

Atmospheric Toxics Webinar Series
Great Lakes Air Deposition Program
November 30, 2010

Development and Application of a Multi-media Screening Model for Chemicals of Emerging Concern in the Great Lakes Basin (GLMOD)

J.V. DePinto, Todd M. Redder


H. Tao, C.L. Turner

LimnoTech, Ann Arbor, MI


D.L. Swackhamer, D.L. Carlson

Environmental Health Sciences, University of Minnesota

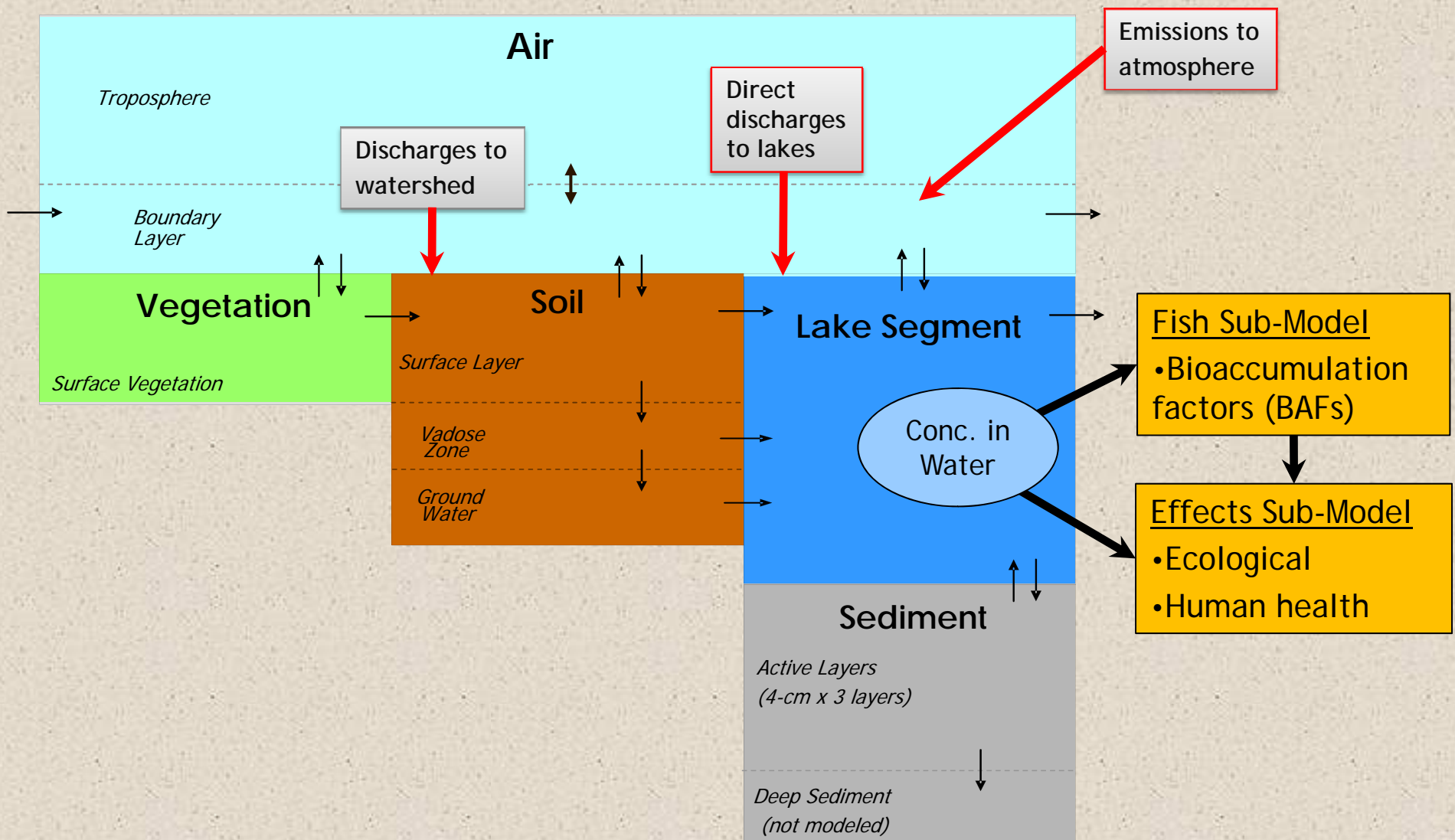
Presentation Outline

- 
- Project Objectives and Overview
 - GLMOD development
 - Conceptual model
 - Configuration to Great Lakes
 - Object-oriented approach
 - Historical PCB field testing (6 congeners)
 - Loads & boundary conditions
 - Model-data comparisons
 - Diagnostic simulations to demonstrate value of GLMOD
 - PCB congeners
 - PBDE congeners
 - Summary

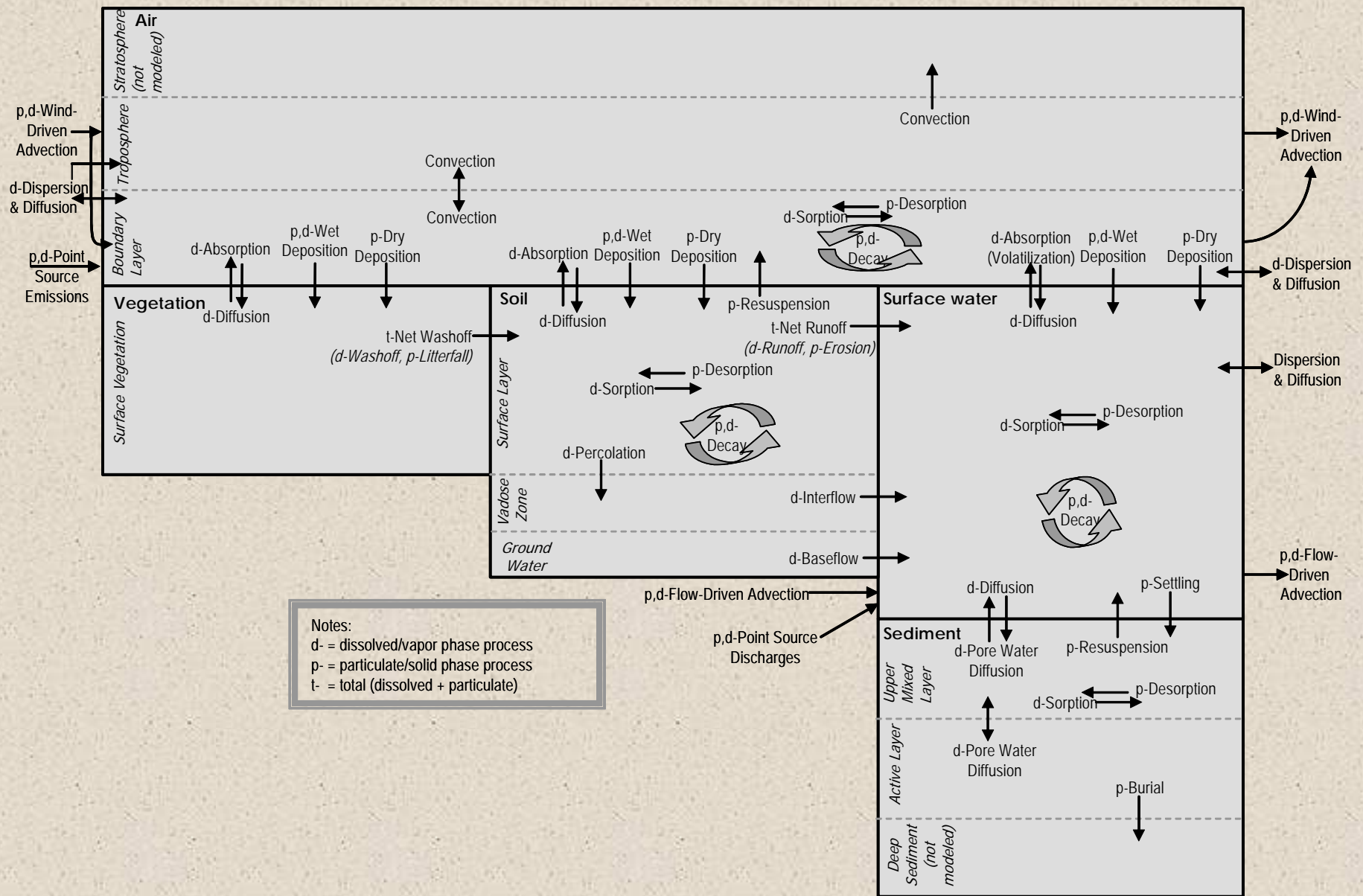
GLMOD Project Objectives

- 
- Develop a physically-based, multi-media, time-dependent model to support assessment and management of chemicals of emerging concern in Great Lakes Basin
 - Tier 2 screening model
 - Establish quantitative source-receptor relationships
 - Identify critical source areas
 - Compare potential exposure pathways
 - Identify locations of highest exposure and risk
 - Evaluate temporal trends
 - Assist in prioritizing research and monitoring programs

