# Jan 5

* Munoz et al estuary study has muscle to whole body conversion (Table S2). And referenced: *de Vos, M. G.; Huijbregts, M. A. J.; van den Heuvel-Greve, M. J.; Vethaak, A. D.; Van de Vijver, K. I.; Leonards, P. E. G.; van Leeuwen, S. P. J.; de Voogt, P.; Hendriks, A. J. Accumulation of perfluorooctane sulfonate (PFOS) in the food chain of the Western Scheldt estuary: Comparing field measurements with kinetic modeling. Chemosphere 2008, 70, 1766−1773*
* Rüdel et al studies
  + Rüdel et al 2022 Chemosphere 292, 133483. Is another ref.
  + A close up of a text

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  + <https://link.springer.com/article/10.1186/s12302-020-0295-9?utm_source=getftr&utm_medium=getftr&utm_campaign=getftr_pilot>A white sheet with black text

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**JBA summer run.**

**Understanding units and calculations**

* In excels (JBA\_Manuscript.xlsx, and PFAS\_Bioaccumulation\_JBA\_V2): Highlight in yellow everything that is used for new model run
  + Brown et al: *Bioaccumulation factors (BAF, L/kg ww) are used to assess the bioaccumulation potential of compounds in individuals, while considering aqueous and dietary exposure routes.58,59 Log BAFs were calculated here using Equation 1:59*

*where CBi is the PFAS concentration in a given fish for taxonomic species i (ng/g wet weight, or “ww”) and CSW is the PFAS concentration in surface water (ng/L). Biota-sediment accumulation factors (BSAF) can provide insight into the transfer of sediment-associated organic compounds into aquatic receptors.58,59 Thus, log BSAFs were calculated using Equation 2:59*

*where CSe is the sediment PFAS concentration (ng/g dry weight, or “dw”). Parameters used to calculate these coefficients can be found in SI Table S3.*

* In Martin et al BAF: *Bioaccumulation factors (BAFs) were calculated by* 
  + *aF/kd*
    - *a = assimilation efficiency*
    - *F = feeding rate*
    - *Kd = depuration rate constants*

Why are units so off? (ng in diet data, vs C\_D), discuss Abby’s data for comparison.

PFDA detection limit?: 0.029 \*

**\*** **Table A8.** Target PFAS, acronyms, accuracy (% recovery), precision (% RSD), and limits of detection and quantification determined from overspikes in SRM 1947 by LC-QTOF.

"PFHxS"

* Sediment: y
* water: y
* fish: y

"PFOS"

* sediment
* water
* fish

"PFOA"

* sediment
* water
* fish

"PFNA"

* sediment
* water
* fish

"PFDA"

* sediment
* water
* fish

"PFUA"

* sediment
* water
* fish

**Running code**

* Customize BMF and BCF run:
* “summer”: June, July data

1. In code:
   * **Ngratios:** unchanged
   * **Consoer\_PFOSratio:** unchanged
   * **Consoer\_PFOAratio:** unchanged
   * **observedData\_BCF:** species specific
   * **observedData\_BMF:** species specific
2. Provided datasets:
   * **dietData:** unchanged
     + *how is Sun et al diet table such low values? C\_D (ng/g)*
   * **organismData:** body mass mean of the species collected in July (no nune collection of fish in JBA) (source: PFAS\_Bioaccumulation\_JBA\_V2)
   * **foodwebTable:** unchanged
   * **chemicalParameters:** unchanged
   * **chemicalData:** C\_WTO, C\_s changed, summer data, mean values (June, July; source: PFAS\_Bioaccumulation\_JBA\_V2)
   * **oceanData:** C\_OX, T, pH changed, only summer data, mean values across all locations (ripple, down, spill, exit) (June, July; source: PFAS\_Bioaccumulation\_JBA\_V2)

* *Using summer variables for:*
  + *Fish weights*
  + *For water temp, DO, etc.*
  + *All others are average.* 
    - *Just a starting point…*
* *Sediment – very low concentrations, minimal contribution to BAF?*
* *Log in excel – just making sure that unlogged values make sense, very high concentrations.*
* *Unsure how the WHOLE body BCF values were obtained from Sun et al.*

Acronyms/ Names of the species:

Sed Sediment

Phy Phytoplankton

Kil Banded Killifish

Chu Creek Chubsucker

Dac Dace sp.

