SUPPORTING INFORMATION

Manuscript Title

A MODEL FOR THE PRESENCE OF POLYCHLORINATED BIPHENYLS (PCBs) IN THE WILLAMETTE RIVER BASIN (OREGON)

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TABLE S1. Key physicochemical properties of selected congeners.

VARIABLE	SYMBOL	CONGENER [CASRN] PCB-077 [32598-13-3]	PCB-118 [31508-00-6]	PCB-169 [32774-16-6]	Ref
Chemical molecular weight (g mol^{-1})	MW	291.99	326.43	360.88	*(1)*
Air-side evaporation MTC parameter a (unitless) [a]	VEWa	0.4032	0.3942	0.3860	*(2)*
Air-side evaporation MTC parameter b (unitless) [a]	VEWb	0.0311	0.0311	0.0311	*(2)*
Water-side evaporation MTC parameter a (unitless) [a]	VEAa	416.43	406.00	395.40	*(2)*
Water-side evaporation MTC parameter b (unitless) [a]	VEAb	0.0035	0.0036	0.0038	*(2)*
Water-to-sediment mass transfer coefficient (m d^{-1})	VD	0.0012 [b]	0.0024	0.0048 [c]	*(3)*
Octanol-water partition coefficient (Log_{10}, unitless)	KOW	6.36	6.69	7.42	*(4,5,6)*
Half-life, water (d)	HLF_{water}	417 [d]	1292	2292 [c]	*(37)*
Half-life, sediment (d)	HLF_{sed}	2292 [d]	2292	7083 [c]	*(37)*
Half-life, soil (d)	HLF_{soil}	708 [d]	4167	22917 [c]	*(37)*
Half-life, leaf (d) [e]	HLF_{leaf}	708 [d]	4167	22917 [c]	*(37)*
Half-life, particles-on-leaf (d) [e]	HLF_{POL}	708 [d]	4167	22917 [c]	*(37)*
Particle scavenging ratio (unitless)	W_P	360000 [f]	330000	240000 [h]	*(7)*
Vapor scavenging ratio (unitless)	W_G	12000 [f]	25000 [g]	53000 [h]	*(7)*
Reaction rate constant (cm^3 $molc^{-1}$ s^{-1})	kA_{ref}	5.90×10^{-13} [d]	3.00×10^{-13}	1.60×10^{-13} [c]	*(37)*
Activation energy in air (J mol^{-1})	Ea_{air}	10460	12920	15380 [c]	*(8)*
Activation energy in other media (J mol^{-1})	Ea_{other}	30000	30000	30000	*(37)*
Henry's Law temperature coefficient (kJ mol^{-1})	ΔH_H	39.229	49.237	163.616	*(1)*
Henry's Law temperature coefficient (kJ mol^{-1} K^{-1})	ΔS_H	0.09	0.13	0.51	*(1)*
Henry's Law constant (Pa m^{-3} mol^{-1}) @ 25° C	H	16.7	36.3	23.4	*(1)*

[a] Assumes a wind speed of 4.5 m s^{-1}
[b] Value for PCB-066
[c] Value for PCB-153
[d] Value for PCB-052
[e] Assumed same as soil per Wania *(34)*
[f] Value for PCB-074
[g] Value for PCB-132
[h] Value for PCB-174
[i] Value for PCB-101

Table S2. Equations used for calculation of rate constants, fluxes, and compartment masses.

Equation	Equation Description (Units)	Ref
RATE CONSTANT CALCULATIONS		
{01} Sediment Burial		
$\mathrm{RATE}_{01} = \mathrm{SA}_{\mathrm{sed}} \cdot \mathrm{VB} \cdot (1 - \mathrm{FDS})/\mathrm{VS}$	Burial rate constant (d^{-1})	*(3)*
$\mathrm{FDS} = 1/(1 + (\mathrm{CSS} \cdot \mathrm{OC}_{\mathrm{sed}} \cdot \mathrm{KOW} \cdot \psi))$	Fraction of chemical freely dissolved in sediment (unitless)	*(3)* [(a)]
{02} Diffusion from Sediment to Water		
$\mathrm{RATE}_{02} = \mathrm{SA}_{\mathrm{sed}} \cdot \mathrm{VD} \cdot \mathrm{FDS}/\mathrm{VS}$	Sediment-water diffusion rate constant (d^{-1})	*(3)*
{03} Re-Suspension from Sediment to Water		
$\mathrm{RATE}_{03} = (\mathrm{RFlux} \cdot \mathrm{CSS}) \cdot (1 - \mathrm{FDS})/(1000 \cdot \mathrm{VS})$	Re-suspension rate constant (d^{-1})	*(3)*
$\mathrm{BFlux} = 1000 \cdot \mathrm{CSS} \cdot \mathrm{SA}_{\mathrm{sed}} \cdot \mathrm{VB}$	Burial flux (kg d^{-1})	*(3)*
$\mathrm{RFlux} = \mathrm{Sflux} - \mathrm{BFlux}$	Re-suspension flux (kg d^{-1})	*(3)*
$\mathrm{SFlux} = 1000 \cdot \mathrm{CPW} \cdot \mathrm{SA}_{\mathrm{water}} \cdot \mathrm{VSS}$	Settling flux (kg d^{-1})	*(3)*
{04} Degradation in Sediment		
$\mathrm{RATE}_{04} = (0.693/\mathrm{HLF}_{\mathrm{sed}}) \cdot \exp\left[\left(\frac{\mathrm{Ea}_{\mathrm{other}}}{8.314}\right) \cdot \left(\frac{1}{\mathrm{T}_{\mathrm{ref}}} - \frac{1}{\mathrm{TA}}\right)\right]$	Temperature-corrected sediment degradation rate constant (d^{-1})	*(37)*
{05} Diffusion from Water to Sediment		
$\mathrm{RATE}_{05} = \mathrm{SA}_{\mathrm{sed}} \cdot \mathrm{VD} \cdot \mathrm{FDW}/\mathrm{VW}$	Water-sediment diffusion rate constant (d^{-1})	*(3)*
{06} Deposition from Water to Sediment		
$\mathrm{RATE}_{06} = (\mathrm{VSS} \cdot \mathrm{SA}_{\mathrm{water}}) \cdot (1 - \mathrm{FDW})/\mathrm{VW}$	Water-sediment deposition rate constant (d^{-1})	*(3)*
$\mathrm{FDW} = 1/(1 + (\mathrm{CPW} \cdot \mathrm{OC}_{\mathrm{sps}} \cdot \mathrm{KOW} \cdot \psi))$	Fraction of chemical freely dissolved in water (unitless)	*(3)*[(a)]
$\mathrm{CPW} = \mathrm{TSS}/1 \times 10^{6}$	Particle concentration in water (kg L^{-1})	---

Table S2. Equations used for calculation of rate constants, fluxes, and compartment masses.

Equation	Equation Description (Units)	Ref
$TSS = 7.2693 \cdot \exp\left(2 \times 10^{-5} \cdot Q\right)$	Total suspended solids concentration (mg L^{-1})	---
{07} River Flow		
$RATE_{07} = VW/\left(Q \cdot 2446.5\right)$	Water residence time (d)	---
$VW = LEN \cdot XSA$	Water volume (m^3)	---
$XSA = \left(A1 \cdot Q^{A2} + A0\right) \cdot 0.0929$	Cross-section area (m^2)	*(11)*
$SA_{water} = LEN \cdot WID$	Water surface area (m^2)	---
$WID = \left(W1 \cdot Q^{W2}\right) \cdot 0.3048$	River width (m)	*(11)*
$VS = AD \cdot LEN \cdot WID$	Sediment volume (m^3)	---
$SA_{sed} = SA_{water}$	Sediment surface area (m^2)	---
{08} Volatilization from Water to Air		
$RATE_{08} = SA_{water} \cdot FDW \cdot VE/VW$	Water-air volatilization rate constant (d^{-1})	*(3)*
$VE = 1/\left(1/VEW + 1/\left(HTD_{water} \cdot VEA\right)\right)$	Volatilization mass transfer coefficient (m d^{-1})	*(3)*
$VEW = VEWa \cdot \exp\left(VEWb \cdot TW\right)$	Water-side volatilization MTC (m d^{-1})	*(3)*
$VEA = VEAa \cdot \exp\left(VEAb \cdot TW\right)$	Air-side evaporation MTV (m d^{-1})	*(3)*
$HTD_{water} = \exp\left(-\Delta H_H/\left(8.314 \cdot TW\right) + \left(\Delta S_H/8.314\right)\right)$	Temperature-dependent dimensionless Henry's law constant, water (unitless)	*(1)*
{09} Degradation in Water		
$RATE_{09} = \left(0.693/HLF_{water}\right) \cdot \exp\left[\left(\frac{Ea_{other}}{8.314}\right) \cdot \left(\frac{1}{T_{ref}} - \frac{1}{TA}\right)\right]$	Temperature-corrected water degradation rate constant (d^{-1})	*(37)*

Table S2. Equations used for calculation of rate constants, fluxes, and compartment masses.

