

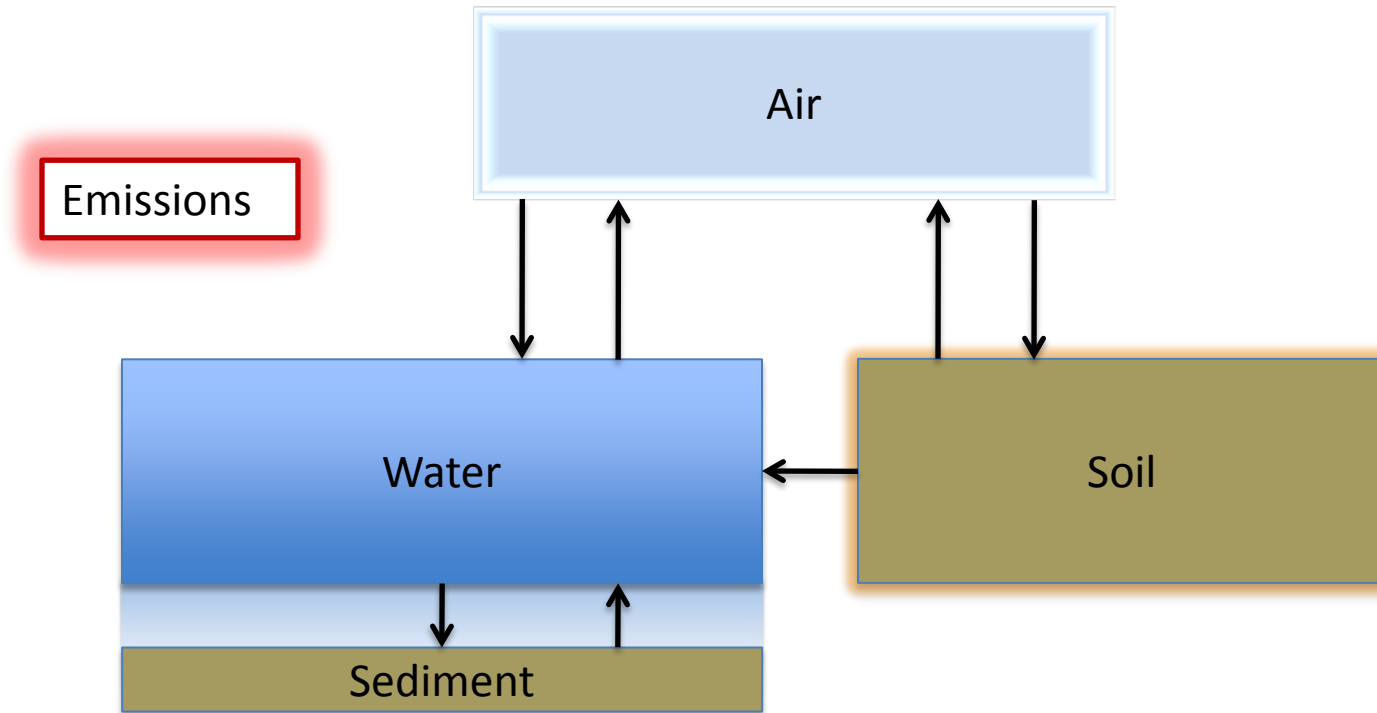
Monte Carlo Based Multi-Media Fate Model for the Great Lakes Ecosystem

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GOALS

- *DESIGN A SIMPLE WEB BASED SCREENING TOOL TO ESTIMATE LEVELS OF CHEMICAL CONTAMINANTS IN EACH OF THE FIVE GREAT LAKES.*
- <http://glad.syrres.com/default.asp>
- California Dept. of Toxic Substance Control:
“The U.S. currently has more than 85,000 chemicals in commerce. There are approximately 2,500 “high production volume” (HPV) chemicals, which are manufactured at a rate of more than one million pounds annually, with nearly 45 percent of these HPV chemicals lacking adequate toxicological studies conducted to evaluate their health effects on humans and wildlife. Further, about 2,000 new chemicals are introduced into commerce annually in the U.S., at a rate of seven new chemicals a day.”