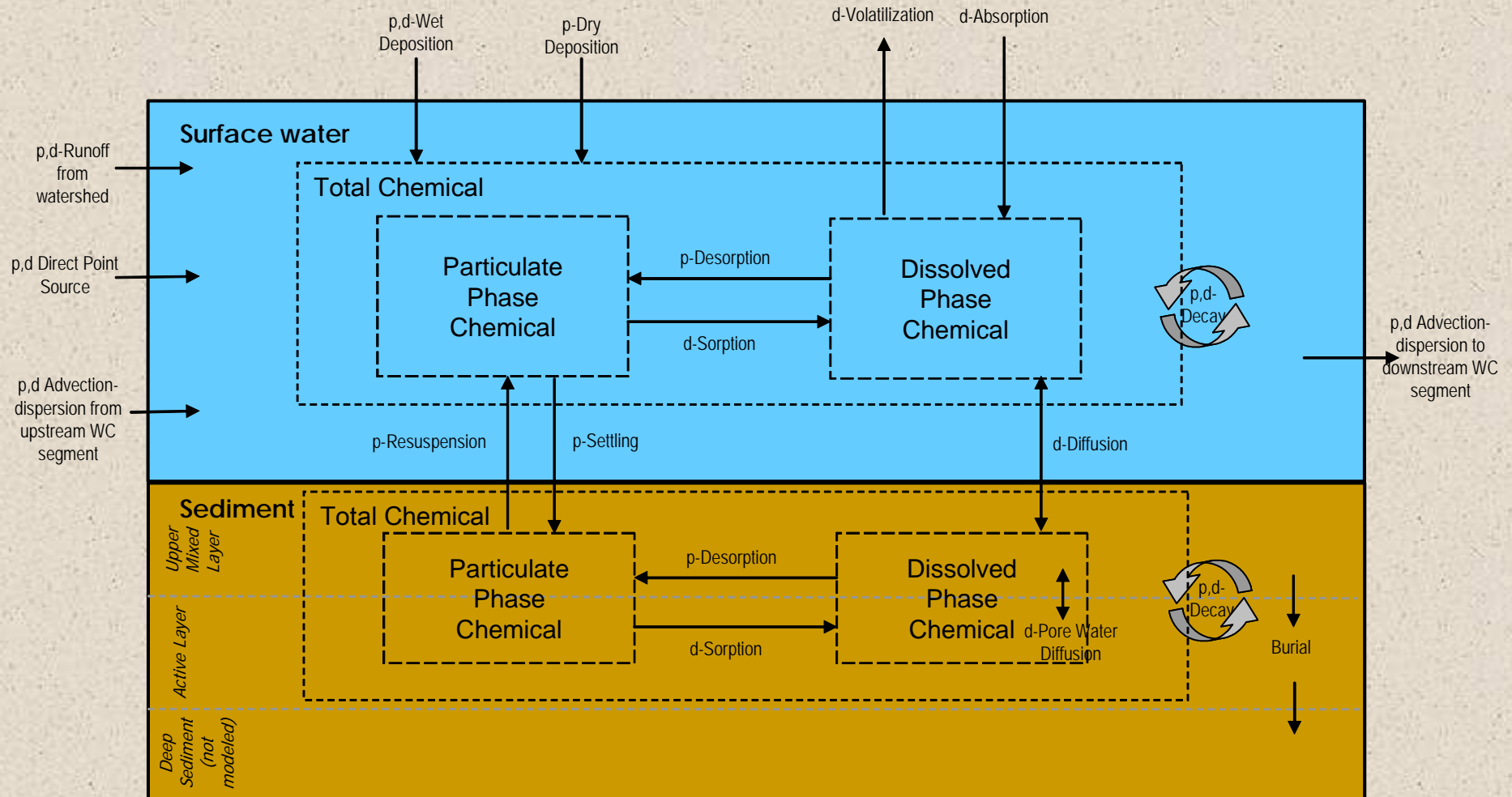
GLMOD Compartments and Inter-Media Pathways



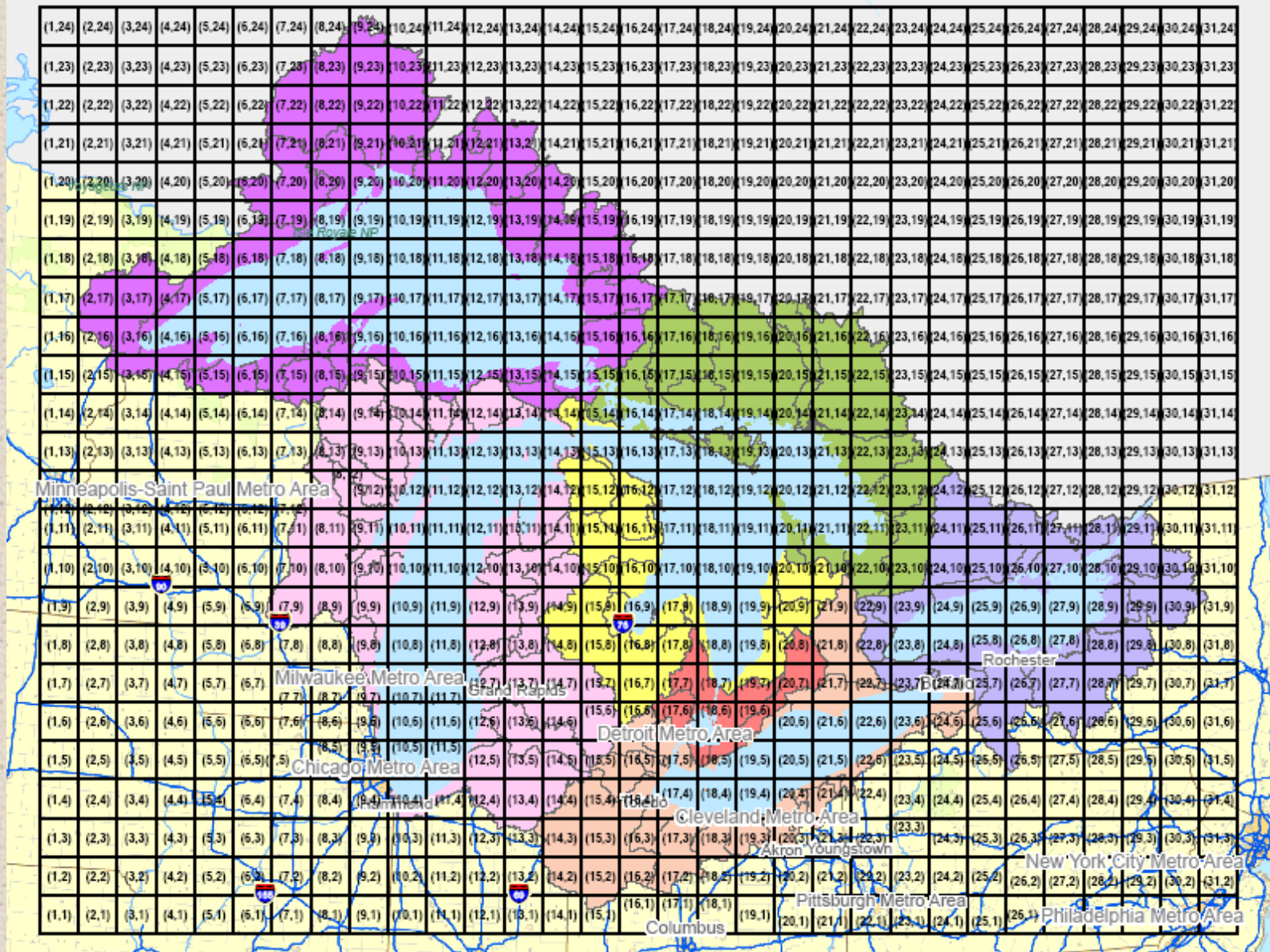
Schematic diagram of GLMOD intra- and inter-compartmental processes



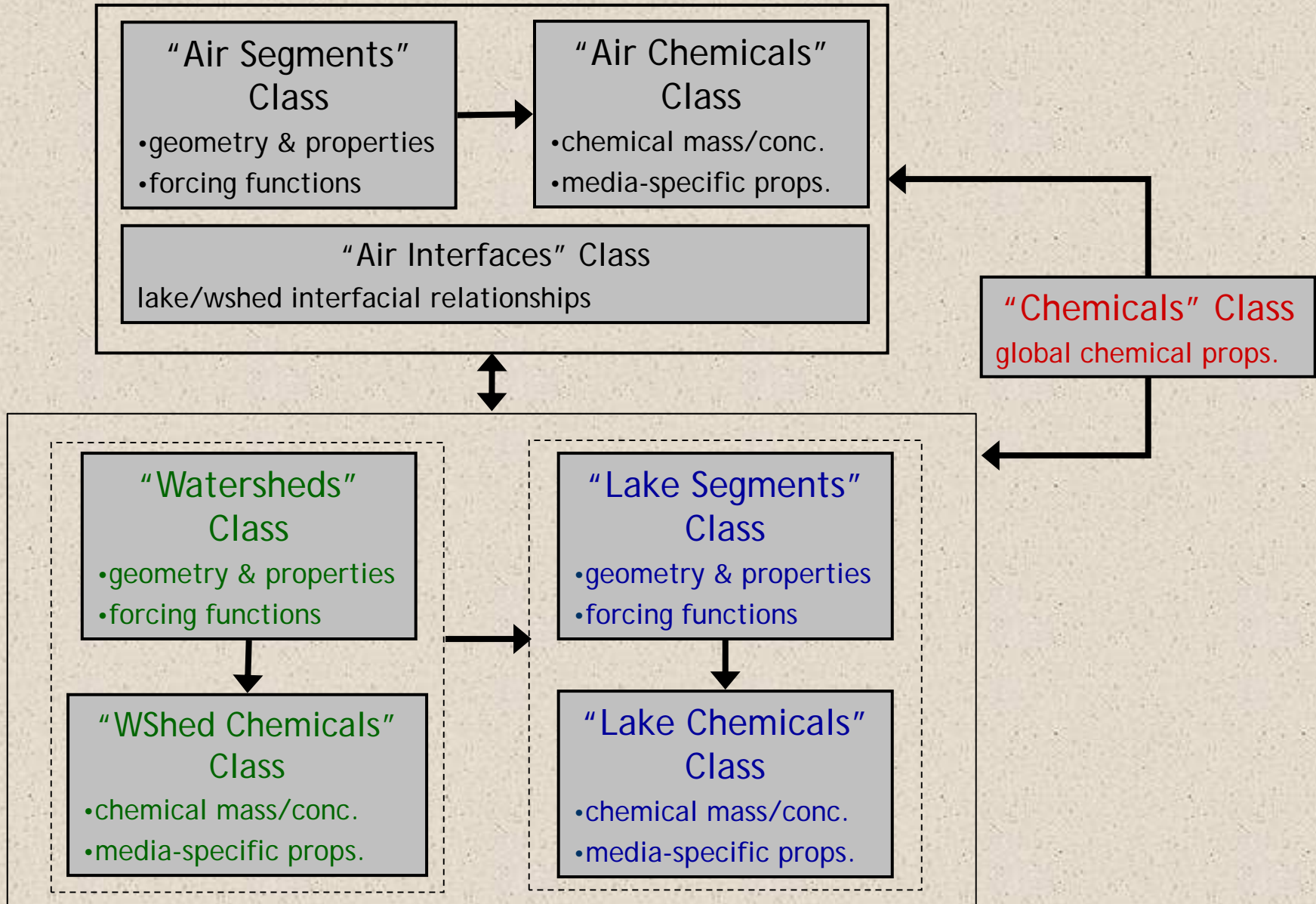
Conceptual mass balance diagram for surface water/sediment compartments