Equation	Equation Description (Units)	Ref
{10} Advective Inflows & Outflows		
$FLUX10_{in} = \left(\left(CTA \cdot u(d) \cdot 86400\right)/1\times10^{18}\right) \cdot LEN \cdot AirHeight$	Advective inflow (kg d^{-1})	*(27)*
$FLUX10_{out} = AIR/\left(VA/\left(u(d) \cdot LEN \cdot AirHeight \cdot 86400\right)\right)$	Advective outflow (kg d^{-1})	*(1)*
{11} Diffusion from Air to Water		
$RATE_{11} = SA_{water}/VA \cdot \left(VE/HTD_{water}\right) \cdot (1-\phi)$	Air-water diffusion rate constant (d^{-1})	*(27)*
$\phi = K_p \cdot TSP/\left(1 - K_p \cdot TSP\right)$	Fraction of chemical bound to dust particles, (unitless)	*(13)*
$K_P = \left(KOW/HTD_{air}\right) \cdot 0.25\times10^{-12}$ {Aerosol Organic Fraction = 20%}	Particle-gas partition coefficient (m^3 μg^{-1})	*(16)*
$HTD_{air} = \exp\left(-\Delta H_H/(8.315 \cdot TA) + (\Delta S_H/8.314)\right)$	Temperature-dependent dimensionless Henry's law constant, air (unitless)	*(1)*
{12, 13, 14} Deposition from Air to Water		
$RATE_{12} = \left(\left(CTA/1\times10^{15}\right) \cdot \phi \cdot SA_{water} \cdot UD\right)/1000$	Dry particulate deposition rate constant (d^{-1})	*(12)*
$RATE_{13} = \left(UR \cdot 0.0254 \cdot SA_{water} \cdot W_P \cdot \phi \cdot \left(CTA/1\times10^{15}\right)\right)/1000$	Wet particulate deposition rate constant (d^{-1})	*(12)*
$RATE_{14} = \left(UR \cdot 0.0254 \cdot SA_{water} \cdot W_G \cdot (1-\phi) \cdot \left(CTA/1\times10^{15}\right)\right)/1000$	Wet gaseous deposition rate constant (d^{-1})	*(12)*
{15} Diffusion from Air to Soil		
$RATE_{15} = ks_{diff} \cdot \left(CTA \cdot 1\times10^{-18}\right)$	Air-soil diffusion rate constant (d^{-1})	---
$ks_{diff} = \left(\left(D_a \cdot SA_{land} \cdot \theta_V\right)/Z_d\right) \cdot 86400 \cdot 1\times10^{-4}$	Diffusive exchange volume (m^3 d^{-1})	*(14)*
$D_a = 1.9/(MW)^{2/3}$	Diffusivity of chemical in air (cm^2 s^{-1})	*(15)*
{16, 17, 18} Deposition from Air to Soil		
$RATE_{16} = \left(CTA/1\times10^{15}\right) \cdot \phi \cdot \left(SA_{nonforest} + SA_{forest} \cdot \left(1 - I_{dry}\right)\right) \cdot UD/1000$	Dry particulate deposition rate constant (d^{-1})	*(27)*
$I_{dry} = 1 - \exp\left[\left(1 - fW_{leaf}\right) \cdot \left(-\alpha VAF \cdot \rho_{area}\right)\right]$	Fraction of dry-depositing chemical intercepted by	*(27)*

Table S2. Equations used for calculation of rate constants, fluxes, and compartment masses.

Equation	Equation Description (Units)	Ref
	canopy (unitless)	
$RATE_{17} = \left(UR \cdot 0.0254 \cdot SA_{nonforest} + SA_{forest} \cdot (1 - I_{wet}) \cdot W_P \cdot \phi \cdot \left(CTA/1\times10^{15}\right)\right)/1000$	Wet particulate deposition rate constant (d^{-1})	*(27)*
$RATE_{18} = \left(UR \cdot 0.0254 \cdot SA_{nonforest} + SA_{forest} \cdot (1 - I_{wet}) \cdot W_G \cdot (1-\phi) \cdot \left(CTA/1\times10^{15}\right)\right)/1000$	Wet gaseous deposition rate constant (d^{-1})	*(27)*
{19, 20} Deposition from Air to POL		
$RATE_{19} = \left(\left(V_{dry} \cdot I_{dry} \cdot SA_{forest}\right)/VA\right) \cdot \left(\phi/(DL/\rho P)\right)$	Dry particulate deposition rate constant (d^{-1})	*(27)*
$VA = SA_{total} \cdot AirHeight$	Basin air volume (m^{-3})	---
$V_{dry} = UD \cdot (DL/\rho P)$	Volumetric dry deposition of particles ($m^3\ m^{-2}$)	*(27)*
$DL = TSP/1\times10^9$	Dust load in air compartment ($kg\ m^{-3}$)	*(27)*
$RATE_{20} = \left(\left(V_{wet} \cdot I_{wet} \cdot SA_{forest}\right)/VA\right) \cdot \left(\phi/(DL/\rho P)\right)$	Wet particulate deposition rate constant (d^{-1})	*(27)*
$V_{wet} = W_P \cdot UR \cdot 0.0254 \cdot (DL/\rho P)$	Volumetric wet deposition of particles ($m^3\ m^{-2}$)	*(27)*
{21} Diffusion from Air to Leaf		
$RATE_{21} = \left((2 \cdot LAI \cdot SA_{forest} \cdot gC + LAI \cdot SA_{forest} \cdot gS) \cdot 1/VA\right)$	Air-leaf diffusion rate constant (d^{-1})	*(27)*
$gB = (D_{air}/1000)/LAP$	Conductance of the air boundary layer ($m\ d^{-1}$)	*(27)*
$gC = \left((1/gB) + (1/g_{cuticle})\right)^{-1}$	Total conductance of the cuticular path ($m\ d^{-1}$)	*(27)*
$g_{cuticle} = \left(P_{cuticle}/(Z_{air}/Z_{water})\right) \cdot 86400$	Conductance of the cuticle ($m\ d^{-1}$)	*(27)*
$gS = \left((1/g_{stomata}) + (1/gB)\right)^{-1}$	Total conductance of the stomatal pathway ($m\ d^{-1}$)	*(27)*
$g_{stomata} = (D_{air}/10000) \cdot Sn$	Conductance of the cuticle ($m\ s^{-1}$)	*(27)*
$P_{cuticle} = 10^{(0.704 \cdot \log KOW - 11.2)}$	Permeance of the cuticle ($m\ s^{-1}$)	*(27)*
$Z_{water} = 1/H$	Fugacity capacity in air vapor ($mol\ Pa^{-1}\ m^{-3}$)	*(27)*

Table S2. Equations used for calculation of rate constants, fluxes, and compartment masses.

Equation	Equation Description (Units)	Ref
$\mathrm{H} = \mathrm{HTD}_{\mathrm{air}} \cdot 8.314 \cdot (273.15 + \mathrm{TA})$	Dimensionless Henry's Law constant (unitless)	---
$\mathrm{Z}_{\mathrm{air}} = 1/(8.314 \cdot (273.15 + \mathrm{TA}))$	Fugacity capacity in total water (mol Pa^{-1} m^{-3})	*(27)*
{22} Deposition from Air to Leaf		
$\mathrm{RATE}_{22} = (\mathrm{SA}_{\mathrm{forest}}/\mathrm{VA}) \cdot \mathrm{UR} \cdot 0.0254 \cdot \mathrm{I}_{\mathrm{wet}} \cdot (\mathrm{Z}_{\mathrm{air}}/\mathrm{Z}_{\mathrm{TotalAir}})$	Wet gaseous deposition rate constant (d^{-1})	*(27)*
{23} Degradation in Air		
$\mathrm{RATE}_{23} = 0.693/(1/\mathrm{kA} \cdot 1//86400)$	Temperature-corrected atmosphere degradation rate constant (d^{-1})	---
$\mathrm{kA} = \mathrm{kA}_{\mathrm{ref}} \cdot \mathrm{OH} \cdot \exp\left[\left(\frac{\mathrm{Ea}_{\mathrm{air}}}{8.314}\right) \cdot \left(\frac{1}{\mathrm{T}_{\mathrm{ref}}} - \frac{1}{\mathrm{TA}}\right)\right]$	Reaction rate constant, air (s^{-1})	*(37)*
{24} Volatilization from Soil to Air		
$\mathrm{RATE}_{24} = \left[\frac{86400}{\mathrm{Z}_{\mathrm{d}} \cdot \mathrm{KOC}_{\mathrm{soil}} \cdot \mathrm{BD}_{\mathrm{soil}}} \cdot \mathrm{HTD}_{\mathrm{soil}}\right] \cdot \left(\frac{\mathrm{D}_{\mathrm{a}}}{\mathrm{Z}_{\mathrm{d}}}\right) \cdot \left[1 - \left(\frac{\mathrm{BD}_{\mathrm{soil}}}{\rho_{\mathrm{soil}}}\right) - \theta_{\mathrm{W}}\right]$	Soil-air volatilization rate constant (d^{-1})	*(15)*
$\mathrm{HTD}_{\mathrm{soil}} = \exp(-\Delta \mathrm{H}_{\mathrm{H}}/(8.315 \cdot \mathrm{TS}) + (\Delta \mathrm{S}_{\mathrm{H}}/8.314))$	Temperature-dependent dimensionless Henry's Law constant, soil (unitless)	*(1)*
$\mathrm{KOC}_{\mathrm{soil}} = \mathrm{KOW} \cdot \mathrm{OC}_{\mathrm{soil}} \cdot \psi$	Organic carbon-water partition coefficient (cm^3 g^{-1})	*(16)*
{25} Erosion from Soil to Water		
$\mathrm{RATE}_{25} = ((\mathrm{XE} \cdot \mathrm{SD} \cdot \mathrm{ER}) \cdot \mathrm{FIP}_{\mathrm{soil}} \cdot 1 \times 10^{-7})/(\mathrm{BD} \cdot \mathrm{Z}_{\mathrm{d}})$	Soil-water erosion rate constant (d^{-1})	*(15)*
$\mathrm{SD}_{\mathrm{k}} = 0.6 \cdot \mathrm{SA}_{\mathrm{land}}^{-0.125}$	Sediment delivery ratio (unitless)	*(15)*
$\mathrm{FIP}_{\mathrm{soil}} = (\mathrm{KOC}_{\mathrm{soil}} \cdot \mathrm{BD}_{\mathrm{soil}})/(\mathrm{HTD}_{\mathrm{soil}} - \theta_{\mathrm{V}} + \theta_{\mathrm{W}} + \mathrm{KOC}_{\mathrm{soil}} \cdot \mathrm{BD}_{\mathrm{soil}})$	Fraction of chemical on soil solids (unitless)	*(14)*

