

Online Model Predicts Chemical Behaviors in the Great Lakes Environment

Syracuse Research Corporation (SRC) has produced an online, interactive modeling application for predicting the fate of chemicals within the Great Lakes environment. The project, led by Dr. Mario Citra of SRC, set out to produce an easy-to-use application that would allow users to determine several important factors relating to how chemicals behave once they have been released into the Great Lakes environment. These include:

- Where in the environment does the chemical tend to accumulate (such as in water, soils, sediments, air or fish)?
- How long is the chemical retained in the Great Lakes environment before it degrades or is transported to another region?
- What concentration in the environment would be produced by a given level of emission?
- What is the potential for a chemical to travel to the Great Lakes region from far away?
- And more.

By providing this capability through an online interface that is easy to access and use, the model gives users a powerful tool for answering their questions about the behavior of a given chemical in the Great Lakes system. The modeling program may be run with as little input as the chemical's Chemical Abstract Service (CAS) identification number (of which 33 million are available) although more detailed characteristics may be input as well. The model's ease of use and availability over the Internet make it a great tool for use in educational settings.

While much information can be generated by the model without specifying chemical quantities, knowing how much of a chemical is emitted into the environment allows a user to obtain even more information, such as predicted concentrations in air, water, soils, sediments and fish. It also allows the user to determine the likelihood that a certain concentration known to be a high-risk level would be exceeded. While users can enter their own emissions information, the website also includes links to pesticide application data from the CropLife Foundation and air emissions data from the Great Lakes Regional Toxic Air Emissions Inventory, which together provide useful release information on more than 350 toxic substances.

While the standard version of the model provides the easiest option for less advanced users, there is also a version that allows the use of Monte Carlo statistical techniques to assess the uncertainty in the model's predictions. This option allows users to enter a range of possible values for important variables, rather than entering a single value. The model then computes the likelihood of possible outcomes given that range of inputs. For example, rather than simply predicting that a given chemical's concentration in water would be 2 grams per liter, the results might say it is 90% likely that the concentration would be between 0.5 and 5 grams per liter, with a most like value of 2. Examples are given on the model's website to assist users in choosing a range of values.

The model is configured to represent each of the five Great Lakes basins (Huron, Ontario, Michigan, Erie and Superior). The user is able to choose which of these five they would like to use as the basis for the model. The program then automatically loads the proper environmental characteristics for that lake basin (such as area and depth of surface water). By modeling with the same inputs but different lake basins selected, comparisons can be made as to how chemicals might behave differently in the different basins. Although the model allows the selection of individual lake basins, the geography within each basin model is not specific enough to allow release points to be defined. Rather, the air and water of each basin are modeled as a single, well-mixed, box.

While other models may be more complex or offer additional capabilities, this modeling program has the advantage of being easy to access and use. Potential applications include investigating the behavior of new or unstudied chemicals; comparing emissions and monitoring data; and calculating expected concentrations of chemicals in the environment or the likelihood that such concentrations will exceed known risk values. It is expected to find uses in places such as governmental agencies, research laboratories and educational classrooms, among others.

The model is available at the SRC website: <http://glad.syrres.com>.

Additional documentation is available at: www.glc.org/glad/projects/citra06

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

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Point Estimate Level III Output

Results

The **Characteristic Transport Distance (CTD)** is: 2,032.9 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 |
| 24.128 | 71.403 | 4.429 | 0.040 | 212.712 | 37.934 | 62.066 |

| Concentration in the Lake Ontario Basin | | | | |
|---|--------------|--------------|-----------------|--------------|
| Air (ng/m ³) | Water (ng/L) | Soil (ng/g) | Sediment (ng/g) | Fish* (ng/g) |
| 0.6183465 | 9.261125E-02 | 6.133979E-04 | 1.874083E-04 | 2.320006E-03 |

*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

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.

An example model output



The project was supported by the Great Lakes Commission's Great Lakes Air Deposition (GLAD) Program with funding originating from the U.S. Environmental Protection Agency. The GLAD Program aims to help regional state governments and their partners better understand and manage the treats of toxic substances that enter the Great Lakes from the atmosphere. For more information, visit www.glc.org