GLMOD Segmentation: Air, Water, & Land



GLMOD Implementation - Object Model



GLMOD Development and Field Testing

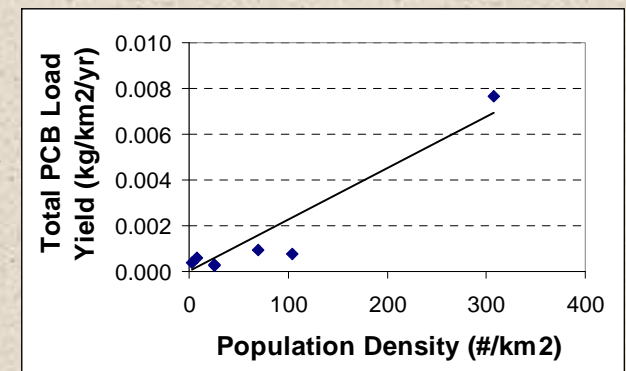
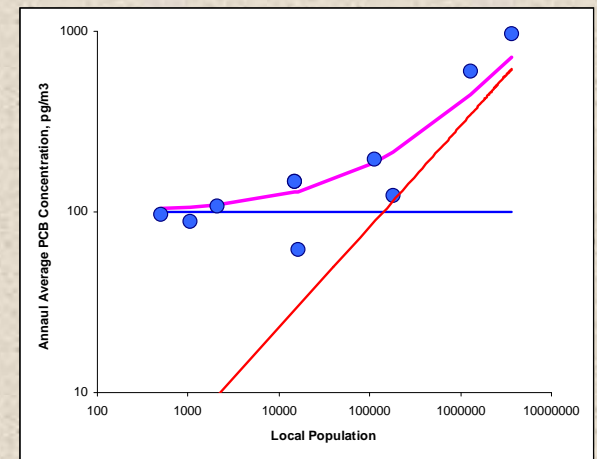
■ Field test model using six PCB congeners:

- Wealth of historical PCB data (e.g., Hornbuckle, et al. 2005)
- Use PCB congeners as “tracers” for constraining inter- and intra-media transfer/transport rates
- Diagnostic analysis of transport, fate, and bioaccumulation as function of chemical properties and basin geography

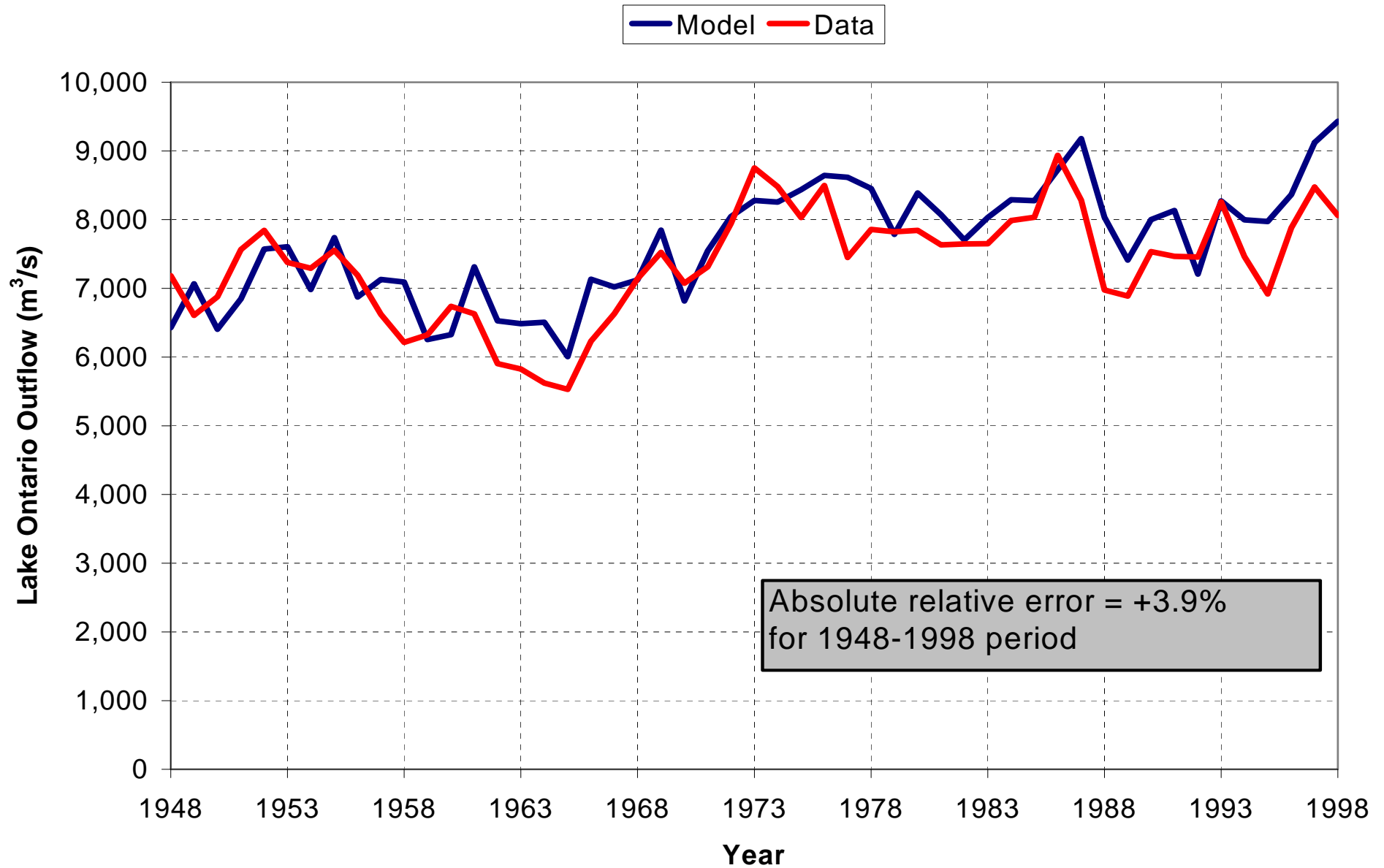
<i>Congener</i>	<i>Substitution Pattern</i>	<i># Chlorines</i>	<i># ortho Chlorines</i>	<i>Molecular Mass (g/mol)</i>	<i>Molar Volume (cm³/mol)</i>	<i>Henry's Law Constant K_H (Pa m³/mol)</i>	<i>Enthalpy of K_H (kJ/mol)</i>	<i>Octanol-Water Partitioning (log K_{ow})</i>	<i>Enthalpy of K_{ow} (kJ/mol)</i>	<i>Organic Carbon Partitioning (log K_{oc})</i>
PCB 18	2,2',5	3	2	257.55	230.1	38	35	5.31	25	4.86
PCB 52	2,2',5,5'	4	2	291.99	247.6	35	31	5.79	20	5.35
PCB 118	2,3',4,4',5	5	1	326.44	265.1	10	50	6.64	20	6.23
PCB 180	2,2',3,4,4',5,5'	7	2	395.33	300.1	12	144	7.28	10	6.89
PCB 201	2,2',3,3',4,5',6,6'	8	4	429.77	317.6	16	145	7.34	5	6.95
PCB 206	2,2',3,3',4,4',5,5',6	9	3	464.22	335.1	10	191	7.97	0	7.60

Historical PCB Field Test Simulation

- 6 congeners (18, 52, 118, 180, 201, 206)
- Historical simulation of PCB washout (1980-1999)
- Air emission loading:
 - Population, yield-based load
 - Seasonal variations, 13% / year decline
- Tributary loading:
 - Population, yield-based load
 - based primarily on LMMBS data
 - Exponential decline of 15% / year
 - "Hot spots" represented with higher yield coefficients (e.g., Fox River)