{26} Runoff from Soil to Water

Table S2. Equations used for calculation of rate constants, fluxes, and compartment masses.

Equation	Equation Description (Units)	Ref
$RATE_{26} = (UR \cdot ROfrac \cdot 2.54) \cdot FIW_{soil} / (\theta_W \cdot Z_d)$	Soil-water dissolved runoff rate constant (d^{-1})	*(15)*
$FIW_{soil} = \theta_W / (HTD_{soil} \cdot \theta_V) + \theta_W + KOC_{soil} \cdot BD_{soil}$	Fraction in soil interstitial water (unitless)	*(14)*
{27} Degradation in Soil		
$RATE_{27} = (0.693/HLF_{soil}) \cdot \exp\left[\left(\frac{Ea_{other}}{8.314}\right) \cdot \left(\frac{1}{T_{ref}} - \frac{1}{TA}\right)\right]$	Temperature-corrected soil degradation rate constant (d^{-1})	*(28)*
{28} Wash-Off from POL to Soil		
$RATE_{28} = (V_{wet} \cdot I_{wet} \cdot SA_{forest}) / V_{leaf}P$	Wash-off rate constant (d^{-1})	*(27)*
$V_{leaf}P = V_{leaf} \cdot 1 \times 10^9$	POL volume (m^3)	*(27)*
{29} Litter-Fall from POL to Soil		
$RATE_{29} = K_{litter}$	POL loss via litterfall rate constant (d^{-1})	*(27)*
{30} Diffusion from POL to Leaf		
$RATE_{30} = K_{POL-leaf}$	POL-leaf diffusion rate constant (d^{-1})	*(27)*
{31} Blow-Off from POL to Air		
$RATE_{31} = ((V_{dry} \cdot I_{dryt} \cdot SA_{forest}) / V_{leaf}P) \cdot RainEvent$	Blow-off rate constant (d^{-1})	*(27)*
$RainEvent \langle \text{if } UR > 0 \text{ then } 1 \text{ else } 0 \rangle$		*(27)*
{32} Degradation in POL		
$RATE_{32} = (0.693/HLF_{POL}) \cdot \exp\left[\left(\frac{Ea_{other}}{8.314}\right) \cdot \left(\frac{1}{T_{ref}} - \frac{1}{TA}\right)\right]$	Temperature-corrected POL degradation rate constant (d^{-1})	*(27, 37)*

{33} Litter-Fall from Leaf to Soil

Table S2. Equations used for calculation of rate constants, fluxes, and compartment masses.

Equation	Equation Description (Units)	Ref
$\mathrm{RATE}_{33} = \mathrm{K}_{\mathrm{litter}}$	Leaf litterfall rate constant (d^{-1})	*(27)*
{34} Diffusion from Leaf to POL		
$\mathrm{RATE}_{34} = 0.01 \cdot \mathrm{K}_{\mathrm{POL-leaf}}$	Leaf-POL diffusion rate constant (d^{-1})	*(27)*
{35} Diffusion from Leaf to Air		
$\mathrm{RATE}_{35} = (2 \cdot \mathrm{LAI} \cdot \mathrm{SA}_{\mathrm{forest}} \cdot \mathrm{gC} + \mathrm{LAI} \cdot \mathrm{SA}_{\mathrm{forest}} \cdot \mathrm{gS}) \cdot 1/\mathrm{V}_{\mathrm{leaf}} \cdot \mathrm{Z}_{\mathrm{air}}/\mathrm{Z}_{\mathrm{leaf}}$	Leaf-air diffusion rate constant (d^{-1})	*(27)*
$\mathrm{V}_{\mathrm{leaf}} = (\mathrm{SA}_{\mathrm{forest}} \cdot \mathrm{LAI} \cdot \rho_{\mathrm{area}})/820$	Volume of leaves (m^3)	*(27)*
$\mathrm{Z}_{\mathrm{leaf}} = 0.18 \cdot \mathrm{Z}_{\mathrm{air}} + \mathrm{Z}_{\mathrm{water}} + 0.02 \cdot \mathrm{Z}_{\mathrm{water}} \cdot \mathrm{KOW}$	Fugacity capacity in total leaf (mol pa^{-1} m^{-3})	*(27)*
$\mathrm{Z}_{\mathrm{TotalAir}} = \mathrm{Z}_{\mathrm{air}} \cdot (1 - \mathrm{DL}/\rho\mathrm{P}) + \mathrm{Z}_{\mathrm{solid}} \cdot (\mathrm{DL}/\rho\mathrm{P})$	Fugacity capacity in total air (mol pa^{-1} m^{-3})	*(27)*
$\mathrm{Z}_{\mathrm{solid}} = \mathrm{Z}_{\mathrm{air}} \cdot (\phi \cdot (1 - \mathrm{DL}/\rho\mathrm{P}))/((1-\phi) \cdot (\mathrm{DL}/\rho\mathrm{P}))$	Fugacity capacity in particulates (mol pa^{-1} m^{-3})	*(27)*
{36} Degradation in Leaf		
$\mathrm{RATE}_{36} = (0.693/\mathrm{HLF}_{\mathrm{leaf}}) \cdot \exp\left[\left(\frac{\mathrm{Ea}_{\mathrm{other}}}{8.314}\right) \cdot \left(\frac{1}{\mathrm{T}_{\mathrm{ref}}} - \frac{1}{\mathrm{TA}}\right)\right].$	Temperature-corrected leaf degradation rate constant (d^{-1})	*(27, 37)*
COMPARTMENT FLUX AND MASS CALCULATIONS		
Air Compartment		
$\mathrm{AIR} = \mathrm{AIR}_{\mathrm{t-dt}} + \left(\begin{array}{l}\mathrm{FLUX}_{08} + \mathrm{FLUX}_{24} + \mathrm{FLUX}_{35} + \mathrm{FLUX}_{31} + \mathrm{FLUX}_{10} - \mathrm{FLUX}_{23} \\ -(\mathrm{FLUX}_{11-14} + \mathrm{FLUX}_{15-18} + \mathrm{FLUX}_{19-20} + \mathrm{FLUX}_{21-22})\end{array}\right) \cdot \mathrm{dt}$	Mass in air compartment (kg)	---
$\mathrm{FLUX}_{08} = \mathrm{WATER} \cdot \mathrm{RATE}_{08}$	Water-air volatilization flux (kg d^{-1})	---
$\mathrm{FLUX}_{11-14} = \mathrm{AIR} \cdot (\mathrm{RATE}_{11} + \mathrm{RATE}_{12} + \mathrm{RATE}_{13} + \mathrm{RATE}_{14})$	Air-water diffusion and deposition flux (kg d^{-1})	---
$\mathrm{FLUX}_{15-18} = \mathrm{AIR} \cdot (\mathrm{RATE}_{16} + \mathrm{RATE}_{17} + \mathrm{RATE}_{18}) + \mathrm{RATE}_{15}$	Air-soil diffusion and deposition flux (kg d^{-1})	---
$\mathrm{FLUX}_{19-20} = \mathrm{AIR} \cdot (\mathrm{RATE}_{19} + \mathrm{RATE}_{20})$	Air-POL deposition flux (kg d^{-1})	---

Table S2. Equations used for calculation of rate constants, fluxes, and compartment masses.

