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

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GOALS

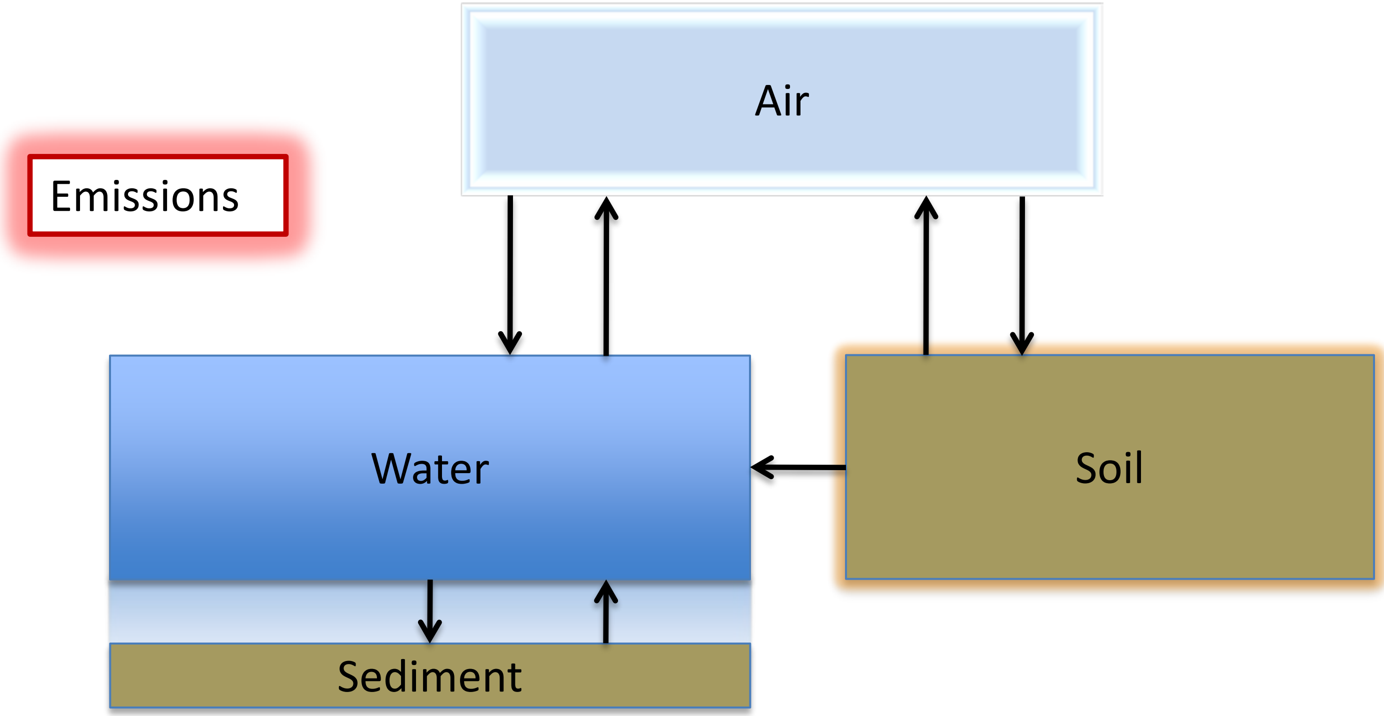
- *DESIGN A SIMPLE WEB BASED SCREENING TOOL TO ESTIMATE LEVELS OF CHEMICAL CONTAMINANTS IN EACH OF THE FIVE GREAT LAKES.*

- 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 (LC_{50}, EC_{50}). http://www.epa.gov/oppt/newchems/tools/21ecosar.htm