Design



REQUIRED USER INPUTS

- ▶ MELTING POINT
- ▶ VAPOR PRESSURE
- ▶ HENRY'S LAW CONSTANT
- ▶ Kow
- ▶ DEGRADATION HALF-LIVES (The program can accept log normal or triangular distributions for the half-lives if desired)
- ▶ EMISSION DATA – Toxic Release Inventory, Regional Air Pollutant Inventory Development System (RAPIDS), National Emission Inventory database (NEI)

OUTPUTS

- ▶ Percentage of the chemical that partitions to each environmental medium
- ▶ Concentration of the chemical in each medium (air, water, soil, sediment)
- ▶ Length of time the substance remains in the environmental model
- ▶ Aquatic toxicity data from estimation software (LC₅₀, EC₅₀).
<http://www.epa.gov/oppt/newchemicals/tools/21ecosar.htm>

General Tips

- ▶ Use the pesticide use maps for emissions to soil (***only includes US data***). Use the 2002 Great Lakes Toxic Air Emissions Hazardous Air Pollutant (HAP) maps or data from the NEI for atmospheric emissions.
- ▶ Use measured values for input parameters when available; otherwise employ the estimation methods to calculate values.
- ▶ EPIWIN Software -
<http://www.epa.gov/opptintr/exposure/pubs/episuitedi.htm>

Using the Program

Monte Carlo Based Multi-Media Fate Model for the Great Lakes Ecosystem - Windows Internet Explorer provided by Yahoo!

http://glad.syrres.com/default.asp

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Monte-Carlo Based Multi-Media Fate Model for the Great Lakes Ecosystem

HOME OVERVIEW PARAMETERS STANDARD LEVEL III CALCULATION MONTE CARLO CALCULATION CONTACT

SRC and PRA Develop a Monte-Carlo Based Fate Model for Great Lakes

Syracuse Research Corporation (SRC), an independent, not-for-profit research and development organization, in collaboration with the Probabilistic Risk Assessment (PRA) Center of Central New York, have developed a Monte Carlo based multi-media fate model for the Great Lakes Commission under the Great Lakes Atmospheric Deposition Program (GLAD).

Fate Model Goals

- Achieve a greater understanding of the atmospheric transport, degradation, and deposition rates for pollutants of concern.
- Develop rational emission reduction strategies for pollutants released to the Great Lakes.
- Aid risk assessors in evaluating potentially hazardous levels of chemicals in the ecosystem.

Corporate Links

- ▶ [Great Lakes Commission](#)
- ▶ [Probabilistic Risk Assessment Center](#)
- ▶ [Syracuse Research Corporation](#)

Developed by the [Syracuse Research Corporation](#) under contract to the [Great Lakes Commission's](#) Great Lakes Air Deposition (GLAD) program, supported by the [U.S. EPA](#).

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http://glad.syrres.com/includes/estimate.asp

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▶ HOME ▶ OVERVIEW ▶ PARAMETERS ▶ STANDARD LEVEL III CALCULATION ▶ MONTE CARLO CALCULATION ▶ CONTACT

Standard Estimate Parameters Form

SMILES Notation

Enter a SMILES notation here or use our [drawing program](#) or [CAS Number lookup program](#) to generate it for you.

NOTE: The drawing applet loads slowly initially.