Equation	Equation Description (Units)	Ref
$FLUX_{21-22} = AIR \cdot (RATE_{21} + RATE_{22})$	Air-leaf diffusion and deposition flux (kg d^{-1})	---
$FLUX_{23} = AIR \cdot RATE_{23}$	Air degradation flux (kg d^{-1})	---
$FLUX_{24} = SOIL \cdot RATE_{24}$	Soil-air volatilization flux (kg d^{-1})	---
$FLUX_{31} = POL \cdot RATE_{31}$	POL-air blow-off flux (kg d^{-1})	---
$FLUX_{35} = LEAF \cdot RATE_{35}$	Leaf-air diffusion flux (kg d^{-1})	---
Fish Compartment		
$FISH = FISH_{t-dt} + (FLUX_{37} - FLUX_{38}) \cdot dt$	Mass in fish compartment, single fish (kg)	---
$FLUX_{37} = (CWT \cdot BSF \cdot k1 \cdot WT_{fish} + C_{diet} \cdot kD \cdot WT_{fish}) \cdot 1 \times 10^{-12}$	Flux into fish (kg d^{-1})	*(10)*
$C_{diet} = CWT \cdot BSF \cdot KOW \cdot L_{diet} \cdot \beta_{fish}$	Concentration in fish diet (ng kg^{-1})	*(10)*
$k1 = 1 / \left((0.01 + (1/KOW)) \cdot \left(WT_{fish}^{\ 0.4} \right) \right)$	Gill uptake rate constant (L kg^{-1} d^{-1})	*(10)*
$kD = \left(0.02 \cdot WT_{fish}^{\ -0.15} \cdot \exp(0.06 \cdot TW) \right) / \left(5.1 \times 10^{-8} \cdot KOW + 2 \right)$	Dietary uptake rate constant (kg kg^{-1} d^{-1})	*(10)*
$BSF = 1 / \left(1 + \left(POC \cdot 1 \times 10^{-6} \cdot \psi_2 \cdot KOW \right) + \left(DOC \cdot 1 \times 10^{-6} \cdot \psi_3 \cdot KOW \right) \right)$	Bioavailable fraction of chemical (unitless)	*(17)*
$POC = PD_{ratio} \cdot DOC$	Concentration of particulate organic carbon (mg L^{-1})	*(10)*
$FLUX_{38} = FISH \cdot (k2 + kE + kG)$	Flux out of fish (kg d^{-1})	*(10)*
$k2 = k1 / (L_{fish} \cdot KOW)$	Elimination rate constant (d^{-1})	*(10)*
$kE = 0.125 \cdot kD$	Fecal egestion rate constant (d^{-1})	*(10)*
$kG = 5.02 \times 10^{-4} \cdot WT_{fish}^{\ -0.2}$	Growth rate constant (d^{-1})	*(10)*

Leaf Compartment

Table S2. Equations used for calculation of rate constants, fluxes, and compartment masses.

Equation	Equation Description (Units)	Ref
$LEAF = LEAF_{t-dt} + (FLUX_{30} + FLUX_{21-22} - FLUX_{34} - FLUX_{33} - FLUX_{35} - FLUX_{36}) \cdot dt$	Mass in leaf compartment (kg)	---
$FLUX_{30} = POL \cdot RATE_{30}$	POL-leaf diffusion flux (kg d^{-1})	---
$FLUX_{33} = LEAF \cdot RATE_{33}$	Leaf-soil litterfall flux (kg d^{-1})	---
$FLUX_{34} = LEAF \cdot RATE_{34}$	Leaf-POL diffusion flux (kg d^{-1})	---
$FLUX_{36} = LEAF \cdot RATE_{36}$	Leaf degradation flux (kg d^{-1})	---
Particle-on-Leaf (POL) Compartment		
$POL = POL_{t-dt} + (FLUX_{34} + FLUX_{19-20} - FLUX_{30} - FLUX_{31} - FLUX_{28-29} - FLUX_{32}) \cdot dt$	Mass in POL compartment (kg)	---
$FLUX_{28-29} = POL \cdot (RATE_{28} + RATE_{29})$	Leaf-soil wash-off and litterfall flux (kg d^{-1})	---
$FLUX_{31} = POL \cdot RATE_{31}$	POL-soil blow-off flux (kg d^{-1})	---
$FLUX_{32} = POL \cdot RATE_{32}$	POL degradation flux (kg d^{-1})	---
Sediment Compartment		
$SED = SED_{t-dt} + (FLUX_{05-06} - FLUX_{01} - FLUX_{02-03} - FLUX_{04}) \cdot dt$	Mass in sediment compartment (kg)	---
$FLUX_{01} = SED \cdot RATE_{01}$	Burial flux (kg d^{-1})	---
$FLUX_{02-03} = SED \cdot (RATE_{02} + RATE_{03})$	Sediment-water diffusion and re-suspension flux (kg d^{-1})	---
$FLUX_{04} = SED \cdot RATE_{04}$	Sediment degradation flux (kg d^{-1})	---
$FLUX_{05-06} = WATER \cdot (RATE_{05} + RATE_{06})$	Water-sediment diffusion and deposition flux (kg d^{-1})	---
Soil Compartment		
$SOIL = SOIL_{t-dt} + (FLUX_{15-18} - FLUX_{33} + FLUX_{28-29} - FLUX_{25-26} - FLUX_{24} - FLUX_{27}) \cdot dt$	Mass in soil compartment (kg)	---
$FLUX_{25-26} = SOIL \cdot (RATE_{02} + RATE_{03})$	Soil-water erosion and runoff flux (kg d^{-1})	---

Table S2. Equations used for calculation of rate constants, fluxes, and compartment masses.

Equation	Equation Description (Units)	Ref
$FLUX_{27} = SOIL \cdot RATE_{27}$	Soil degradation flux (kg d^{-1})	---
Water Compartment		
$WAT = WAT_{t-dt} + \begin{pmatrix} FLUX_{02-03} + FLUX_{11-14} + FLUX_{25-26} + FLUX_{38} \\ - FLUX_{05-06} - FLUX_{08} - FLUX_{09} - FLUX_{07} - FLUX_{37} \end{pmatrix} \cdot dt$	Mass in water compartment (kg)	---
$FLUX_{07} = (WATER/RATE_{07})$	River flow flux (kg d^{-1})	---
$FLUX_{09} = WATER \cdot RATE_{09}$	Water degradation flux (kg d^{-1})	---
MISCELLANEOUS CALCULATIONS		
$CWT = (WATER/VW) \cdot 1 \times 10^{9}$	Total concentration in water (ng L^{-1})	---
$CTA = (AIR/VA) \cdot 1 \times 10^{18}$	Total concentration in air (fg m^{-3})	---
$CST = SED/(VS \cdot CSS \cdot 1000) \cdot 1 \times 10^{9}$	Total concentration in sediment (µg kg^{-1})	---
$CSD = (CST/OC_{sed}/(KOW \cdot \psi))$	Concentration in sediment pore water (µg L^{-1})	---
$C_{soil} = (SOIL/(SA_{land} \cdot BD_{soil} \cdot 1000 \cdot (Zd/100))) \cdot 1 \times 10^{12}$	Total concentration in surface soil (ng kg^{-1})	---
$CB_{fish} = (FISH/WT_{fish}) \cdot 1 \times 10^{9}$	Concentration in fish (µg kg^{-1})	*(10)*
$CTV = ((LEAF/V_{leaf})/\rho_{leaf}) \cdot 1 \times 10^{15}$	Concentration in leaves (pg kg^{-1})	---
$SA_{forest} = SA_{land} \cdot ForestFrac$	Surface area of forested land (m^{2})	---
$SA_{land} = SA_{total} - SA_{water}$	Surface area of land (m^{2})	---
$SA_{nonforest} = SA_{land} \cdot (1 - ForestFrac)$	Surface area of non-forested land (m^{2})	---

[a] Equation corrected per conversation with the author.

Table S3. Summary of model input variables.

Variable	Description (units)	Value	Note / Ref
ψ	Organic carbon-water partition coefficient (unitless)	0.41 [(a)]	(*16*)
ψ_2	Particulate organic carbon proportionality constant (unitless)	0.35 [(a)]	Eq. 4 (*17*)
ψ_3	Dissolved organic carbon proportionality constant (unitless)	0.08	Eq. 4 (*17*), (*18*)
ρ_{area}	Above-ground vegetation biomass inventory (kg m^{-2})	2	Eq. 7-2 (*27*)
ρ_{leaf}	Density of leaves (kg m^{-3})	820	(*27*)
βfish	Overall food web biomagnification factor (unitless)	PCB-077: 2.75 PCB-118: 6.0 PCB-169: 2.75	Calibrated with the region-specific Gobas-type food web model (*10*)
ρ_P	Dust particle density (kg m^{-3})	1400	Eq. 7-2 (*27*)
ρ_{soil}	Solids particle density (g cm^{-3})	2.7	Table B-2-6 (*15*)
θ_V	Soil void fraction (unitless)	0.3	(*14*)
αVAF	Vegetation attenuation factor (m^2 kg^{-1})	2.9	Eq. 7-2 *(27)*
θ_W	Soil volumetric water content (ml cm^{-3})	0.2	Table B-2-6 (*15*)
A0	Cross section area coefficient (unitless)	0	(*11*)
A1	Cross section area coefficient (unitless)	5.86	(*11*)
A2	Cross section area coefficient (unitless)	0.69	(*11*)
AD	Active sediment depth (m)	0.03	Assumed maximum depth of chemically active zone
BD_{soil}	Soil bulk density (kg L^{-1})	1.5	Willamette soils data (*22*)
CSS	Concentration of solids in sediment (kg L^{-1})	0.4	Assumes a mean porosity of 0.83 and mean sediment density 2350 kg m^{-3}
DOC	Dissolved organic carbon concentration in water (mg L^{-1})	Graphical function	Time series water quality data from USGS gage 14211000 (RM 12.8)
ER	Particle enrichment ratio (unitless)	3	Table B-2-3 (*15*)
ForFrac	Fraction of land area covered by coniferous forest	0.7	NRCS data for the Willamette Valley (*32*)
fW_{leaf}	Water content of leaf (kg kg^{-1})	0.8	Eq. 7-2 *(27)*
AirHeight	Mixing height of air column (m)	5000	*(27)*
I_{wet}	Plant interception fraction of wet deposition (unitless)	0.2	*(27)*

Table S3. Summary of model input variables.