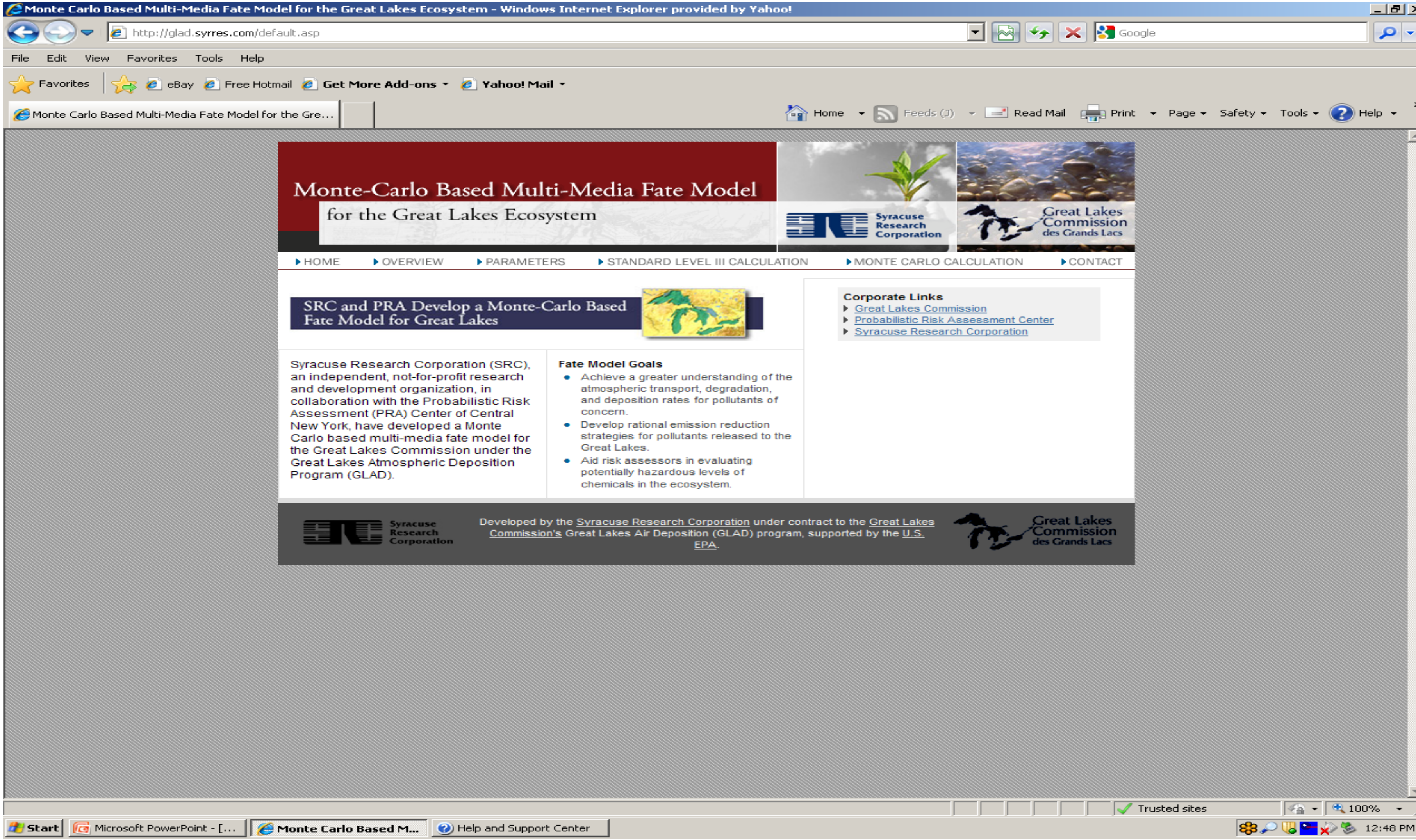
General Tips

- 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.

