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Integrated Modeling: Examining the Fate and Transport of Contaminants in Canadian Lakes and Rivers.

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Abstract

With the ever increasing introduction of chemicals to the environment (approx. 4000 new chemicals are registered each day), scientists and program managers are faced with an apparently endless and overwhelming task of examining the possible ecological risks of these new chemicals as well as the existing chemicals in aquatic ecosystems. It is also well recognized that no single model will be capable of dealing with all of the different types of chemicals and the environments that these chemicals are released into. It is therefore necessary to be able to integrate a spectrum of best practice models into a system that allows the user to model the fate and transport of contaminants in an optimized way. This is best done in a decision support system framework that contains not only the core models, but also the data, knowledge, and supplementary tools that are required to run the models and to evaluate their results. ChemSim (Chemical Simulation) has been developed in support of implementing the Canadian Environmental Protection Act (CEPA). The ChemSim modeling system is modular in design with currently seven main components: 1) Drainage Area Ratio Analysis Tool**;** 2) Discharge Site Analysis Tool; 3) Spatial database; 4) Water Quality Module; 5) Sediment Module; 6) Physical-Chemical Database and 7) Integrated Lakes Modeling Tool. The system has been developed using a well tested decision support system frame work and models. The system has already been used to evaluate over 25,000 chemicals and continues to be developed to allow greater realism of exposure characterization. The paper provides a description of the decision support framework and the system components.

Keywords: Integrated modeling; risk assessment.

1. INTRODUCTION

ChemSim is similar to the Probabilistic Dilution Model (PDM) (U.S. EPA) in its ability to combine geographical data on industry release estimates and river systems in order to calculate expected aqueous concentrations. ChemSim also allows users to select facilities by Standard Industrial Code (SIC). The advantage of using ChemSim is that it estimates the concentration of substances within the mixing zone (i.e. plume) at different distances from the point of discharge; estimates would not be based simply on the concept of immediate and complete mixing with the receiving watercourse. While it can be simply applied in conducting initial screening assessments, the more advanced components (detailed and site specific models) allow application of ChemSim in more complex or site-specific applications. The new ILMS module now allows the system to evaluate discharges to lakes.

2. ChemSim

2.1 System Design

The ChemSim modeling system was developed within the EnSim Hydrologic system that was originally developed by the Canadian Hydraulics Centre (CHC, 2003) of the National Research Council of Canada. ChemSim includes seven main components, which are fully integrated:

- **Drainage Area Ratio Analysis Tool**: Allows for the estimation of streamflows in locations where gauging information is unavailable. This method calculates the downstream or upstream

flow by means of linear interpolation based on the drainage area ratio method.

- **Discharge Site Analysis Tool**: Allows for the estimation and visualization of dispersion plumes as well as prediction of other parameters such as peak concentrations downstream from the point of discharge and the percentage of the width of the watercourse where it is predicted that the effects thresholds will be exceeded.

- **Spatial Database**: The database contains maps and data on industrial facilities, sewage treatment plants, and stream-flow gauging stations. Industrial dischargers are grouped by Standard Industrial Codes, and are identified as direct or indirect dischargers of their effluent (National Pollutant Release Inventory (NPRI), Environment Canada). The data regarding Sewage Treatment Plants (STP) includes STP location, effluent flow volume, receiving watercourse and treatment types. Information on treatment types is also available for some of the STPs. The HYDAT database from Environment Canada contains measurements at all stage and discharge gauging stations in Canada. The hydrology data includes watercourse information and various stream-flow statistics. A relationship exists between these three data sources so information can be interrelated to assist in characterizing the entry pathway, transport and dispersion of substances released to watercourses.

- **Water Quality Module**: The water quality module was developed by Environment Canada's National Water Research Institute (NWRI). The goal of this module is to account for various fate and degradation processes that would influence the concentrations in the water column. Specifically, this model allows users to account for biodegradation, volatilization, hydrolysis, photolysis, and adsorption to sediment. Users have the option of entering user specified rates or from selecting values from a database of existing substances.

- **Sediment Module**: The sediment module was developed by NWRI to estimate the concentration of substances that would be present in sediments downstream from the point of discharge. Specifically, the sediment module is a steady-state advection – diffusion and adsorption model that solves for chemicals in water and suspended sediments. Taking into account adsorption/desorption and degradation, this module solves for the suspended sediment concentration first using a settling velocity, then it uses the suspended sediment concentration with a normalized partitioning coefficient to solve for the chemical total, particulate and dissolved concentrations with a specified decay rate.

