Sensitivity of 2,3,7,8 Bioaccumulation model to Log Kow

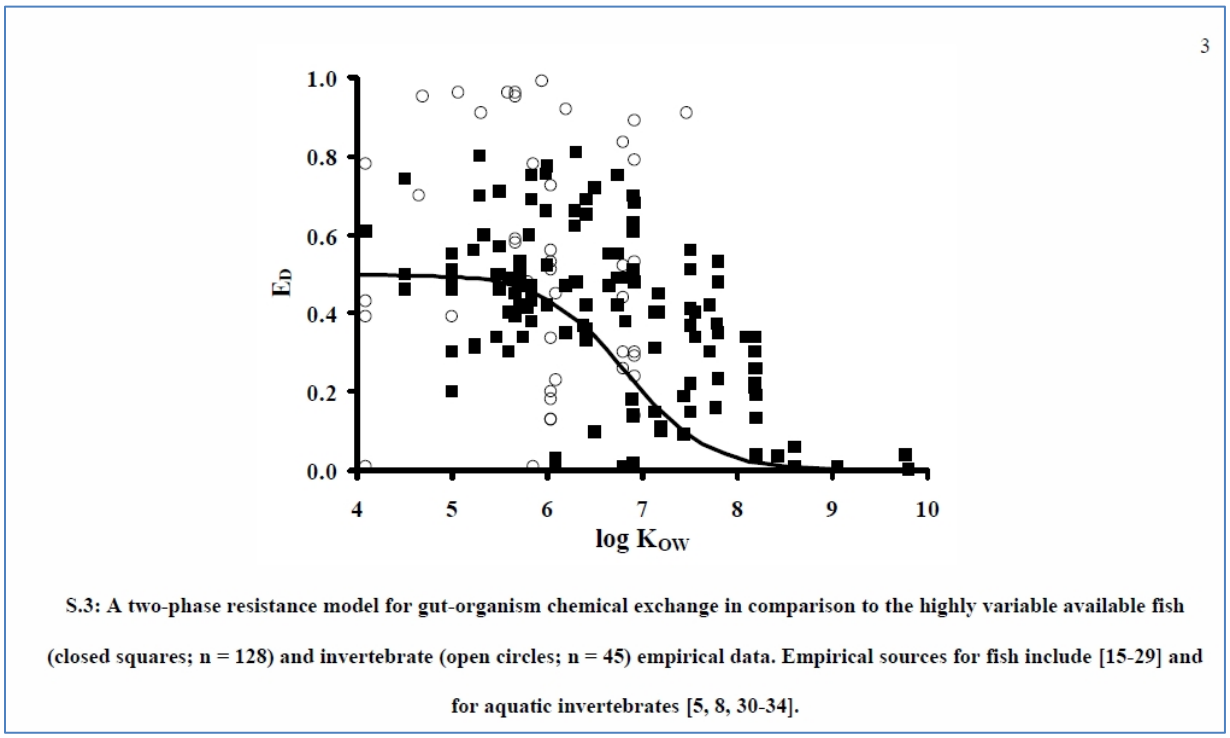
In the presentation of March 28, CPG noted that optimal calibrations for 2378-TCDD occur at low Log Kow (~5.5) and high Log Kow (~7.5) relative to the best estimate for Log Kow (~6.4 as shown on slide 12 of the March 28 presentation). The EPA team wanted to understand the reason for this model behavior, which we also reproduced in our experimentation with the model.

This model behavior seems to be driven by the model overpredicting concentrations in organisms at Log Kow ~6.5. (The model predicts concentrations that are a factor of 3 to 8 times lower in game fish at Log Kow ~5.5 and Log Kow~7.5 than it does at Kow 6.5. This results in significantly improved model fit at 5.5 and 7.5.)

The driver for this parabolic curve (in predicted fish-tissue concentrations relative to Log Kow) is the dietary uptake rate which also has a parabolic shape relative to Kow. Dietary uptake is predicted to be about a factor of four higher at Log Kow 6.5 than it is at either Log Kow ~5.5 or Log Kow ~7.5.

To further break down the cause for this parabolic shape, the EPA team examined the two pieces of the dietary uptake-- the k_D or "clearance rate constant via ingestion of food and water," and the weighted average of contamination in the food ($\sum P_i \times C_{D,i}$). Our discovery was that from Kow 5.5 to 7.5 the predicted k_D declines by an order of magnitude, while the contamination in the food increases by an order of magnitude. The combination of these two effects creates the parabolic relationship.