Variable	Description (units)	Value	Note / Ref
K_{litter}	Litterfall rate constant, conifers (d^{-1})	0.0021	*(27)*
$K_{POL\text{-}leaf}$	Transfer factor, POL to leaf compartment (d^{-1})	0.3	*(27)*
LAI	Leaf-area index (m^2 m^{-2})	9.3	*(29, 30)*
LAP	Thickness of air boundary layer (m)	0.001	Eq. 7-12 *(27)*
L_{diet}	Lipid content of fish diet (unitless)	0.01	*(10)*
LEN	River (main stem) length (m)	225,000	USGS watershed data
L_{fish}	Lipid content of fish (unitless)	0.05	Mean from *(31)*
OC_{sed}	Organic carbon content of bottom sediment (unitless)	0.0037	Willamette River Mercury TMDL (www.deq.state.or.us/lab/wqm/wb mercurystudy.htm, accessed June 2007)
OC_{soil}	Fraction of organic carbon in soil (unitless)	U(0.01, 0.03) [(b)]	(*22*)
OC_{sps}	Organic carbon content of suspended solids (unitless)	0.03	Appendix A (*15*)
OH	Hydroxyl (OH) radical concentration (molec cm^{-3})	Winter: 2×10^6 Spring: 0.8×10^6 Summer: 0.09×10^6 Fall: 0.8×10^6	Mean value in 2000 m surface layer at 45°N *(9)*
Q	Mean of daily mean flow (ft^3 s^{-1})	Graphical function	Time series flow data from USGS guage at Corvallis, Oregon
PD_{ratio}	Ratio of POC to DOC in water (unitless)	U(0.17, 0.36) [(b)]	Measured ratio of POC to DOC at Willamette RM 12.8
RO_{frac}	Fraction of precipitation becoming runoff (unitless)	0.4	(*24*)
SA_{total}	Land surface area (m^2)	2.90×10^{10}	USGS watershed data
Sn	Stomatal area (m^{-1})	200	Eq. 7-14 *(27)*
TA	Mean daily air temperature (°C)	Graphical function	Time series air temperature data from Corvallis, Oregon (Oregon State University), 1953-2006
TS	Mean daily maximum soil temperature at 2" depth (°C)	Graphical function	Time series soil temperature data from Hyslop Farm, Oregon, 1973-1984 (*25*)
TSP	Total suspended particulates (μg m^{-3})	Graphical function	Time series data for PM2.5 from ODEQ monitors in the Willamette Basin, 2003-2006

Table S3. Summary of model input variables.

Variable	Description (units)	Value	Note / Ref
TSS	Total suspended solids in water (mg L^{-1})	Function of flow	Relationship derived from USGS data collected at RM 12.8
TW	Water temperature (C°)	Graphical function	Time series water temperature data from USGS gauge at RM 84.1
UD	Dry deposition velocity (m d^{-1})	500	Default for dioxin in (*27*)
u(d)	Wind speed, average annual (m s^{-1})	3.81	Oregon Climate Service (Oregon State University): 1985 - 2005
UR	Daily mean rainfall (in)	Graphical function	Time series precipitation data from Corvallis, Oregon (Oregon State University), 1889-2006
VB	Sediment burial mass transfer coefficient (m d^{-1})	0.0	Assumption that burial in deep sediment unlikely in an active river
VD	Water-to-sediment mass transfer coefficient (m d^{-1})	0.0024	*(3)*
VSS	Suspended solids settling rate (m d^{-1})	1.1	Estimated assuming a mean sediment particle diameter of 4 μm and a mean sediment density of 2.65 g cm^{-3}
W1	River width coefficient 1 (unitless)	18.1	(*11*)
W2	River width coefficient 2 (unitless)	0.374	(*11*)
WT_{fish}	Body weight of fish (kg)	0.65	Mean from *(31)*
XE	Unit soil loss (kg km^{-2} d^{-1})	Graphical function	Value varies seasonally around a basin-wide annual average of ≈ 1480, based on observations in *(32, 35, 36)*
Z_d	Soil depth (cm)	2	Table B-2-3 (*15*)

[a] These values should be the same (see Karichoff *(39)* or Seth *(40)*). Their disparity reflects that between the original publications cited.
[b] U(LB, UB) = Lower (LB) and upper (UB) bounds of a uniform random variable. When data suggest a range of values, but no distributional information is provided, a uniform distribution is the most parsimonious way to represent this range.

Table S4. Summary of available Willamette Basin congener-specific PCB data, and data sources, by media type.

Congener	ENVIRONMENTAL MEDIA						
	Air [(a)]	Surface Soil [(b)]	Terrestrial Vegetation	Surface Water [(c,g)]	Bed Sediment [(c,g)]	Suspended Sediment [(d)]	Fish [(e,f,g)]
008	---	ub	---	ph	ub	lb	---
018	---	ub	---	ph[018/030]	ub, ph	lb	ph[018/030]
077	ub	ub	---	ph	ph	lb	lb, ph
101	---	ub	---	---	ub	lb	lb, ph
105	ub	ub	---	ph	ph	lb	lb, ph
110	---	ub	---	ph[110/115]	ub, ph	lb	ph[110/115]
118	ub	ub	---	ph	ph[106/118]	lb	---
126	ub	ub	---	ph	ph	---	ph, lb
128	---	ub	---	ph[128/166]	ub, ph[128/162]	---	lb, ph[128/166]
153	---	ub	---	ph[153/168]	ub, ph	lb	lb, ph
156	ub	ub	---	---	ph	---	lb, ph
157	ub	ub	---	---	ph	---	---
169	ub	ub	---	---	ph	---	lb, ph
∑PCB	---	---	---	ub	---	---	lb, ph

<u>Sampling Locations</u>
ub Upper Basin (> RM 26.5)
lb Lower Basin (< RM 26.5, ~RM 12.8)
ph Portland Harbor Superfund site (RM 3.5-9.5)

[(a)] Cleverly et al. (*19*); [(b)] U.S. EPA (*20*); [(c)] Villeneuve et al. (*21*); [(d)] Morace (*26*); [(e)] Sethajintanin et al. (*33*); [(f)] Henny et al. (*31*); [(g)] LWG (*38*)