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http://glad.syrres.com/standard/standardcalcproperties.asp

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Standard Level III Estimated Parameter Values

Select a lake (the default is Lake Ontario):

- Lake Ontario
- Lake Erie
- Lake Huron
- Lake Superior
- Lake Michigan

Chemical Name:	<input type="text" value="Not Entered"/>		
CAS Number:	<input type="text" value="Not Entered"/>		
SMILES Notation:	<input type="text" value="c1ccccc1"/>		

Property	Value	Units	Type
Henry's Law constant (atm-m3/mol):	<input type="text" value="0.0056"/>	567.42 Pa/m ³ mole	Measured
log Kow:	<input type="text" value="2.1"/>		Measured
Vapor Pressure (atm):	<input type="text" value="0.12"/>	91.2 mm Hg	Measured
Melting Point (Kelvin):	<input type="text" value="278.65"/>	(5.5 degrees C)	Measured
Bioconcentration Factor:	<input type="text" value="8.7"/>		Estimated
Molecular Weight:	<input type="text" value="78.11"/>	g/mol	
Emission rate (kg/hr) air:	<input type="text" value="1"/>		
Emission rate (kg/hr) water:	<input type="text" value="0"/>		
Emission rate (kg/hr) soil:	<input type="text" value="100"/>		

Half-life of the chemical (in hours) in air, water, soil, and sediment.

Air: <input type="text" value="170"/> (7.3 days)	Water: <input type="text" value="900"/> (38 days)	Soil: <input type="text" value="1800"/> (75 days)	Sediment: <input type="text" value="8100"/> (340 days)
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OPTIONAL: Enter a level of concern (LOC) for this chemical in the lake in ng/L.

Using the Program

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http://glad.syrres.com/standard/standardexec.asp

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Point Estimate Level III Output

Input Values

Parameter	Value	Comment
Chemical Name:	Not Entered	
Henry's Law Constant(atm m ³ /mol):	0.0056	
log Kow:	2.1	
Vapor Pressure (atm):	0.12	
Melting Point (Kelvin):	278.65	
Molecular Weight:	78.11	
Air Half-life (hrs):	170	
Water Half-life (hrs):	900	
Soil Half-life (hrs):	1800	
Sediment Half-life (hrs):	8100	
Air Emission Rate (kg/hr):	1	
Water Emission Rate (kg/hr):	0	
Soil Emission Rate (kg/hr):	100	
LOC in lake (ng/L):	1	

Results


The [Characteristic Transport Distance \(CTD\)](#) is: 3,527.7 km
The [Long Range Transport \(LRT\)](#) potential is: high

Partitioning in Environmental Media and Environmental Persistence						
% Air	% Water	% Soil	% Sediment	Persistence Time (hours)	% Degraded	% Advected
48.740	9.906	41.352	0.002	76.608	17.025	82.975


Concentration in the Lake Michigan Basin				
Air (ng/m ³)	Water (ng/L)	Soil (ng/g)	Sediment (ng/g)	Fish* (ng/g)
21.42715	0.1554772	0.1129786	1.169913E-04	9.785891E-04

*The fish compartment is a minor subunit of the total water compartment

The current emission rates are unlikely to result in a water concentration greater than the LOC

 Syracuse Research Corporation

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Case Studies Atrazine

- ▶ Surface water levels of atrazine monitored in the Great Lakes (2005-2007)
 - Perihan B et al. 2010. Metolachlor and Atrazine in the Great Lakes. Environ. Sci. Technol. 44: 4678-4684.

	Range (ng/L)	Median (ng/L)	Predicted Levels (Emission solely to US soil) (ng/L)
L. Superior	5.1-6.0	5.4	0.0066
L. Huron	4.7-32	13.2	2.2
L. Michigan	48-71	55	10.3
Lake Erie	17-92	41	84.2
L. Ontario	29-151	59	13.4

Metolachlor

Surface water levels of metolachlor monitored in the Great Lakes (2005-2007)

- Perihan B et al. 2010. Metolachlor and Atrazine in the Great Lakes. Environ. Sci. Technol. 44: 4678-4684.

	Range (ng/L)	Median (ng/L)	Predicted Levels (Emission solely to US soil) (ng/L)
L. Superior	0.2-1.0	0.25	0.0016
L. Huron	1.0-6.6	3.0	0.83
L. Michigan	11-17	13	2.7
Lake Erie	5.6-23	18	17.4
L. Ontario	5.4-21	10	3.6