Dar Darter sp.

Min Eastern Mudminnow

Fal Fallfish

Bas Large Mouth Bass

Mad Margined Madtom

Pum Pumpkinseed

Swa Swallowtail Shiner

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**To change:**

**Organism specific uptake:”**

**Steady state model L67-77**

**# \*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Organism specific chemical uptake here \*\*\*\*\*\*\*\*\*\*\***

## Diet = sum(P \* t(C\_D)) + (Pd \* chemdata$C\_s)

* P = Fraction of the diet consisting of prey item ‘i' **unitless**
* Pd = Fraction of the diet consisting of detritus **unitless**
* C\_D = Contaminant concentration in the diet **ng/g**
* C\_s = Contaminant concentration in sediment. **ng/g**
* **Units: ng/g**

## Water = (org$m\_O \* chemdata$Phi \* chemdata$C\_WTO + (1-org$m\_O) \* C\_WDP)

* m\_O = Fraction of respiration from overlying water (always 1 in the data?) **unitless**
* Phi = Fraction of chemical in the dissolved phase (assumed 1) **unitless**
* C\_WTO = Total chemical concentration in the water column above the sediments
  + **(g/L)!! was written in the code**
  + **(ng/mL) provided in the datasheet and provided in SI**
* C\_WDP = C\_SOC / K\_OC, where C\_SOC = C\_s / OCS and is the chemical concentration in sediment normalized for OC content (g/kg-OC). **Units :** **ng/mL**

## FeedRate = G\_D / org$W\_B

* W\_B = body weight (kg)
* G\_D = Feeding rate, used for k\_D. [calculated in class ‘**New\_organism’**].

*Sun et al: “*Note that several studies have observed decreasing concentrations with increasing fish length w/in the same species. This could potentially be due to growth dilution, ontogenetic shifts, or other processes, not necessarily feeding rate”

Depends on settings: chooseStudyType == 'Martin BCF' G\_D = 1.5% body weight.

Otherwise: **0.022 \* W\_B^0.85 \* exp(0.06\*env$T)**

* **Units:** 
  + **G\_D: kg/d\*kg**

## Gill\_uptake = k\_1 \* (org$m\_O \* chemdata$Phi \* chemdata$C\_WTO + (1 - org$m\_O) \* C\_WDP)

* Units: k1; **L/kg/d \* ng/mL** = g chemical/kg fish/day
* the second part of the equation is the same as [**‘Water’**](#_Water_=_(org$m_O) above
* **k\_1** = is the clearance rate constant **(L/kg/d)** for chemical uptake via respiratory area [from **SSC\_B**]
* **k\_1** = E\_W \* G\_V / W\_B [kg/d]

description: (E\_W = gill chemical uptake efficiency \* G\_V = ventilation volume? [L/day]) / body mass

* + E\_W = Fish gill uptake efficiency (%, **unitless 0-1 values**) Used to calculate k1 clearance rate constant for fish, invertebrates, and zooplankton
  + G\_V = ventilation rate **(L/d)**

## Dietary\_uptake = k\_D \* (sum(P \* t(C\_D)) + (Pd \* chemdata$C\_s))

# kg food/kg org \* ng/g (or g/kg food) = g chemical/kg fish/day

* **k\_D =** E\_D \* [G\_D / org$W\_B] [calculated in class ‘**New\_organism’;** [feedRate] kg/d.

Description: dietary chemical transfer efficiency \* feeding rate divided by body mass

* the second part of the equation is the same as [**‘Diet’**](#_Diet_=_sum(P) above
  + E\_D = Dietary chemical transfer efficiency (%, unitless, 0-1 values) Used to calculate kd uptake rate constant. Empirical values for PFAAs differ for juvenile and adult fish
  + G\_D = Feeding rate, used for k\_D. [calculated in class ‘**New\_organism’**].