Figure S1

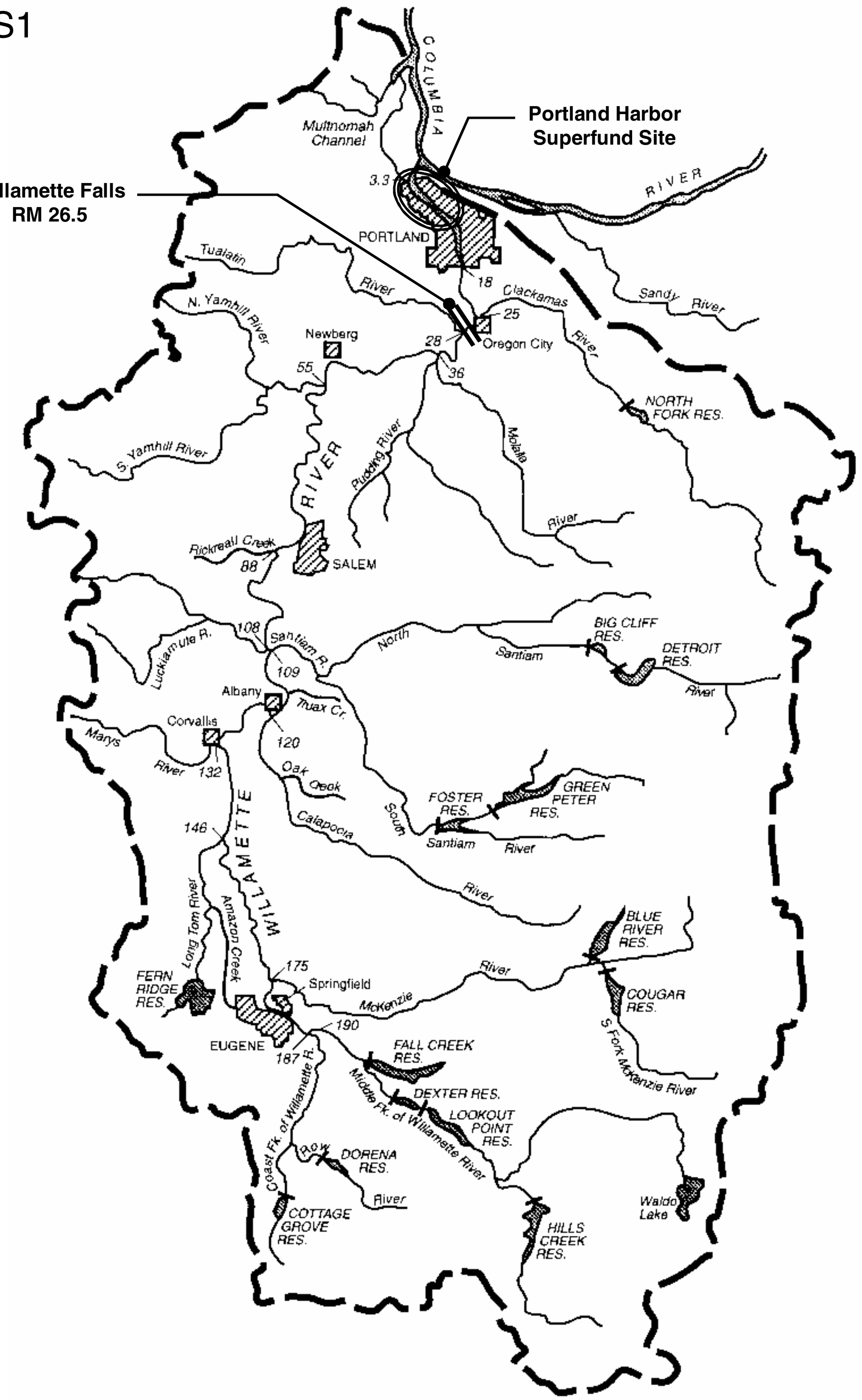

Portland Harbor
Superfund Site
Willamette Falls
RM 26.5
COLUMBIA
RIVER
Multnomah
Channel
3.3
PORTLAND
18
Clackamas
River
25
Oregon City
28
36
Sandy
River
Tualatin
River
N. Yamhill River
Newberg
55
NORTH
FORK RES.
Molalla
River
Pudding River
S. Yamhill River
RIVER
Rickreall Creek
88
SALEM
108
Santiam R.
109
North
Santiam
River
BIG CLIFF
RES.
DETROIT
RES.
Luckiamute R.
Albany
Truax Cr.
Corvallis
120
Marys
River
132
Oak
Creek
South
FOSTER
RES.
GREEN
PETER
RES.
Santiam
River
Calapooia
River
146
WILLAMETTE
Long Tom River
Amazon Creek
BLUE
RIVER
RES.
175
Springfield
River
McKenzie
COUGAR
RES.
FERN
RIDGE
RES.
EUGENE
187
190
FALL CREEK
RES.
DEXTER RES.
LOOKOUT
POINT
RES.
S Fork McKenzie River
Coast Fk. of Willamette R.
Middle Fk. of Willamette River
Row
DORENA
RES.
River
COTTAGE
GROVE
RES.
HILLS
CREEK
RES.
Waldo
Lake

Figure S2

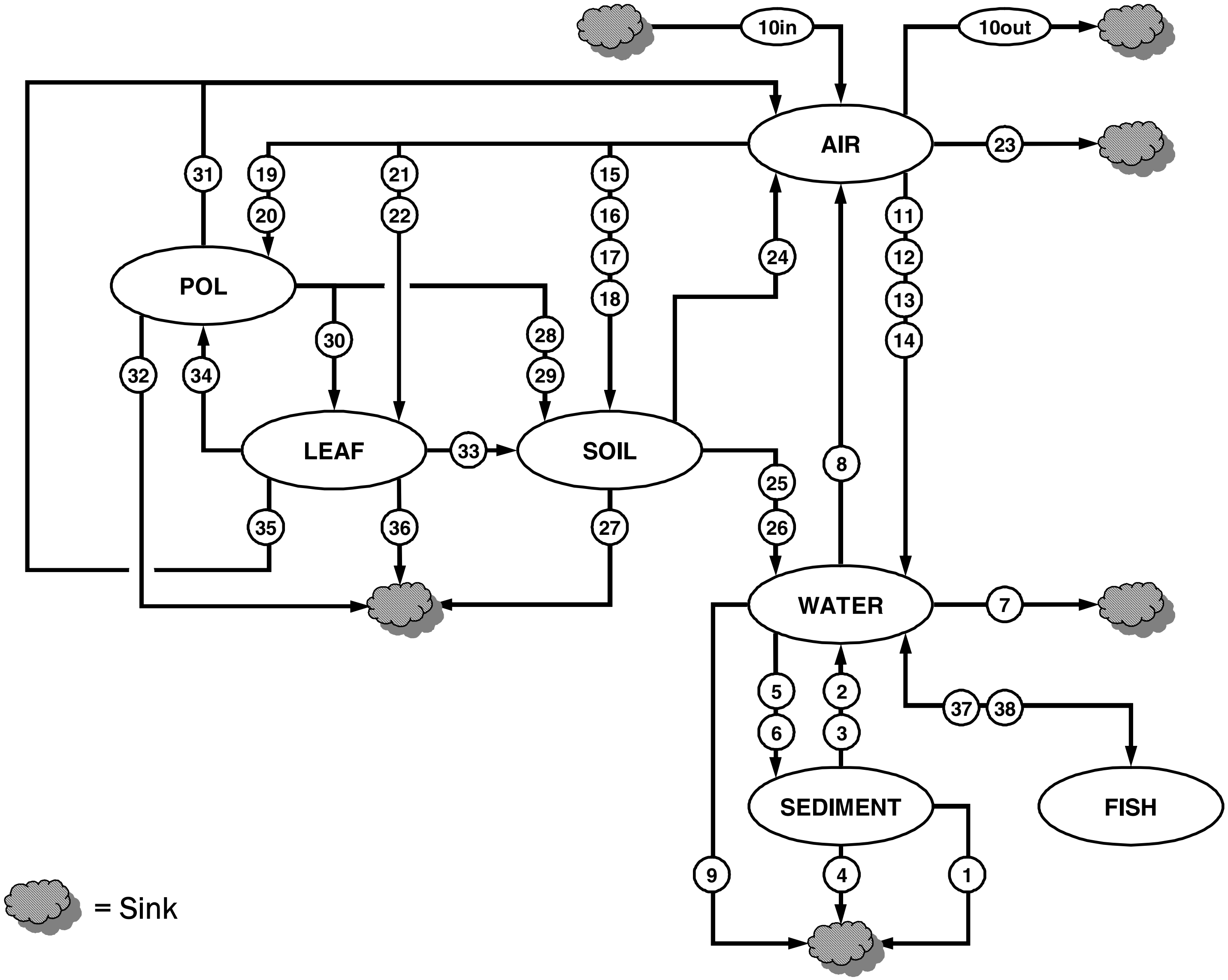

10in
10out
AIR
23
31
19
20
21
22
15
16
17
18
24
11
12
13
14
POL
30
28
29
32
34
LEAF
33
SOIL
8
25
26
35
36
27
WATER
7
5
6
2
3
37
38
SEDIMENT
FISH
9
4
1
= Sink

Figure S2. Schematic representation of the environmental compartments and chemical fate processes in the model and list of fluxes.