Our focus then went to the prediction of k_D as a function of Log Kow. This relationship in the Arnot Gobas 2004 model [$K_D = (E_D * G_D) / W_B$] is governed by the fit to data for E_D shown below.



S.3: A two-phase resistance model for gut-organism chemical exchange in comparison to the highly variable available fish (closed squares; n = 128) and invertebrate (open circles; n = 45) empirical data. Empirical sources for fish include [15-29] and for aquatic invertebrates [5, 8, 30-34].

Figure 1. Figure S.3 from (Arnot and Gobas 2004).

Our observation about this fit is that it contains ample room for interpretation of, and calibration of, the E_D parameter.

Rather than using a generic fit to Log Kow to estimate the E_D (the unitless dietary chemical transfer efficiency) for 2378-TCDD it may be warranted to use literature observations of E_D specifically for 2378-TCDD. This could provide a constraint to the model that is based on chemical-specific data rather than an estimate based on a loose fit to Kow.

Our preliminary literature search found an estimate from (Morrison et al. 1999) of a E_D of **0.41** for 2,3,7,8 TCDD. The citation for this estimate was the average of data from (Gobas et al. 1988; Hawkes and Norris 1977; Kleeman et al. 1986). Looking at those papers, the 1988 Gobas paper finds an E_D of **0.34** for 2,3,7,8 TCDD, and cites the Hawkes paper as the source for that estimate.

The Kleeman and Hawkes/Norris papers do not seem to have specific estimates of E_D within them. These papers do have experimental data showing the speed and extent of dietary uptake of 2,3,7,8 TCDD in rainbow trout. Using the data in these papers and a "generic" time-varying bioaccumulation model (see below), our own (initial) estimate of E_D was **0.32** from data in Hawkes and Norris paper, and **0.33** from the data in Kleeman. Another source (Batterman et al. 1989) would result in E_D in the range of **0.38** to **0.45.** The Batterman study did include some sediment exposure, meaning these E_D values may be overestimated.

Another study (Fisk et al. 1997) results in very high estimates of E_D reported at 0.7 to 0.93, but these estimates appear to be lipid normalized compared to other studies. When calculating on a non-lipid normalized basis the K_D values seem to exceed 1.0. This study should perhaps be discounted due to the fact that exposures were limited to 30 days.

(Jones et al. 2001) reported assimilation efficiencies that "ranged **between 8 and 11%** in the early phases of the exposure." Fitting a time varying model to the Jones data set resulted in E_D values of **0.18, 0.12, and 0.3.**

With the caveats that most these data are for rainbow trout which is not relevant to the LPR study area, it may be worth considering the E_D for 2,3,7,8 TCDD as a calibration parameter, independent of Kow, and **potentially varying from 0.12 to 0.45** based on the literature search above.

On another note, most of these papers also contain information about kinetic rates of uptake and depuration. These data may be useful to verify the predictions of the non-steady-state model when that model is being developed and tested. Specifically, model-predicted half lives and uptake rates can be compared against the experimental data to ensure that predicted uptake and depuration rates within the model are reasonable. For juvenile rainbow trout, the half-lives reported ranged from 70-105 days. For adult fish, half-lifes would be much slower (i.e. >346 days in adult trout, 300-325 days in carp) (Tietge et al. 1998)

The EPA team wanted to ensure that CPG model calibrations are not artificially constrained by the fit shown in Figure 1, and instead could potentially be parameterized by data specifically relevant to 2,3,7,8 TCDD.

"Generic" time varying bioaccumulation model

$$\frac{dM_B}{dt} = \left\{ W_B \cdot \left(k_1 \cdot \left[m_O \cdot C_{WD,O} + m_P C_{WD,P} \right] + k_D \cdot \sum_i \left(P_i \cdot C_{D,i} \right) \right) \right\} - \left(k_2 + k_E + k_M \right) \cdot M_B$$

$K_D = E_D * (G_D / W_B)$

where

- G_D is the feeding weight and W_B is the wet weight of the organism
- Therefore E_D is multiplied by the ingestion rate in (g/(g day)) multiplied by the concentration of contaminant within the food to get K_D
- $(K_2+K_E+K_M)$ is calculated based on experimental half-life data or reported loss rates.
- K_1 is assumed to be zero as these are dietary-uptake studies

This model was approximately fit to reported experimental data to estimate E_D values listed above.

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