*Sun et al: “*Note that several studies have observed decreasing concentrations with increasing fish length w/in the same species. This could potentially be due to growth dilution, onotogenetic shifts, or other processes, not necessarily feeding rate”

Depends on settings: chooseStudyType == 'Martin BCF' G\_D = 1.5% body weight.

Otherwise: 0.022 \* W\_B^0.85 \* exp(0.06\*env$T)

## Uptake = Gill\_uptake + Dietary\_uptake

## Gill\_uppct = Gill\_uptake / Uptake

## Diet\_uppct = Dietary\_uptake / Uptake

## TotalElim\_rate = (k\_2 + k\_E + k\_M + k\_G)

* **k\_2 = (k\_2 = k\_1 / D\_BW )**
  + D\_BW = Body-water distribution coefficient
  + **Units: (L/kg\*d)**
  + **k\_1 = k\_1** is the clearance rate constant (L/kg\*d) for chemical uptake via respiratory area
    - k\_1 only for uptake, not ELIMINATION
* **k\_E =** the rate constant (1/d) for chemical elimination via excretion into egested feces [calculated in class ‘**New\_organism’**]
  + **k\_E** = G\_F \* E\_D \* K\_GB / W\_B
    - G\_F = Fecal egestion rate
    - E\_D = Chemical absorption efficiency across the gut membrane (gut or dietary chemical absorption efficiency)
    - K\_GB = is the partition coefficient of the chemical between the contents of GIT and the oragnism
* **k\_M =** 0 Elimination through biotransformation
* **k\_G =** is the growth rate constant, ‘dilution’ factor[calculated in class ‘**New\_organism’**]
  + conditional calculations

**`k\_R = renal elimination calculated elsewhere.**

**brainstorm: UNITS**

**C\_B = ((k\_1 \* (org$m\_O \* chemdata$Phi \* chemdata$C\_WTO + (1 - org$m\_O) \* C\_WDP) +**

**k\_D \* (sum(P \* as.numeric(unlist(C\_D))) + (Pd \* chemdata$C\_s))) / (k\_2 + k\_E + k\_M + k\_G+ k\_R\_est))**

(k\_1 \* (org$m\_O \* chemdata$Phi \* chemdata$C\_WTO + (1 - org$m\_O) \* C\_WDP)

+ m\_o = unitless

+ Phi = unitless

+ C\_WTO = ng/ml

+ C\_WDP = ng/ml

+ k\_1 = water uptake: L/kg/d

**L/kg/d \* ng/ml**

k\_D \* (sum(P \* as.numeric(unlist(C\_D)))

+ k\_D = dietary uptake: **kg/kg/d**

+ C\_D = ng/g

(Pd \* chemdata$C\_s))) /

+ C\_s = ng/g

**kg/kg/d \* ng/g**

(k\_2 + k\_E + k\_M + k\_G+ k\_R\_est))

+ all elimination rates = / **per day**

**A diagram of a fish

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**# \*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Organism specific chemical uptake here \*\*\*\*\*\*\*\*\*\*\***

**Incorporating metabolism in the model:**

**Goals:**

* G\_V – ventilation rate depends on the metabolic rate
* G\_D – feeding rate depends on temperature

**Feed intake rate (calories)**

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**Rubalcaba et al model 2020 PNAS**