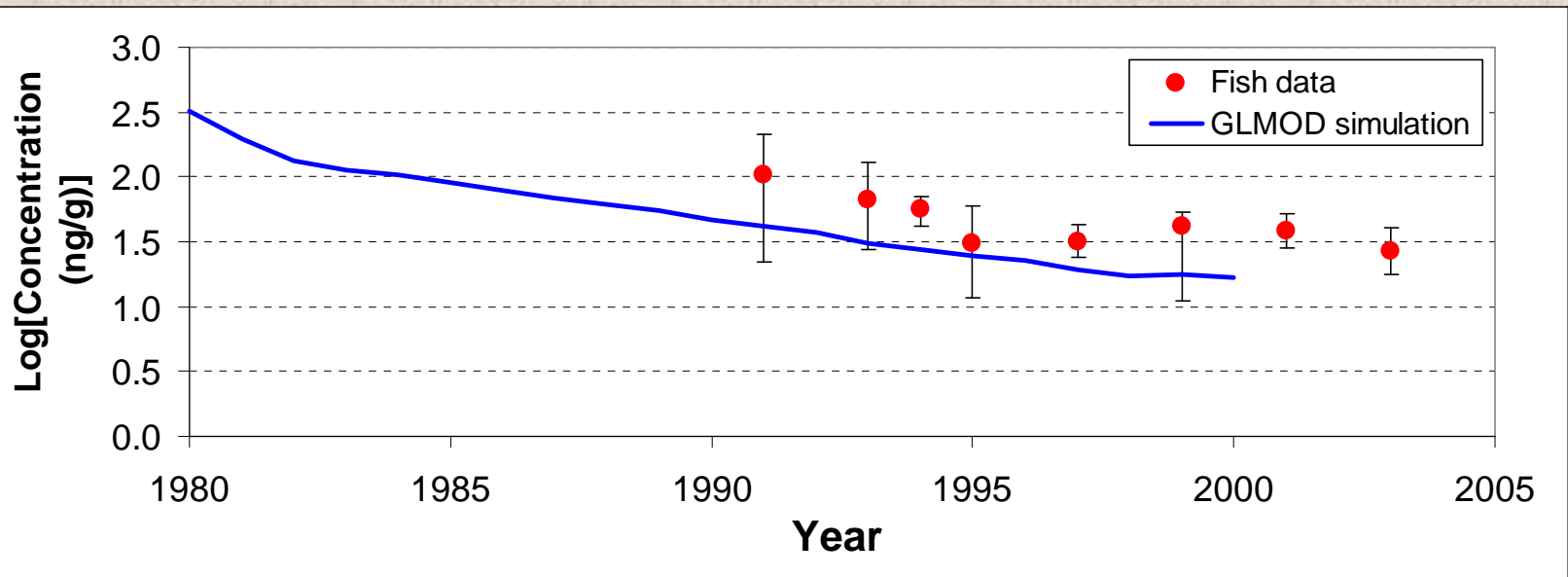


Results of Basin Hydrology Sub-model

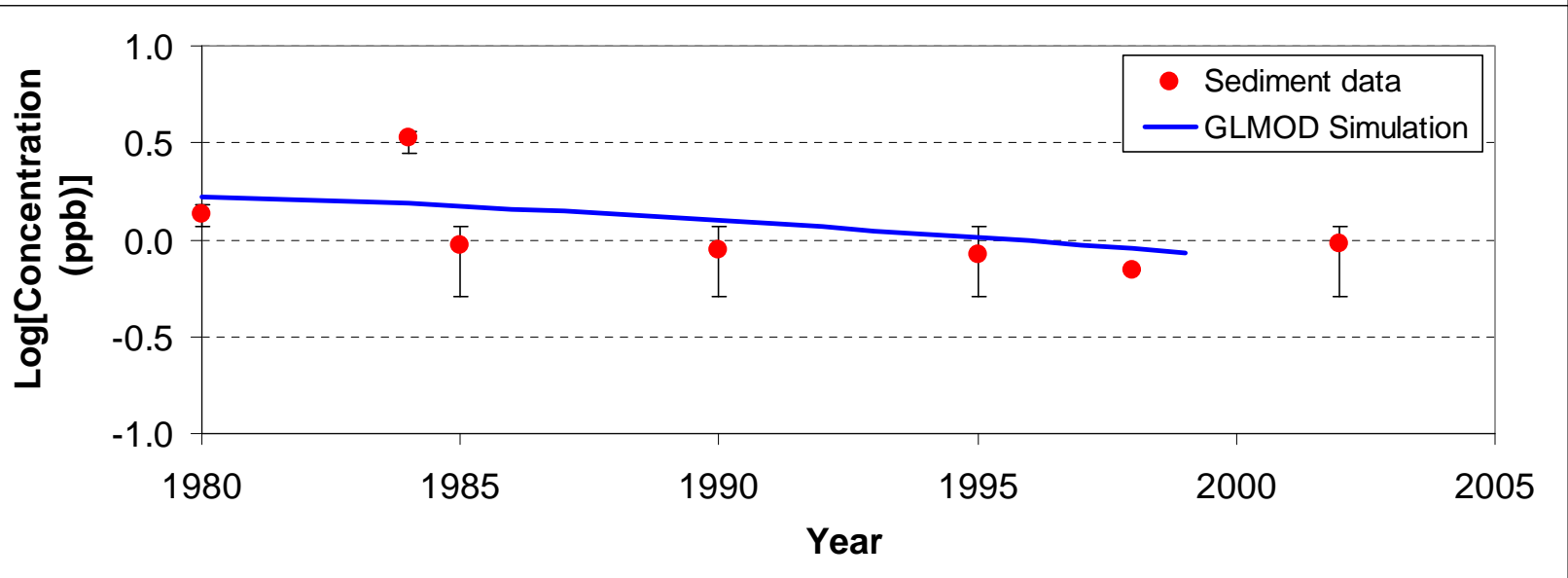


PCB Hindcast Field Test Results: Lake Michigan (south): Congener 52

Fish Results

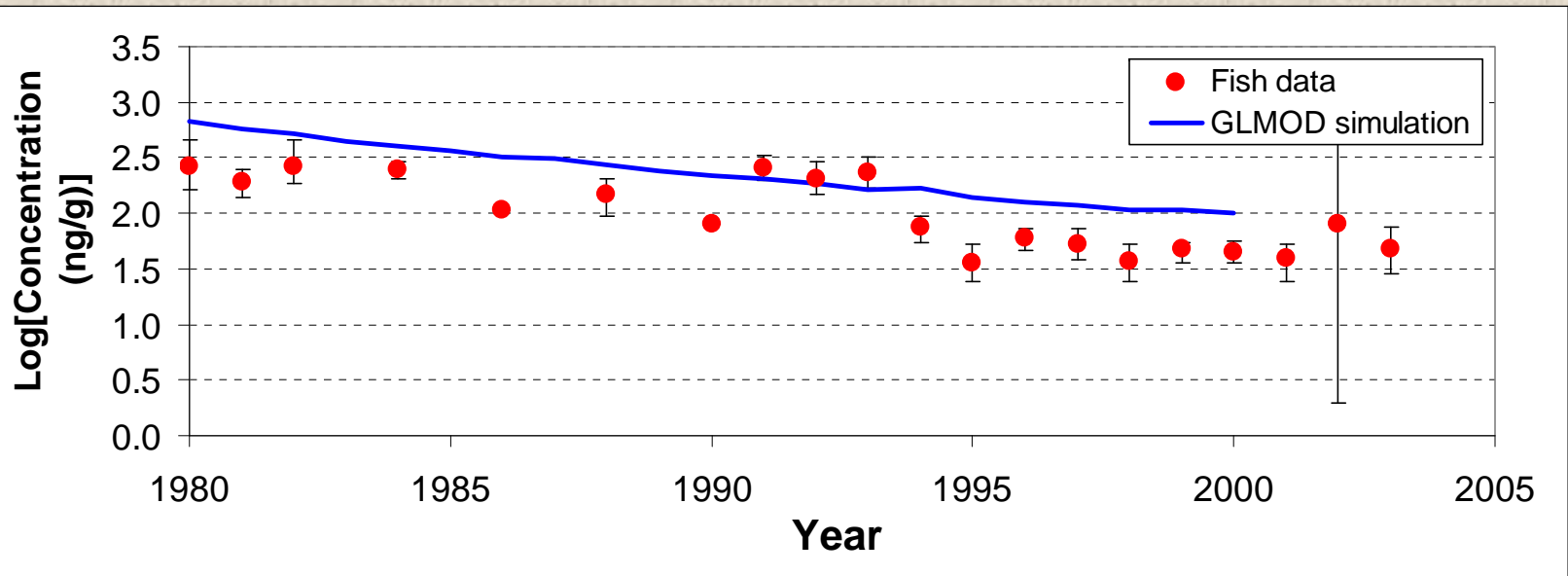


Sediment Results

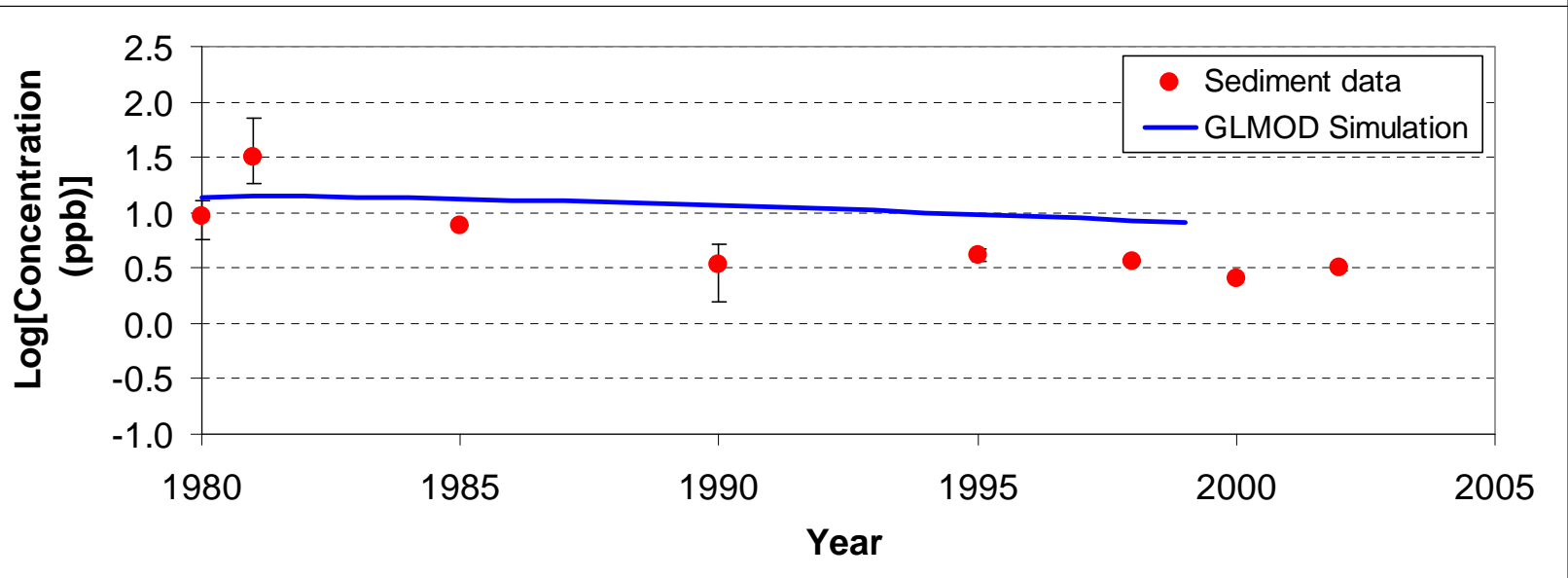


PCB Hindcast Field Test Results: Lake Ontario: Congener 118

Fish Results



Sediment Results



Diagnostic Model Analysis Demonstrates:

- Quantifying the relative distribution of chemicals among media (air, water, sediment, fish, etc.) and specific geographic segments (e.g., Lake Michigan northern basin);
- Quantifying the residence time of chemicals in various Great Lakes media and segments;
- Quantifying the potential for long-range transport of chemicals from their release point;
- Identifying the geographic location of exposure “hotspots”; and
