MODELING BIOACCUMULATION AS A POTENTIAL ROUTE OF RIVERINE FOODWEB EXPOSURES TO PFOS

B. Rashleigh (rashleigh.brenda@epa.gov)[1], R.A. Park[2], J. Clough[3], M.C. Wellman[1], R. Bringolf[4], P.J. Lasier[5]
[1]U.S. Environmental Protection Agency, [2]EcoModeling, [3]Warren Pinnacle Consulting, Inc.. [4]University of Georgia, [5]U.S. Geological Survey

United States Environmental Protection Agency

OVERVIEW

Perfluoralkyl acids (PFAAs) are compounds of interest as bioaccumulators; these persistent chemicals have been found in humans and animals throughout the world

Perfluoroctane sulfonate (PFOS) has an especially high bioaccumulation factor in fish

Few models are available for modeling the effects of PFOS on aquatic ecosystems; one is AQUATOX

AQUATOX has been used to simulate PFOS in an estuary. Here, we use it for **exploratory analysis for a river site**; future work uses a spatially explicit linked-segment version

PFOS

PFOS, a manmade florosurfactant that is hydrophobic and lipophobic, is used for its antiwetting and antistaining properties in a wide array of products

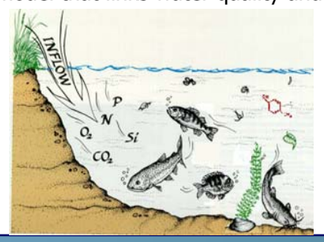
PFOS is taken up by protein rather than lipids (Kannan et al. 2001), so its kinetics cannot be modeled as functions of octanol-water partition coefficient. **Equations based on perfluoroalkyl chain length** (Martin et al. 2003) are used in AQUATOX

AQUATOX MODEL

An integrated simulation model that links water quality and aquatic life

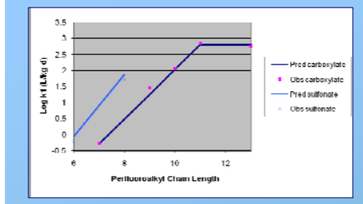
AQUATOX predicts:
- Fate of stressors
- Exposure of toxics
- Effects on biota

(Park et al. 2008, US EPA 2009)



PFOS PROCESSES IN AQUATOX

Uptake through Gill

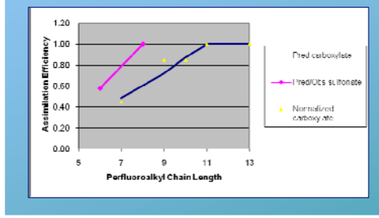


$GillUptake = WetToDry \cdot SizeCorr \cdot k1 \cdot StVarAnimal \cdot e^{-6}$

$\log k1 = -5.85 + 0.966 \cdot ChainLength$

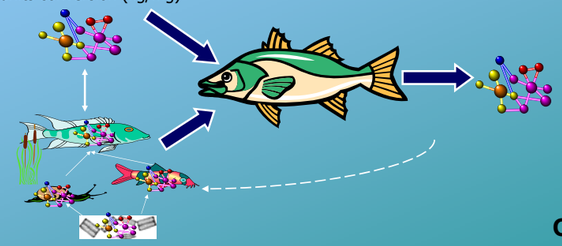
GillUptake = uptake of toxicant by gills (µg/L d)
WetToDry = conversion factor for wet to dry weights
k1 = uptake transfer rate (L/kg d)
ChainLength = length of perfluoroalkyl chain (integer)
SizeCorr = allometric correction for size (unitless)
StVarAnimal = biomass of given animal (mg/L)
1 e-6 = units conversion (kg/mg)

Uptake from Diet



$GutEff = -0.68 + 0.21 \cdot ChainLength$

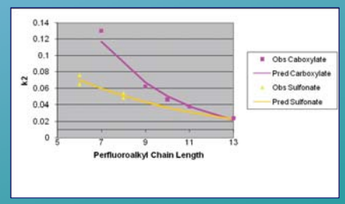
GutEff = Dietary Assimilation
User inputs organic matter partition coefficient
Sorption to algae and macrophytes are modeled empirically



Depuration

$\log k2 = -0.733 - 0.07 \cdot ChainLength$

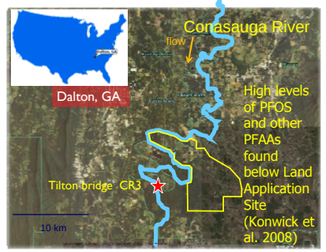
k2 = depuration rate (1/d)

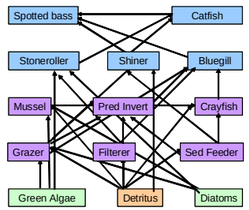


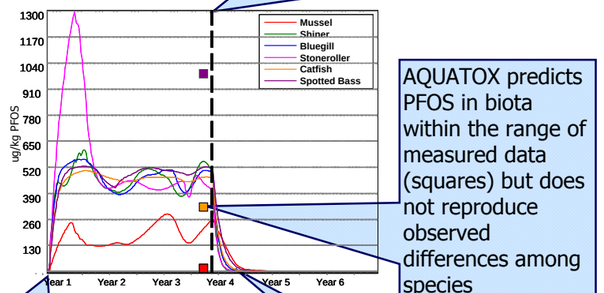
Other losses

Predation, mortality, spawning, biotransformation to different forms

PFOS IN RIVERS







REFERENCES

Kannan, K., J. Koistinen, K. Beckman, T. Evans, J. F. Gorzelany, K. J. Hansen, P. D. Jones, E. Helle, M. Nyman, and J. P. Giesy. 2001. Accumulation of Perfluorooctane Sulfonate in Marine Mammals. Environ. Sci. Technol. **35: 1593-1598.**

Konwick, BJ, GT Tomy, N Ismail, JT Peterson, RJ Fauver, D Higginbotham, and AT Fisk. 2008. Concentrations and Patterns of Perfluoroalkyl Acids in Georgia, USA Surface Waters Near and Distant to a Major Use Source. Environ Toxicol Chem **27:2011-2018**.

Martin, J. W., S. A. Mabury, K. R. Solomon, and D. C. G. Muir. 2003. Bioconcentration and Tissue Distribution of Perfluorinated Acids in Rainbow Trout (*Oncorhyncus mykiss*). Environmental Toxicology and Chemistry **22: 196-204.**

Park, R. A., J. S. Clough, and M. C. Wellman. 2008. AQUATOX: Modeling Environmental Fate and Ecological Effects in Aquatic Ecosystems. Ecological Modelling **213:1-15.**

U.S. Environmental Protection Agency. 2009. AQUATOX (Release 3) Modeling Environmental Fate and Ecological Effects in Aquatic Ecosystems, Volume 2: Technical Documentation. EPA-823-R-09-004, U.S. Environmental Protection Agency, Office of Water, Office of Science and Technology, Washington DC.
http://www.epa.gov/waterscience/models/aquatox/