c(2.8613636, 2.8000000, 0.7776578),
                              c(1.5763636, 1.5000000, 0.3829208),
                              c(7.152273, 5.600000, 6.632916),
                              c(2.2590909, 2.1000000, 0.8216031),
                              c(1.6463636, 1.6000000, 0.6162908),
                              c(0.5012273, 0.4100000, 0.3635252),
                              c(0.4275000, 0.4300000, 0.1926453),
                              c(0.2195455, 0.2100000, 0.1122695)), digits = 3
)
rownames(serum_df) <- c("Mean","Median","SD")
colnames(serum_df) <- c("PFOA_yr1","PFOA_yr6","PFOA_yr10","PFOS_yr1","PFOS_yr
6","PFOS_yr10","PFHxS_yr1","PFHxS_yr6","PFHxS_yr10")

# Age dependent weight from CDC growth function (kg)
weight_at_age1    <- (0.00005*(1*52.14)^2 + 0.0235*(1*52.14) + 10.9775)
weight_at_age6    <- (0.00005*(6*52.14)^2 + 0.0235*(6*52.14) + 10.9775)
weight_at_age10.5 <- (0.00005*(10.5*52.14)^2 + 0.0235*(10.5*52.14) + 10.9775)

# Age dependent median weight of the child cohort (kg)
weight_1yr    <- weights_df$"Median weight at one year"[]
weight_6yr    <- weights_df$"Median weight at six years"[]
weight_10.5yr <- weights_df$"Median weight at ten years"[]

# Weight adjustment factor
adj_BW_10.5to11 <- weight_10.5yr/(0.00005*(10.5*52.14)^2 + 0.0235*(10.5*52.14
) + 10.9775)

######## Select compound parameters ########

# Which compound?
if (Compound==1) {
  PFOS       <-1
  PFOA       <-0
  PFHxS      <-0
} else if (Compound==2) {
  PFOS       <-0
  PFOA       <-1
  PFHxS      <-0
} else if (Compound==3) {
  PFOS       <-0
  PFOA       <-0
  PFHxS      <-1
}

# Volume of distribution (L/kg)
PFOS_VD_BW  <- 0.235
```

```
PFOA_VD_BW  <- 0.200
PFHxS_VD_BW <- 0.235

# Selection of the correct volume of distribution
VD_BW <- PFOS*PFOS_VD_BW + PFOA*PFOA_VD_BW + PFHxS*PFHxS_VD_BW


# Half lives (h)
PFOS_HL  <- 4.35*365*24
PFOA_HL  <- 2.2*365*24
PFHxS_HL <- 8.5*365*24

# Selection of the correct volume of distribution
HL <- round((PFOS*PFOS_HL + PFOA*PFOA_HL + PFHxS*PFHxS_HL), digits = 1)

# Elimination rate constant (h^-1)
EL_cons <- round((log(2)/HL), digits = 7)

######## FUNCTIONS ########

# Function for child weight; translates the timestep of the loop (h) into unt
is of weeks
BW_C_fun <- function(t,adj_BW_fac = adj_BW_10.5to11){
  BW_C_vec[t] <<- (0.00005*(t*0.005952)^2 + 0.0235*(t*0.005952) + 10.977 *adj
_BW_fac)
  Bodyweight <<- BW_C_vec[seq(from = 1, to = length(BW_C_vec), by = 168)]
} # 0.005952 equivalent to hourly steps in units of weeks

# Function for bodyweight adjusted volume of distribution (L), L/kg * kg = L
VD_fun <- function(t){VD_vec[t] <<- signif(BW_C_vec[t]*VD_BW, digits = 4)
Volumeofdistribution <<- VD_vec[seq(from = 1, to = length(VD_vec), by = 168)]
}

# Body Burden (ng), selects for the correct scenario & initial serum concentr
ation to calculate bodyburden, ng/mL * 1000 mL/L * L = ng
AMT_fun <- function(t = child_age_vec, amtprev = (PFOS*serum_df$PFOS_yr1[2] +
PFOA*serum_df$PFOA_yr1[2] + PFHxS*serum_df$PFHxS_yr1[2])*(1000*VD_vec[child_a
ge_vec]),
                    intake = Intake*weight_10.5yr){
  AMT_vec[t] <<- round((amtprev + intake)-((amtprev + intake)*EL_cons), digit
s = 4) # ng
  Bodyburden <<- AMT_vec[seq(from = 1, to = length(AMT_vec), by = 168)]/1000
# ug
}

# Serum Concentration (ng/mL), ng/L * 0.001 L/mL = ng/mL
CON_fun <- function(t=child_age_vec){
  CON_vec[t] <<- round(((AMT_vec[t]/VD_vec[t])/1000), digits = 4)
  Serumconcentration <<- CON_vec[seq(from = 1, to = length(CON_vec), by = 168
)]
}