[1] Sediment Burial

[2] Sediment to Water via Diffusion

[3] Sediment to Water via Resuspension

[4] Sediment Degradation

[5] Water to Sediment via Diffusion

[6] Water to Sediment via Deposition

[7] River Flow

[8] Water to Air via Volatilization

[9] Water Degradation

[10in] Advective Inflow

[10out] Advective Outflow

[11] Air to Water via Diffusion

[12] Air to Water via Dry Particulate Deposition

[13] Air to Water via Wet Particulate Deposition

[14] Air to Water via Wet Gaseous Deposition

[15] Air to Soil via Diffusion

[16] Air to Soil via Dry Particulate Deposition

[17] Air to Soil via Wet Particulate Deposition

[18] Air to Soil via Wet Gaseous Deposition

[19] Air to Particles-on-Leaf (POL) via Dry Particulate Deposition

[20] Air to POL via Wet Particulate Deposition

[21] Air to Leaf via Diffusion

[22] Air to Leaf via Wet Gaseous Deposition

[23] Air Degradation

[24] Soil to Air via Volatilization

[25] Soil to Water via Particulate Erosion

[26] Soil to Water via Dissolved Runoff

[27] Soil Degradation

[28] POL to Soil via Wash-off

[29] POL to Soil via Litter-fall

[30] POL to Leaf via Diffusion

[31] POL to Air via Blow-off

[32] POL Degradation

[33] Leaf to Soil via Litter-fall

[34] Leaf to POL via Diffusion

[35] Leaf to Air via Diffusion

[36] Leaf Degradation

[37] Water to Fish via Uptake

[38] Fish to Water via Excretion

Figure S3

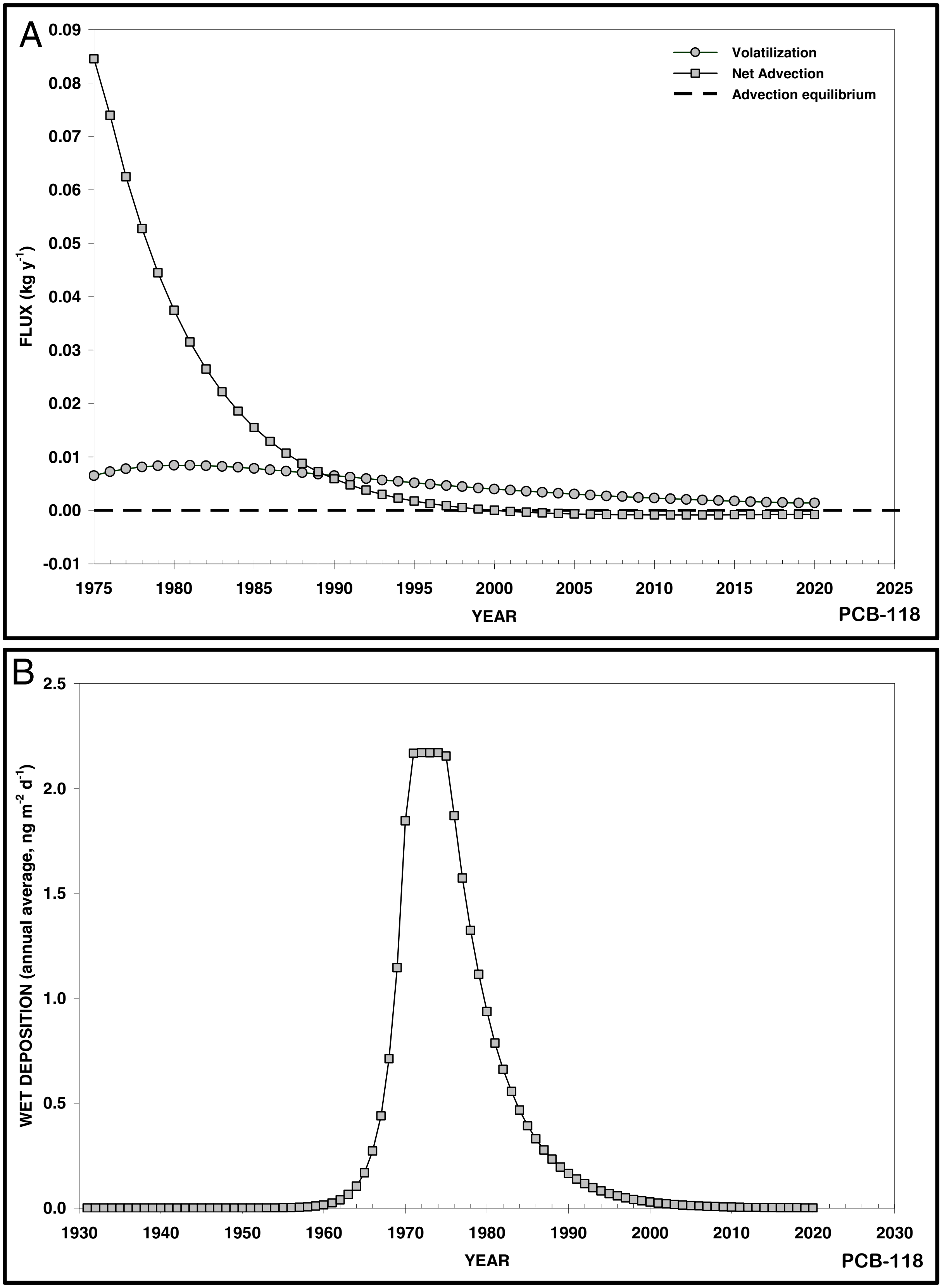
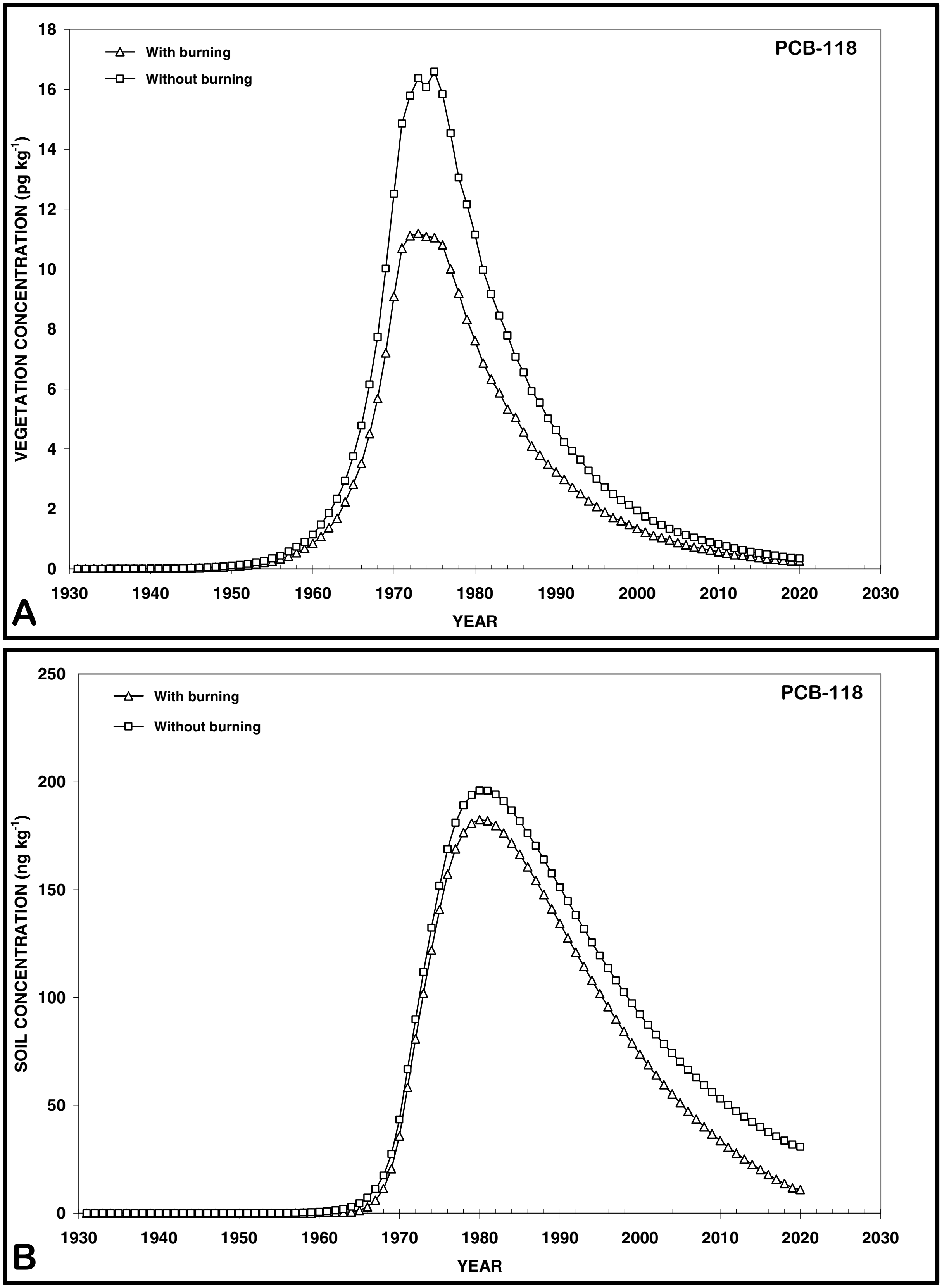
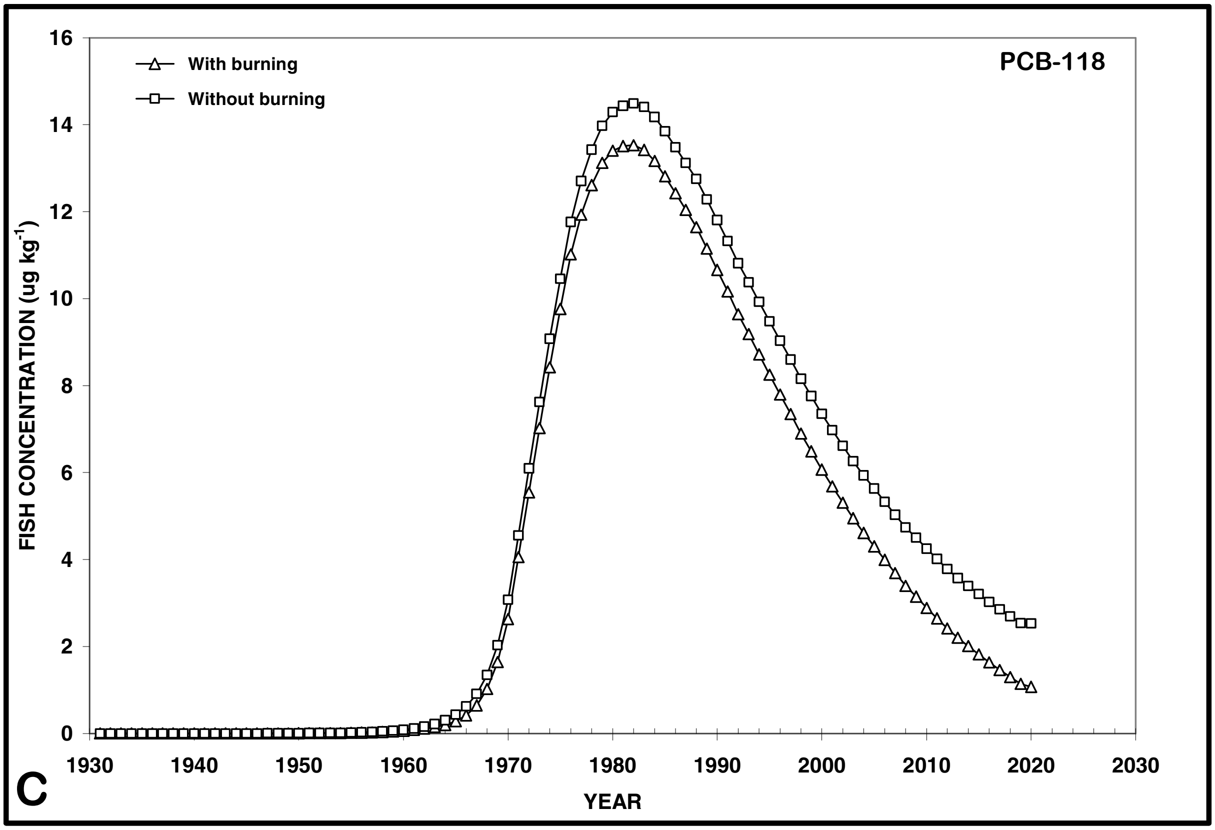