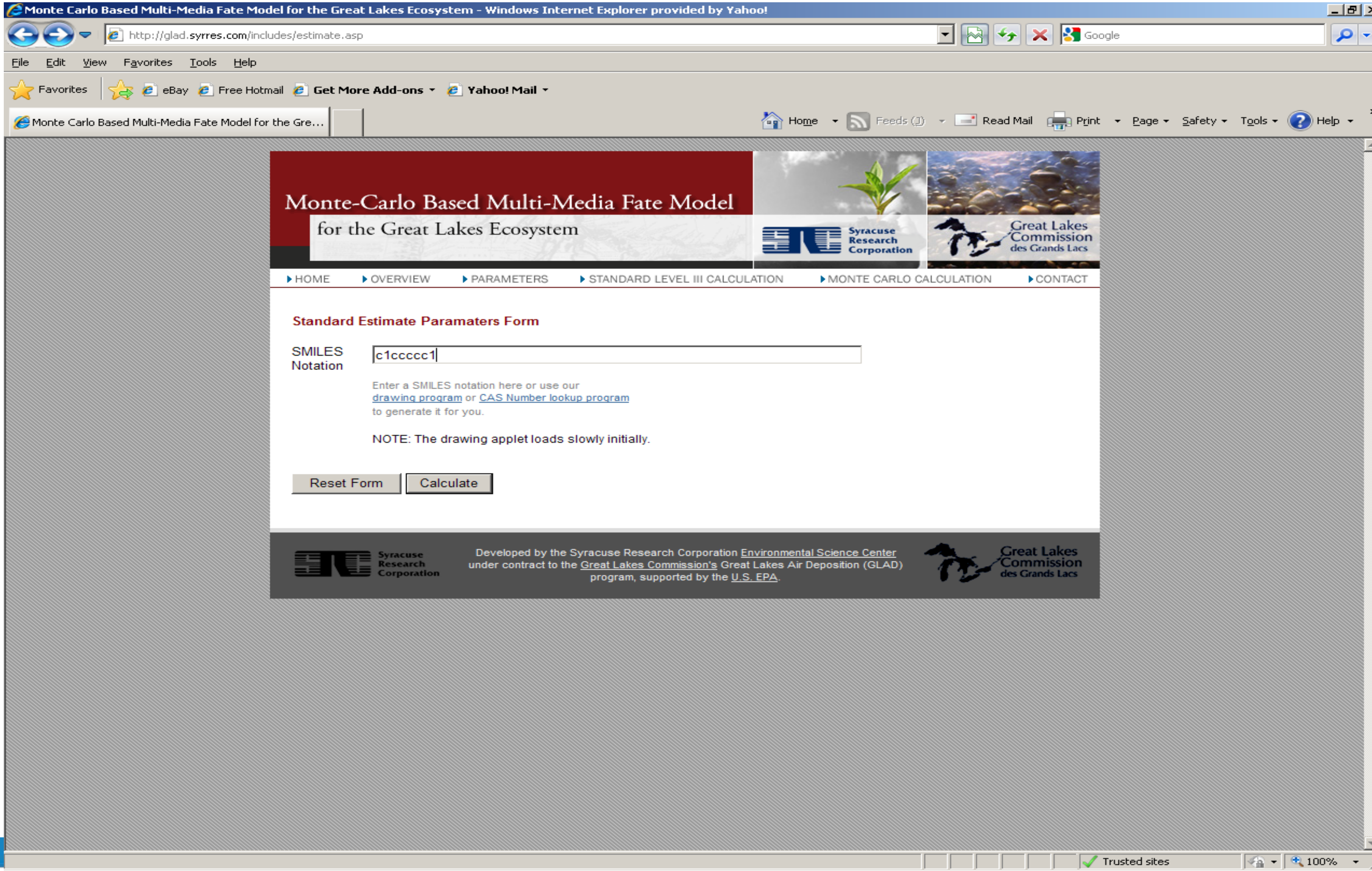
- Use measured values for input parameters when available; otherwise employ the estimation methods to calculate values.