# Scenario dependent total median intake of the child cohort, units: ng/kg BW
```

```
/d to ng/kg BW/h
if(Exposure == 1){
  Intake <- ((1-biotrans)*((PFOS*0.15 +
                              PFOA*0.16 +
                              PFHxS*0.0026)/24)) +
    ((biotrans)*((PFOS*0.165 +
                    PFOA*0.16064 +
                    PFHxS*0.0026)/24))
} else if(Exposure == 2){
  Intake <- ((1-biotrans)*((PFOS*0.19 +
                              PFOA*0.19 +
                              PFHxS*0.0032)/24)) +
    ((biotrans)*((PFOS*0.201 +
                    PFOA*0.1938 +
                    PFHxS*0.0032)/24))
} else if(Exposure == 3){
  Intake <- ((1-biotrans)*((PFOS*0.53 +
                              PFOA*0.53 +
                              PFHxS*0.19)/24)) +
    ((biotrans)*((PFOS*0.545 +
                    PFOA*0.545 +
                    PFHxS*0.19)/24))
}

BW_C_vec             <- vector()
Bodyweight           <- vector()
child_age_vec        <- vector()
VD_vec               <- vector()
Volumeofdistribution <- vector()
AMT_vec              <- vector()
Bodyburden           <- vector()
CON_vec              <- vector()
Serumconcentration   <- vector()

######## Simulation ########

for(y in 8760:model_run_length){
  if(y == 8760) {
    child_age_vec <- 1
    BW_C_fun(t = child_age_vec)
    VD_fun(t = child_age_vec)

    AMT_fun()
    CON_fun()
  }
  if(y <= child_10.5yrs){
    child_age_vec <- child_age_vec + 1
    BW_C_fun(t = child_age_vec)
    VD_fun(t = child_age_vec)

    AMT_fun(amtprev = AMT_vec[child_age_vec-1])
    CON_fun()
  }
```

```
  if(y > child_10.5yrs){
    child_age_vec <- child_age_vec + 1
    BW_C_fun(t = child_age_vec)
    VD_fun(t = child_age_vec)

    AMT_fun(amtprev = AMT_vec[child_age_vec-1])
    CON_fun()
  }
}

# Save the simulated serum concentrations at 6 years & 10.5 years of age
Serumconc_6yrs    <- CON_vec[52560] # ng/mL
Bodyburden_6yrs   <- AMT_vec[52560]/1000 # ng * 0.001 ug/ng = ug

Serumconc_10yrs   <- CON_vec[91980] # ng/mL
Bodyburden_10yrs  <- AMT_vec[91980]/1000 # ng * 0.001 ug/ng = ug

# Save the model output
Intake              <- Intake*24  # ng/kg/h * 24 h/d = ng/kg BW/d

child_age           <- seq(1,(length(Serumconcentration)))+52.14
output_df           <- data.frame(child_age, Serumconcentration, Bodyburden,
Bodyweight, Volumeofdistribution)
colnames(output_df) <- c("Child Age (week)","Serum Concentration (ng/mL)", "B
ody Burden (ug)","Weight (kg)", "Weight adjusted Volume of Distribution (L)")

output_scenarios_df           <- data.frame(Compound, Exposure, biotrans, Int
ake)
colnames(output_scenarios_df) <- c("Which Compound? (1 : PFOS, 2: PFOA, 3: PF
HxS)","Exposure scenario (1: low, 2: intermediate, 3: high)", "Consider Precu
rsor Biotransformation (1: yes, 0: no)","Total Intake (ng/kg BW/d)")

if(Compound == 1){
  Serum <- serum_df[,c(4:6)]
} else if (Compound==2) {
  Serum <- serum_df[,c(1:3)]
} else if (Compound==3) {
  Serum <- serum_df[,c(7:9)]
}

print("Summary of set parameters")
print("VD_BW (L/kg)")
print(VD_BW)
print("HL(h)")
print(HL)
print("Compound")
print(Compound)
print("Exposure")
print(Exposure)
print("Biotransformation")
print(biotrans)

# Make sure the package "ggplot2" is installed in R
```

```
# Open ggplot2
library(ggplot2)
# Create plot (cannot be computed by using the source command)
ggplot() +
  geom_line(data = output_df, mapping = aes(x = output_df[,1]/52.14, y = outp
ut_df[,2]), size = 0.7) +
  geom_pointrange(data = Serum, mapping = aes(x = c(1), y = Serum[2,1], ymin
= Serum[2,1]-Serum[3,1], ymax = Serum[2,1]+Serum[3,1] )) +
  geom_pointrange(data = Serum, mapping = aes(x = c(6), y = Serum[2,2], ymin
= Serum[2,2]-Serum[3,2], ymax = Serum[2,2]+Serum[3,2] )) +
  geom_pointrange(data = Serum, mapping = aes(x = c(10.5), y = Serum[2,3], ym
in = Serum[2,3]-Serum[3,3], ymax = Serum[2,3]+Serum[3,3] )) +
  labs(x = "Age (years)", y = "Serum concentration (ng/mL)", title = "Simulat
ed serum concentration (line) vs measured serum concentration (median +- SD)"
) +
  scale_x_continuous(breaks = c(1,6,10.5), labels = c("1","6"," 10.5")) +
  theme_classic()
```

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