- Quantifying the rate of change of chemical concentrations in fish, water, and air once air emissions or land-based loadings have changed.



PCB Diagnostic Simulations

■ Diagnostic Simulations

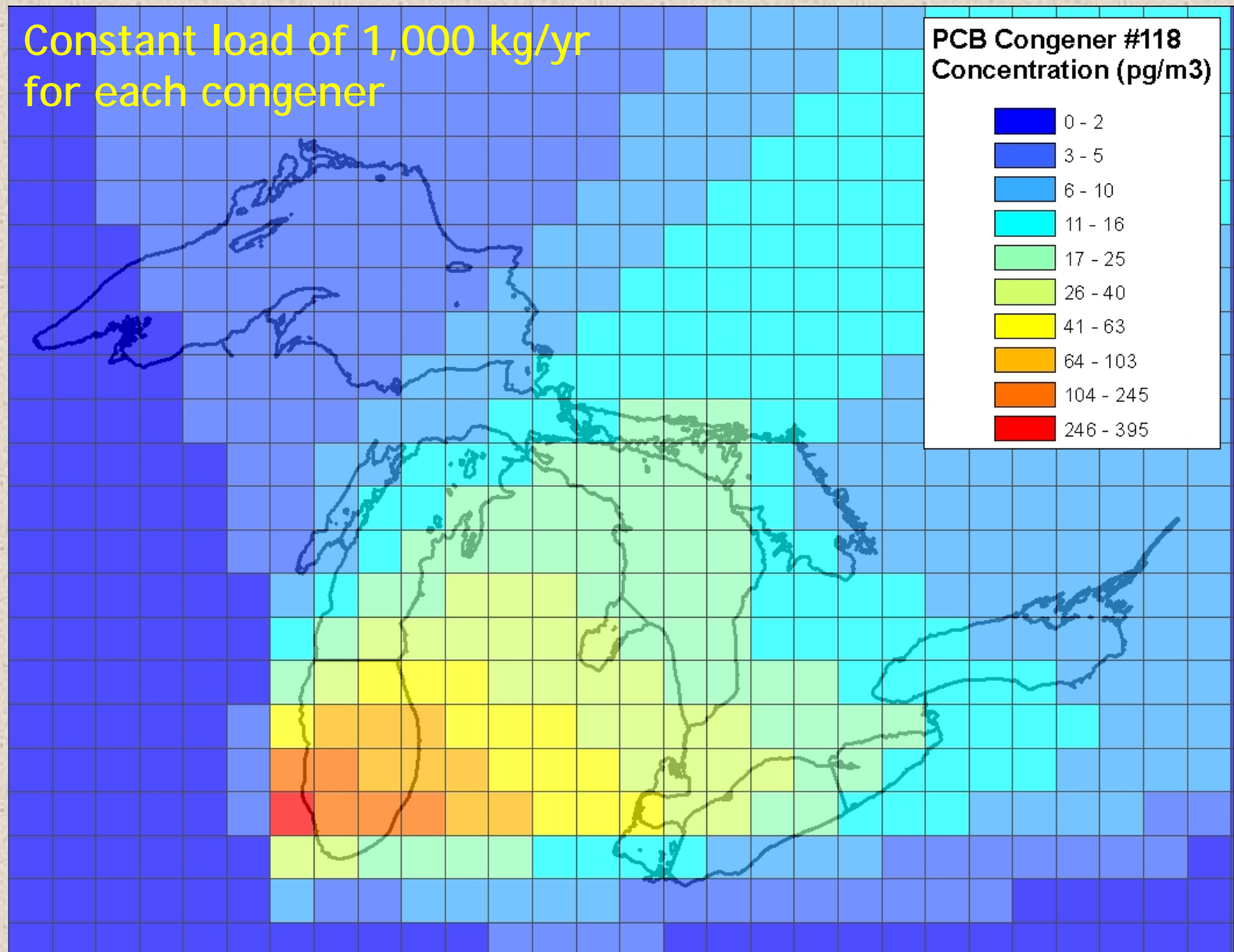
- Diagnostic #1: Constant emission loading of 1,000 kg/yr (for each PCB congener) to the air segment above the Chicago metropolitan area for a 20-year period;
- Diagnostic #2: Constant emission loading of 1,000 kg/yr (for each PCB congener) to the air segment above the Detroit metropolitan area for a 20-year period; and
- Diagnostic #3: Constant loading of 1,000 kg/yr (for each PCB congener) from the Fox River basin to Green Bay.

- Each diagnostic simulates all six PCB congeners in all media for a 20 year period with zero initial conditions



Diagnostic #1: Emission to air over Chicago Air Simulation Results (July - year 20)