- **Physical-Chemical Properties Database:** The water quality database has been developed from a large number of existing databases as well as other reference sources. The largest and most comprehensive physical property and chemical fate databases have been obtained from the Syracuse Research Corporation (SRC).

- **Integrated Lakes Modelling tool:** It has been developed to simulate the fate and transport (e.g. volatilization, adsorption, hydrolysis, biodegradation, etc.) of substances that are released to lakes. There are seven lake models to cover a range of conditions. It may operate independently from the other tools but shares common databases and graphics modules. It also contains an expert system for model selection developed using the RAISON Decision Support System (Booty and Wong, 1994).

The design is generic so that existing databases can be upgraded and additional databases integrated into the system. The system provides information to the user on the applicability and validation of each method.

2.2 Model Operation

The basic steps involved in running ChemSim are:

- display the discharge sites
- select a site and retrieve site description information (where available)

- retrieve, enter or calculate hydraulic and dispersion data
- select a chemical by group, name or CAS#
- retrieve, enter or calculate decay and mass loss rates, which allows the system to calculate half-life and loading mass lost; this includes selecting input parameter values and methods
- specify release mass and method
- display results

Depending on the desired level of complexity, users have the option to (1) estimate predicted environmental concentrations in the water column based on simple dispersion, (2) account for fate and degradation processes with the water quality module, or (3) account for interaction with the sediments and estimate concentrations in the water column and the sediments.

2.3 ChemSim Outputs

ChemSim generates three forms of output: (1) the peak concentration downstream from the point of discharge, (2) the area of the plume greater than user-specified effects thresholds, and (3) the percentage of the width of the river where the estimated concentration is greater than the effects thresholds. These output data are presented both graphically and in tabular format. An example 2-D output of a thematic graph of the spatial extent of the peak concentrations downstream from the source for pentachlorophenol is shown in Figure 1.

3. ILMS

3.1 System Design

The ILMS is being developed to simulate the fate and transport (e.g. dispersion, volatilization, adsorption, hydrolysis, biodegradation, etc.) of substances that are released to lakes. The system is being designed to be able to estimate the concentrations of substances in the water column, sediments, and biota. A series of seven lake models is used to simulate a range of conditions as shown in Table 1. These seven categories of models are based on potential lake characteristics such as volume, depth, turnover rate, etc. as well as the nature of the discharge. An expert system model selection interface has been developed. The current expert system interface relies on the user to answer questions about data availability and the desired type of calculations. By answering these questions, the interface will suggest which model(s) to use.

3.2 Example Outputs

An example output from model 3 is shown in Figure 2. This shows the steady-state mass balance of the discharged chemical in Clearwater Lake with the concentrations and mass in each of the various lake ecosystem media.

Figure 3 is an example output from model 7 for the central basin of Lake Erie showing the horizontal total concentration gradients. Some of the items available on the 2-D thematic maps include:

- legend - can be interactively adjusted by the user to change interval ranges and colours.
- date-time clock can also be displayed and repositioned.
- map coordinates can be shown on the map grid lines.
- user can zoom in and out and move map interactively.
- if the parameter being thematically mapped varies in time, then it can be animated so that changes can be seen through time. The clock will show the time changes.

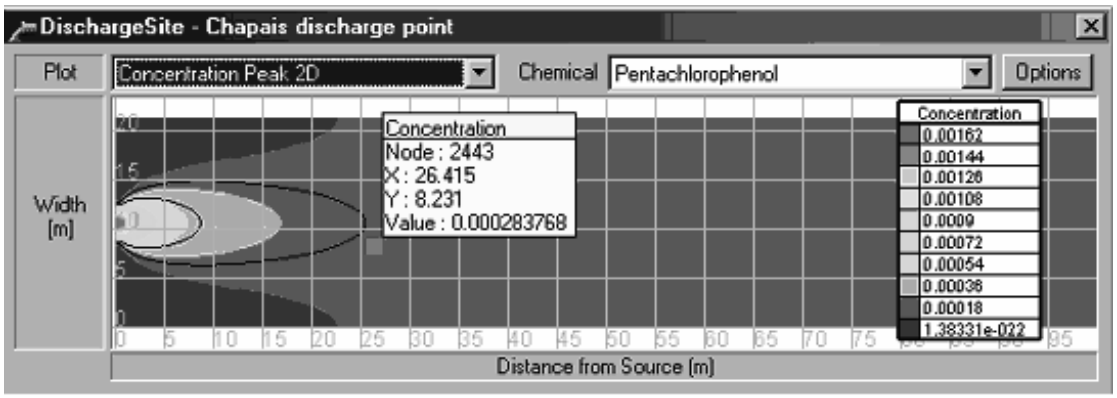

Figure 1 A thematic graph of the spatial extent of the peak concentrations downstream from the source