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|  |  |  |
| --- | --- | --- |
| b0 |  |  |
| δ | (FAS = MMR/RMR)  *unitless* | Constant representing the increase in metabolic demand above the minimum (e.g., due to activities such as locomotion, feeding, or fighting). \*\*\* |
| M | kg | Mass of the fish |
| b |  | Scaling exponent |
| **E**/kT |  | E = activation energy (eV), k = the Boltzma |
| **E**/**k**T |  | The Boltzmann’s constant |
| E/k**T** | K | Temperature |
| *ρ*O2gill\* | mg m−3 | concentration of oxygen at the gill surface |
| *ρ*O2water | mg m−3 | the concentration of oxygen in the environment, i.e., the product of partial pressure and solubility calculated as a function of water **temperature** |
| H |  |  |
| KM |  | Michaelis constant representing the concentration at which the reaction velocity is half of Vmax |
| A | m2 | Gill respiratory surface area |
| hm | m s-2 | Mass transfer coefficient |
| µ | Pa s | Viscosity of water |
| ρ | kg m−3 | Density of water |
| D | m2 s−1 | diffusion coefficient of oxygen |
| L | m | Length of the lamellae (geometry of the gill) |
| v |  | Water velocity at the gill, influenced by ventilation rate |
|  |  |  |

\*\*\* δ = 1 thus represents the minimum metabolic requirements (resting metabolic rate, RMR), whereas δ > 1 simulates increasing metabolic demand (up to maximum metabolic rate, MMR). Thus, the parameter δ is equivalent to the factorial aerobic scope (FAS = MMR/RMR), which provides a means to investigate the effect of oxygen limitation at different activity levels.

**Next steps:**

1. Change ventilation rate as function of mass, temp, and oxygen
   1. **Units**: L/d (liters/day)
   2. Van Rooj Videler

<https://www-int-res-com.proxy.library.ucsb.edu/articles/meps/132/m132p031.pdf>

A screenshot of a paper

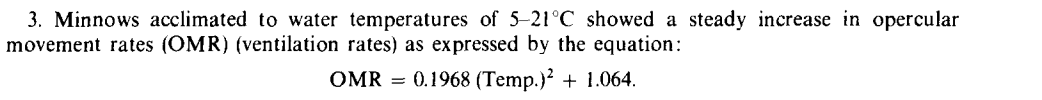
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* 1. Wares and ingram 1986 <https://deepblue.lib.umich.edu/bitstream/handle/2027.42/23722/0000694.pdf?sequence=1>

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* 1. Predict metabolic rate from the ventilation rate (metabolism 🡨 Vent rate (G\_D)
  2. Milidine et al CJFAS: <https://cdnsciencepub-com.proxy.library.ucsb.edu/doi/pdf/10.1139/F08-118>

1. Change feeding frequency as function of mass, temp, and oxygen
   1. Use the existing one in the model (not specific to Martin et al study, take ‘chooseStudyType out’
   2. Incorporate activity in the model
2. Food web inspiration:
   1. <https://dspace.wlu.edu/bitstream/handle/11021/33393/RG38_Nettere_ENV_2016.pdf?sequence=1>

**TO DO:**

double check the food web

Simulate temperatures

Simulate DO

Get metabolism in model?

Check notes from meeting with Chris

Plot the error with sample size

Size in kg !! (the bio conc C\_D part of food web) – min max .. adjust correct

BCF data (max and min the same?)

Is BCF and bioconcentrations the same thing?

Get organic carbon data

Get dissolved carbon data

Change Koc (Koc: Sediment organic carbon-water partition coefficient)

Change Kd (Kd: Sediment-water partition coefficient)

**Willow Grove data**

Assumptions:

1. Carcass proportions in body: <https://onlinelibrary.wiley.com/doi/pdf/10.1111/j.0906-6691.2004.00031.x>

* GSI = (gonad weight / full body weight)\* 100
  + 1 (mean female male …) %
* HIS = (liver weight / full body weight)\* 100
  + 0.9 %
* MI = (muscle weight / full body weight)\* 100
  + 45%
* Blood volume = assumed
  + 4% BW

1. Prey weight: no data 5g
2. DO: no data – 8 mgO2/L
3. pH: no data 7.5
4. Tissue concentrations (C\_D), average from all tissues (muscle, liver, and gonad)
5. BAF? Not log in the data?
6. Units for TOC

|  |  |
| --- | --- |
| **UNITS:** | **Abbi's data: (TOC ) = mg/kg** |
|  | **Needed for model: ( OC ) = kg/L** |

Get organic carbon data

Get dissolved carbon data