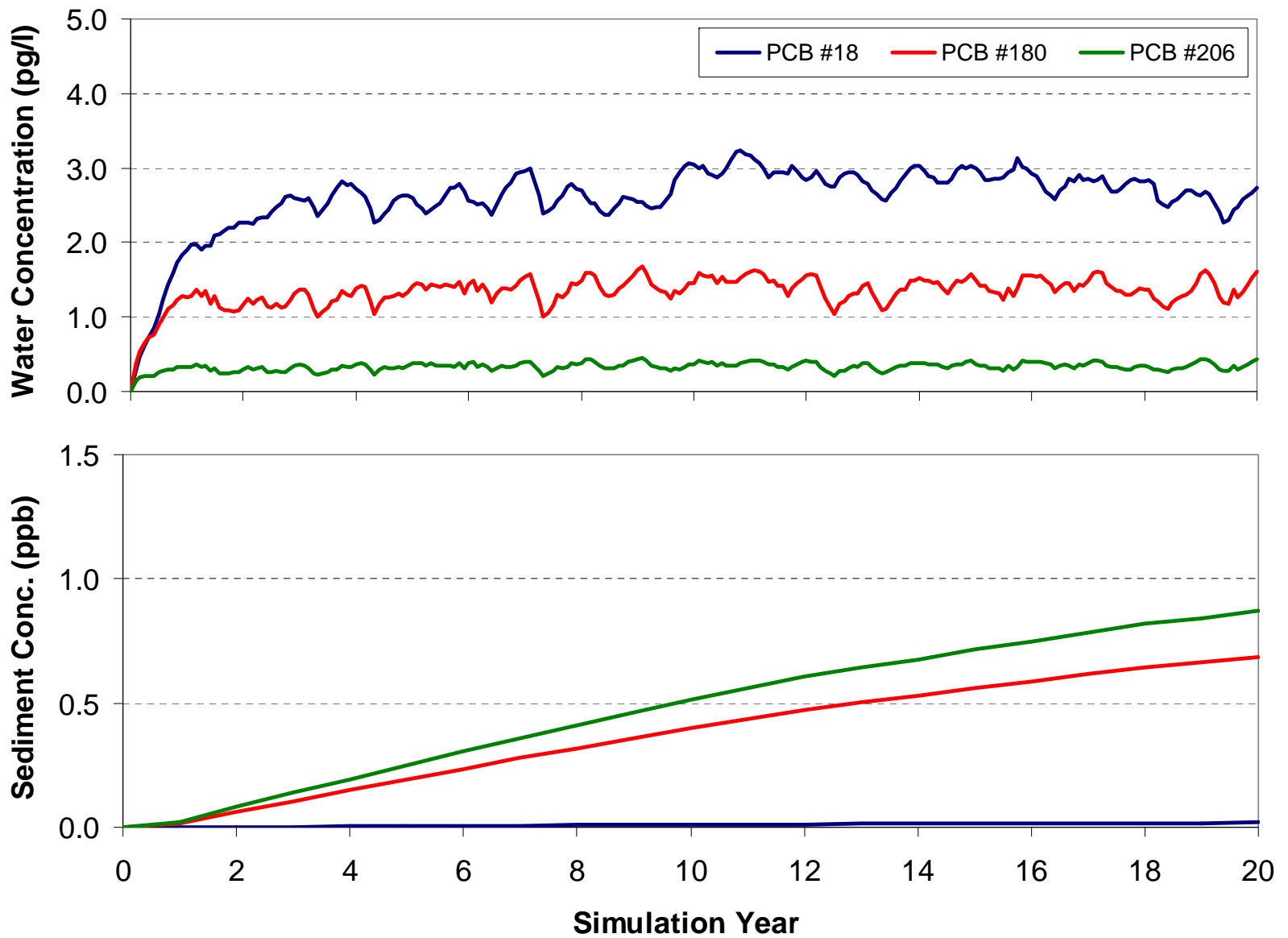
Constant load of 1,000 kg/yr
for each congener



Diagnostic #1: Emission to air over Chicago Lake Michigan (south) results

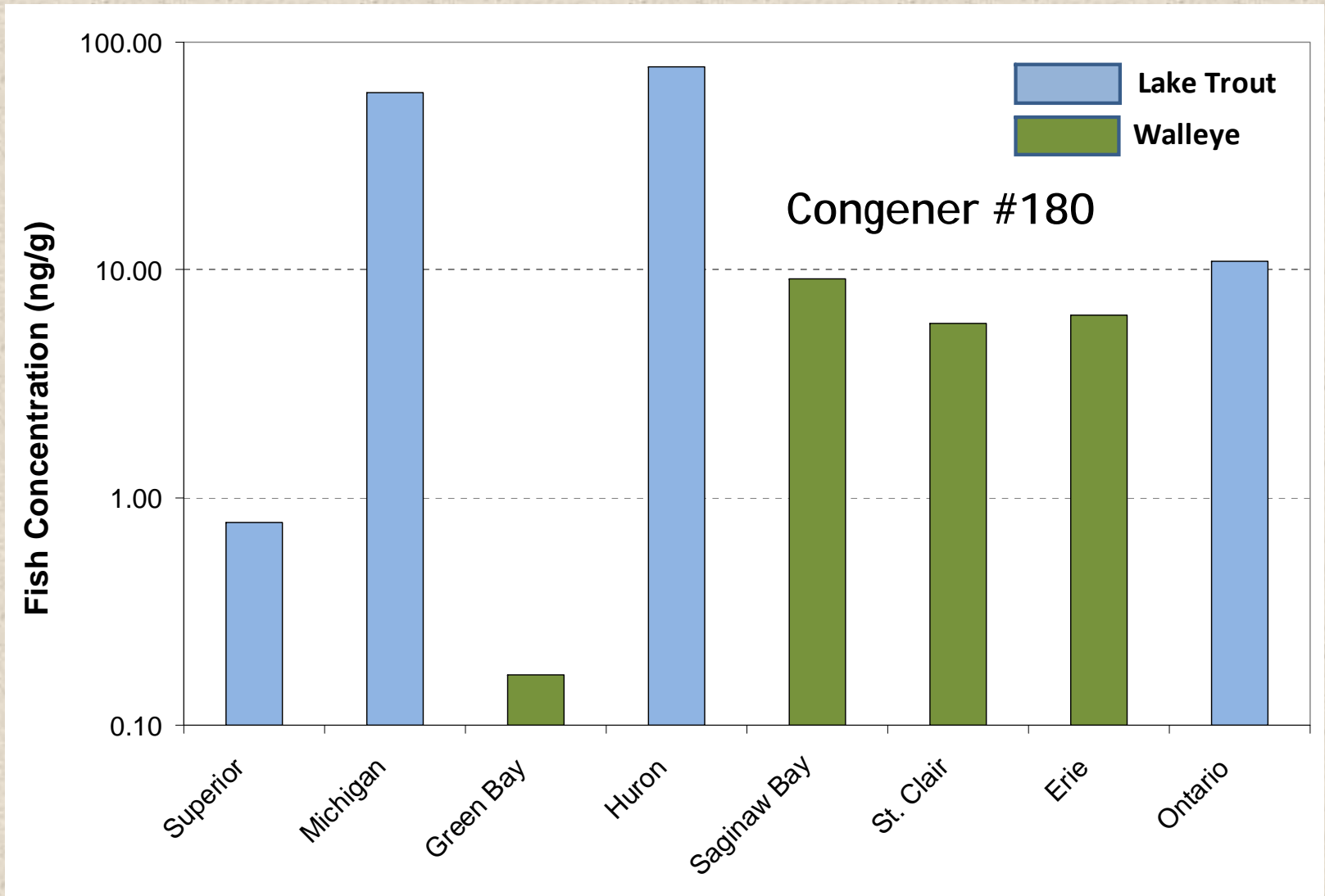
Water Results

Sediment Results



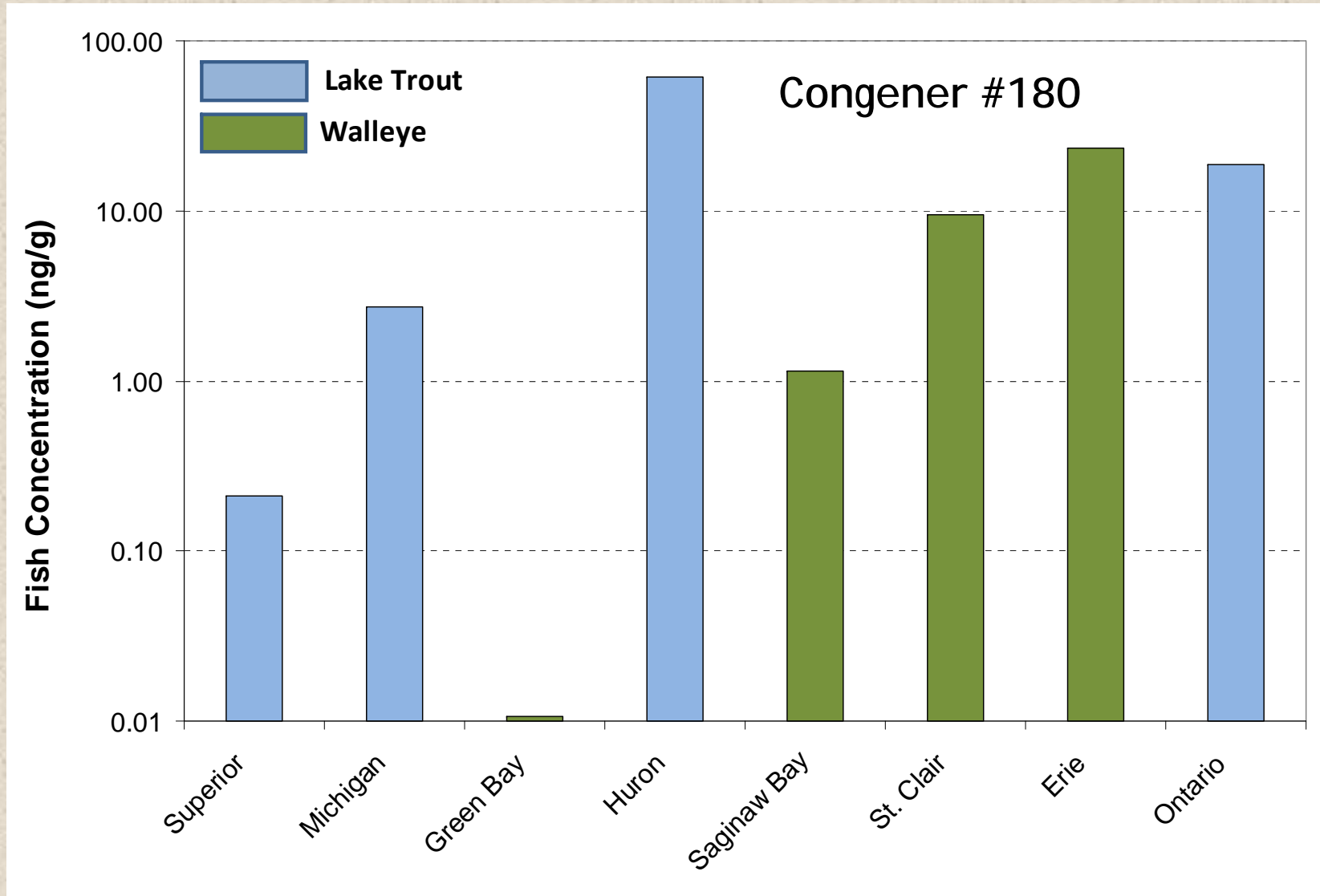
Diagnostic #1: Emission to air over Chicago Fish Simulation Results (after 20 years)