- EPIWIN Software - http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm

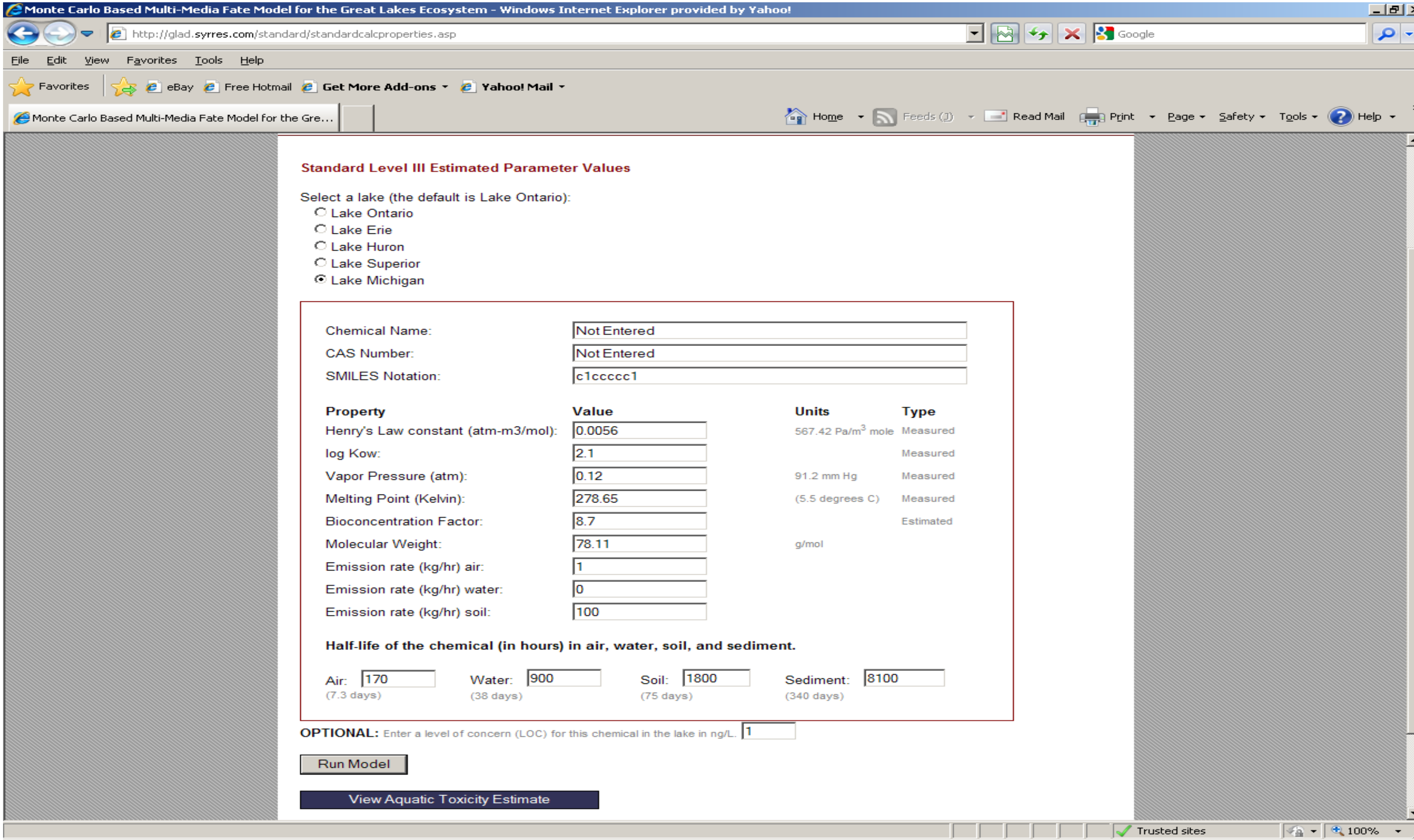
Using the Program



Using the Program



Using the Program



Defense › Environment › Intelligence

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/standard/standardexec.asp

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

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

Great Lakes Commission des Grands Lacs

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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