A
Volatilization
Net Advection
Advection equilibrium
FLUX (kg y^{-1})
YEAR
PCB-118
B
WET DEPOSITION (annual average, ng m^{-2} d^{-1})
YEAR
PCB-118

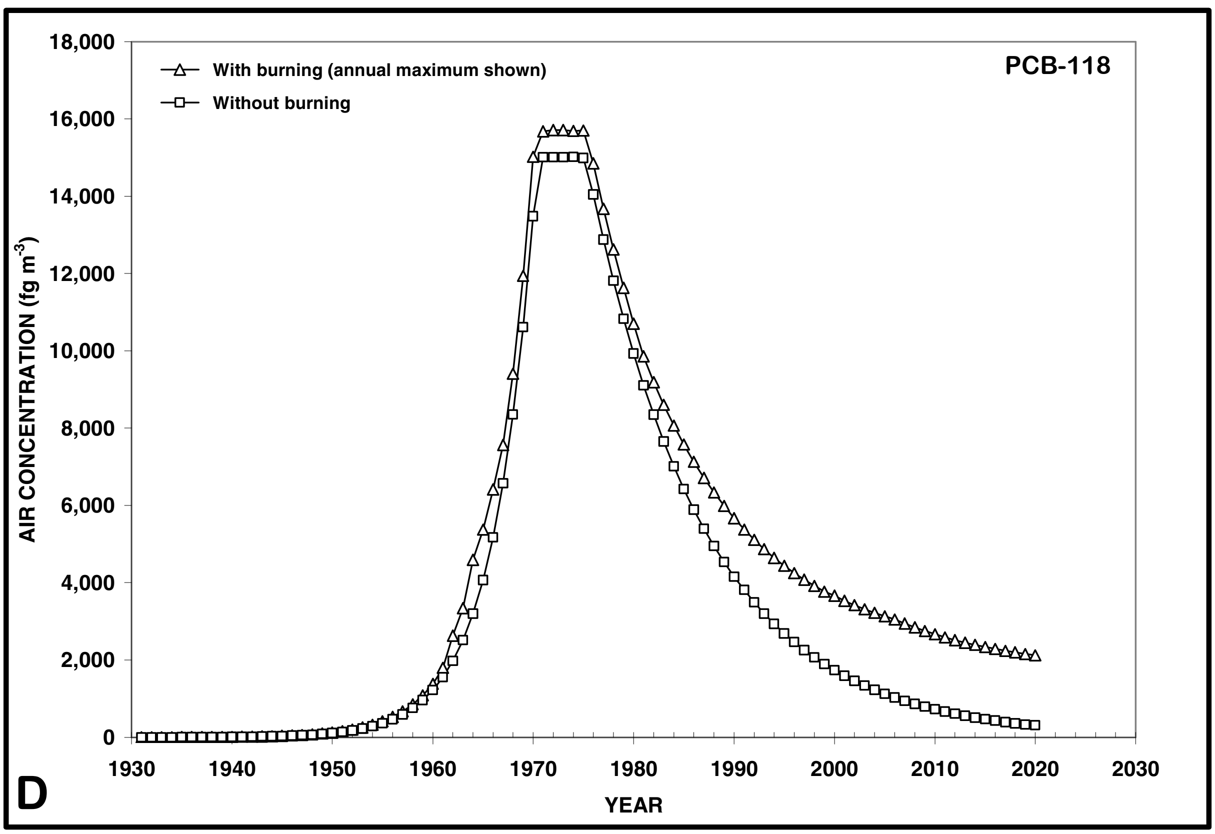
Figure S4



With burning
Without burning
PCB-118
VEGETATION CONCENTRATION (pg kg^{-1})
YEAR
A
With burning
Without burning
PCB-118
SOIL CONCENTRATION (ng kg^{-1})
YEAR
B

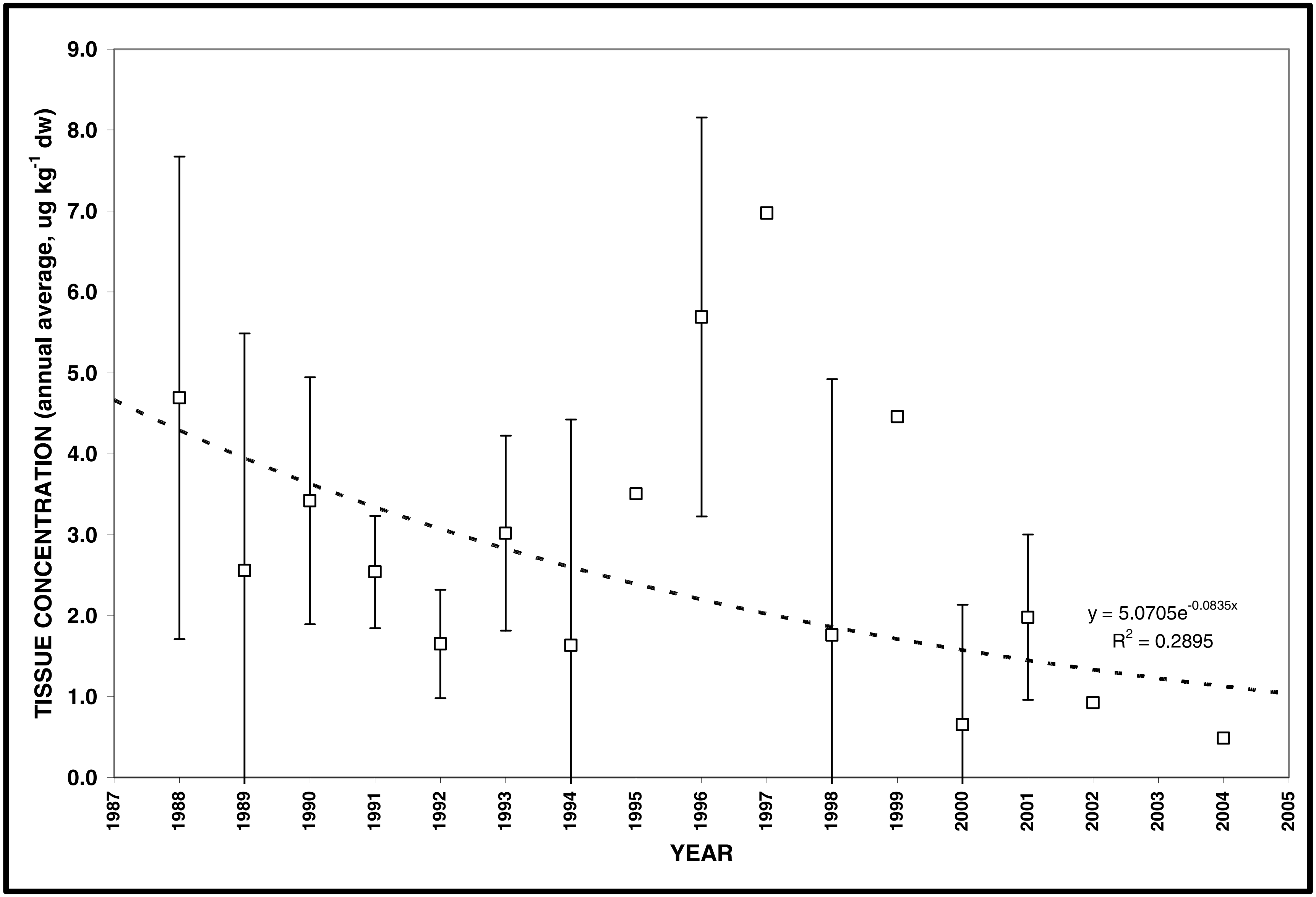


16
14
12
10
8
6
4
2
0
FISH CONCENTRATION (ug kg-1)
With burning
Without burning
PCB-118
1930
1940
1950
1960
1970
1980
1990
2000
2010
2020
2030
YEAR
C



18,000
16,000
14,000
12,000
10,000
8,000
6,000
4,000
2,000
0
AIR CONCENTRATION (fg m-3)
With burning (annual maximum shown)
Without burning
PCB-118
1930
1940
1950
1960
1970
1980
1990
2000
2010
2020
2030
YEAR
D

Figure S5


9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
TISSUE CONCENTRATION (annual average, ug kg-1 dw)
1987
1988
1989
1990
1991
1992
1993
1994
1995
1996
1997
1998
1999
2000
2001
2002
2003
2004
2005
YEAR
y = 5.0705e-0.0835x
R2 = 0.2895

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