Constant load of 1,000 kg/y for each congener



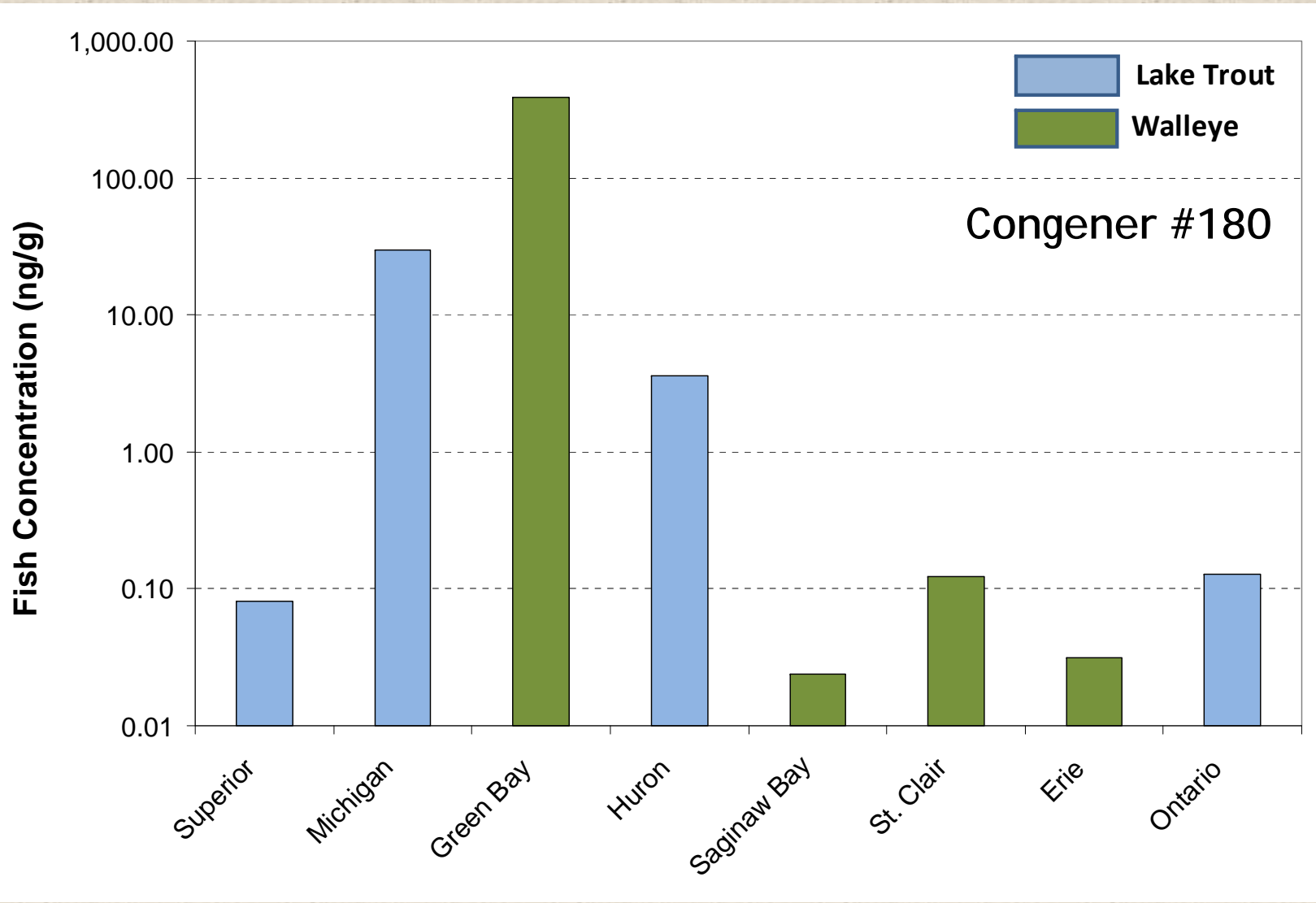
Diagnostic #2: Emission to air over Detroit Fish Simulation Results (after 20 years)

Constant load of 1,000 kg/y for each congener




Diagnostic #3: Fox River Load to Green Bay Fish Simulation Results (after 20 years)

Constant load of 1,000 kg/y for each congener

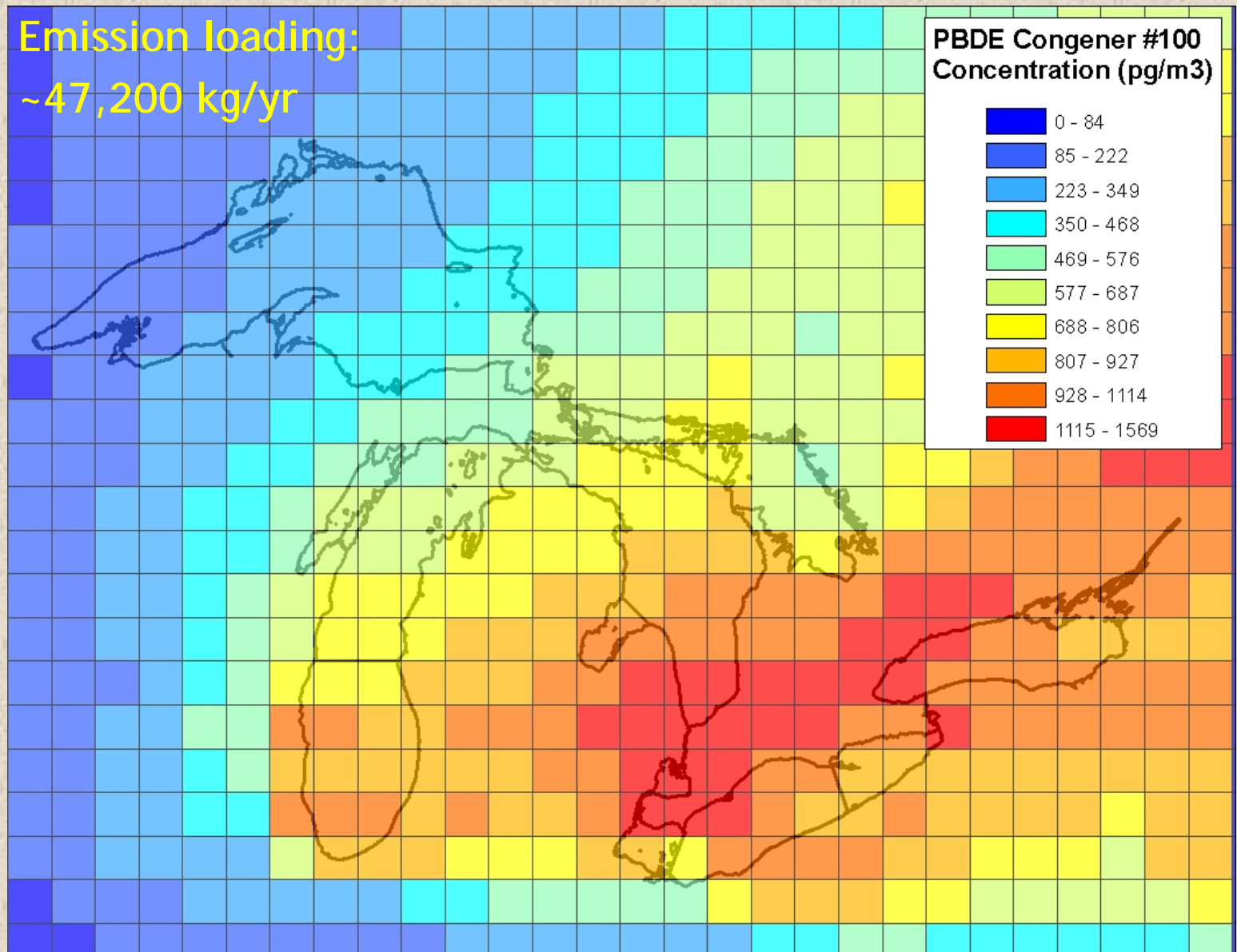


Example Emerging Chemical (PBDE) Simulation

- 
- Polybrominated diphenyl ethers (PBDEs)
 - class of chemicals used as flame retardants, plastics in consumer electronics, etc.
 - Seven PBDE congeners simulated
 - #28, #47, #99, #100, #153, #154, #209
 - Used range of measured chemical properties
 - Synthetic air emission loading scenario:
 - Load proportional to local population density
 - Total annual emission load: ~47,200 kg/yr
 - Run to steady-state (40-year simulation)
 - Predict relative distribution of PBDEs in:
 - Air boundary layer
 - Watershed (soil, vegetation, etc.)
 - Lake surface water, bottom sediments

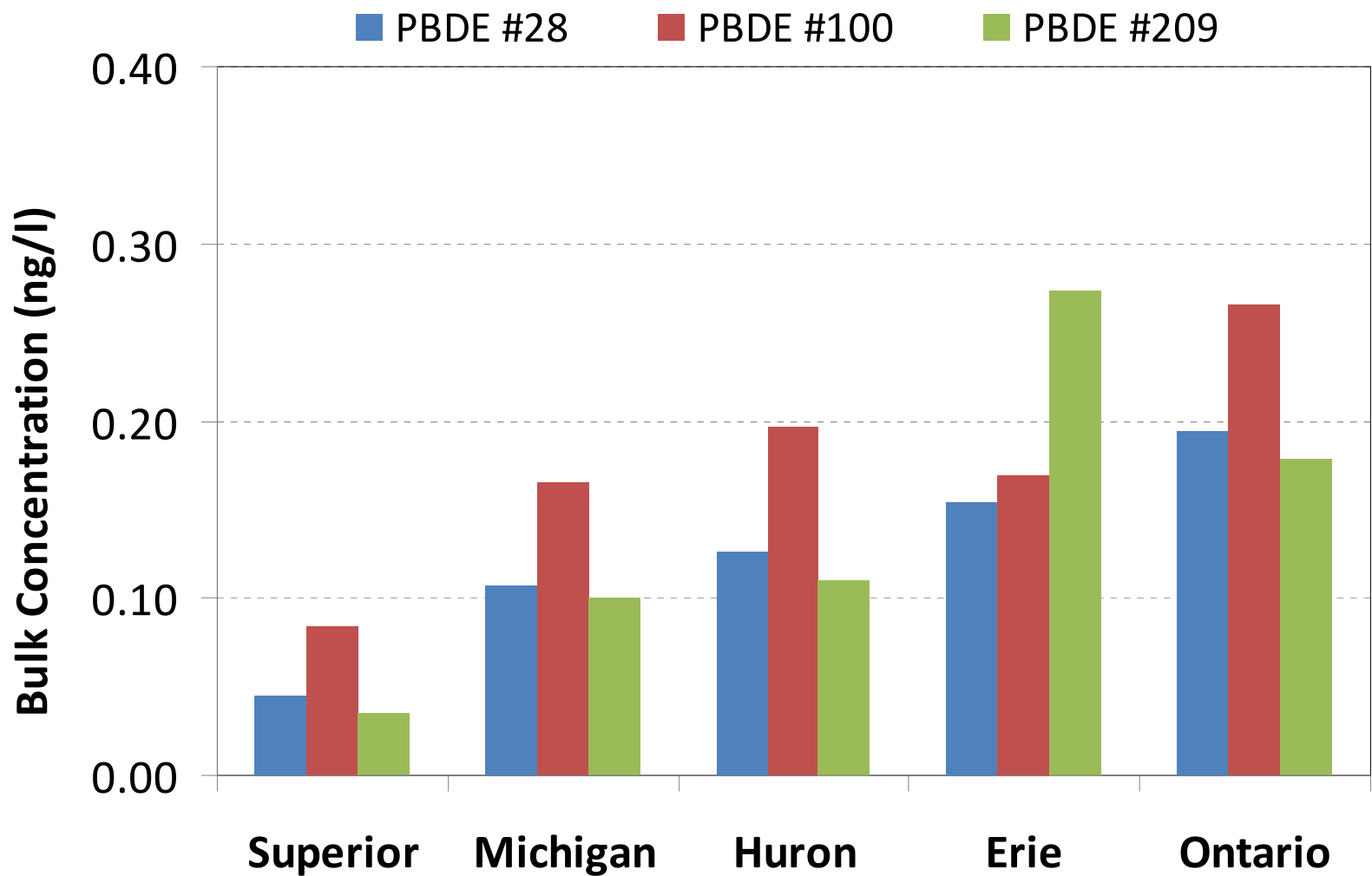
PBDE Diagnostic: Air Concentrations (Congener #100, Year 20 - July)

Emission loading:
~47,200 kg/yr



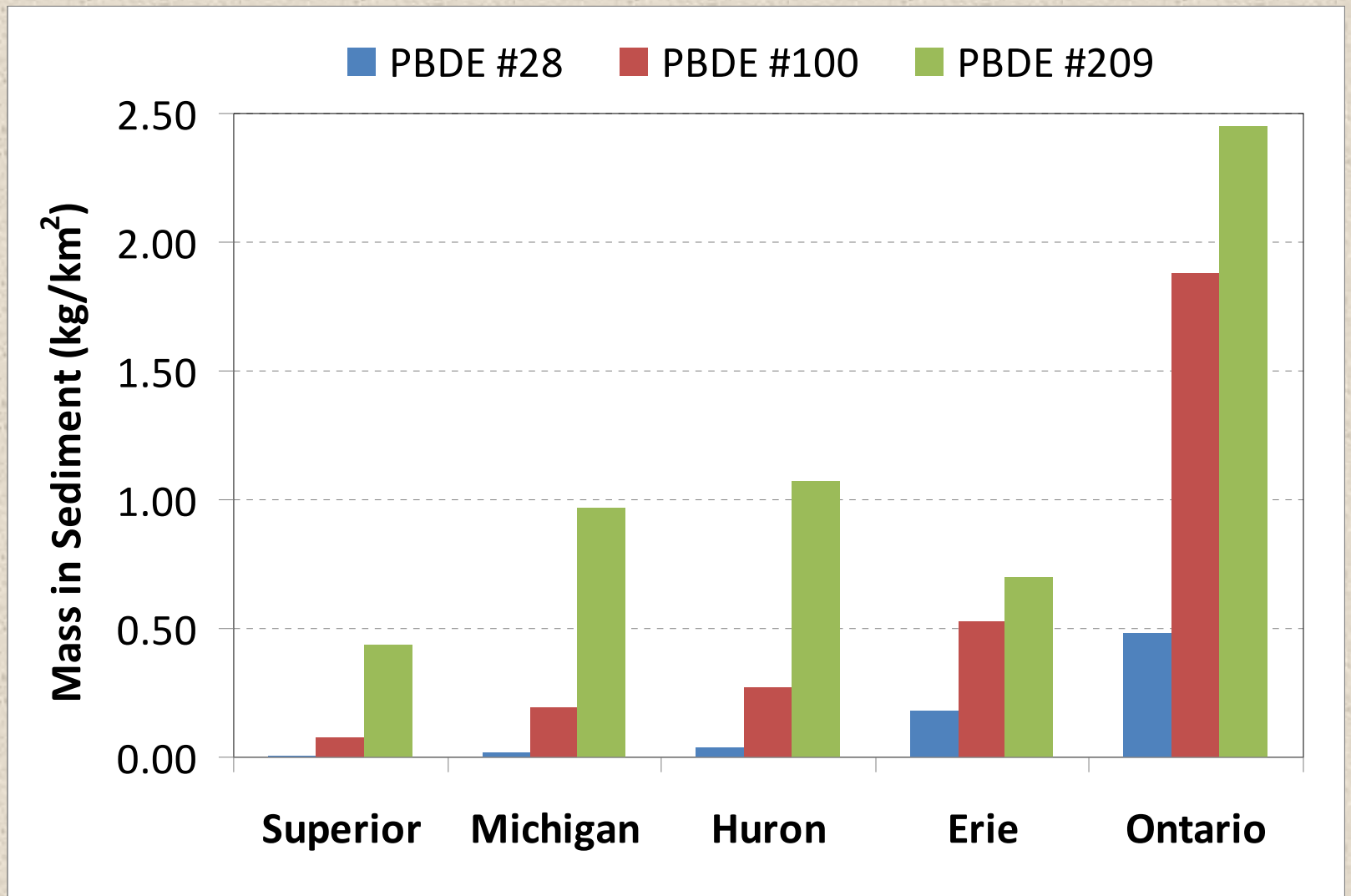
PBDE Diagnostic: Lake Water Results

Water Column Concentration (year 40)




PBDE Diagnostic: Lake Sediment Results


Sediment Mass Inventory (year 40)



Value of a Great Lakes Multi-Media Screening Level Model (GLMOD)

- 
- Assess the potential basin-wide and location-specific impact of emerging chemicals
 - Framework within which to synthesize all research and monitoring data
 - Assess relative importance of various exposure pathways
 - Based on chemical properties, receptor location
 - Relative contributions of sources inside and outside the basin
 - Assess progress toward achievement of specific risk reduction targets of emerging chemicals in the Great Lakes
 - Estimate concentrations of bioaccumulative chemicals in sport fish and compare them to toxicity benchmarks
 - Assist in prioritizing research and monitoring programs
 - determining chemical properties, measuring sources, evaluating exposure pathways, evaluating trends

Summary

- 
- Developed a physically-based, process oriented multi-media model for transport, exposure, and effects of chemicals in the Great Lakes basin
 - Prototype developed using object-oriented programming approach
 - Field testing for six PCB congeners spanning range of K_{ow} and Henry's constants
 - Model can serve as a "tier 2" screening model for chemicals of emerging concern in the Great Lakes Basin
 - Next Steps
 - Use to synthesize and interpret developing CEC database and prioritize further research and monitoring
 - Link to CHARM model (NOAA-GLERL) and evaluate climate change scenarios

Questions?

■ Acknowledgements:

- Funding: EPA-Great Lakes Air Deposition (GLAD) Program
 - <http://www.glc.org/glad/>
 - Project Officer: Jon Dettling, Great Lakes Commission
- Sharing *Large Basin Runoff Model* (LBRM) for hydrology of basin: Tom Croley (NOAA-GLERL)

■ Contact Information:

Joe DePinto

LimnoTech

Ann Arbor, MI

jdepinto@Limno.com