Model	Model Type (complexity)	What does the model do	Time Domain	Spatial Domain	Inputs	Outputs
(1)	Box model Low	Calculates steady-state dissolved concentrations for a simple (limited geometry) lake	Steady state	1-D	Volume, flows, loads	Dissolved concentrations in water column
(2)	Box model Low	Calculates time-variable concentrations in dissolved and particulate forms for a simple (limited geometry) lake	Time variable	1-D	Volume, flows, loads, suspended solids	Dissolved and particulate concentrations
(3)	Whole lake mass balance (medium)	Calculates steady-state concentrations in water, sediment and biota for a fully mixed lake	Steady state	1-D	physical data, S-S loads, rate constants	S-S concentrations in water, sediment and biota
(4)	Whole lake mass balance (medium)	Calculates time-variable concentrations in water, sediment and biota for a fully mixed lake	Time variable	1-D	Physical data, temporal loads, rate coefficients	Temporal concentrations in water, sediment and biota
(5)	Lagrangian/ Eularian nearfield/ farfield transport (medium)	Calculates nearfield and farfield concentrations in water for buoyant and sinking plumes over time	Steady State or Time variable	3-D	Geometry data of outfall and receiving body, current data, flows and loads	Concentration in time and space within the dissolved phase of discharge plume
(6)	Vertically stratified (high)	Calculates vertical concentration gradients for a whole lake	Time variable	2-D	Vertical profiling data, loads	Concentrations at depth over time for dissolved and particulate phases

(7)	2-D whole lake (very high)	Calculates horizontal concentration gradients over a vertically mixed lake	Time variable	2-D	Boundary conditions, met data, temporal and spatial loads	Concentrations over time and horizontally across the lake for water and sediment

Table 1 Integrated Lake Modeling System

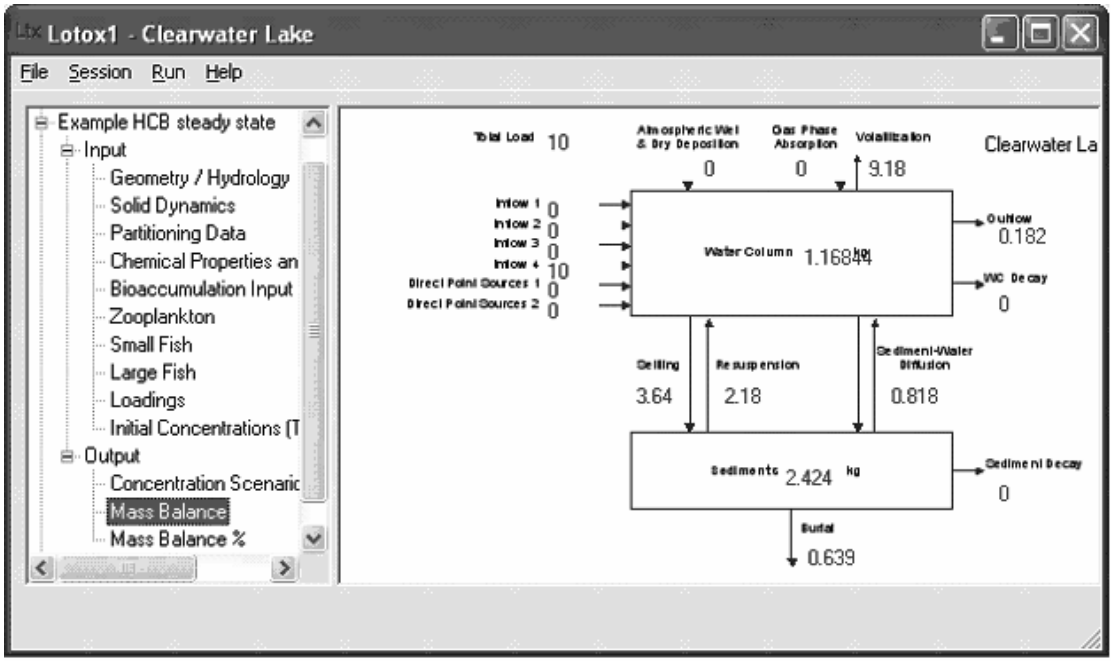

Figure 2 Mass balance diagram output for model 3

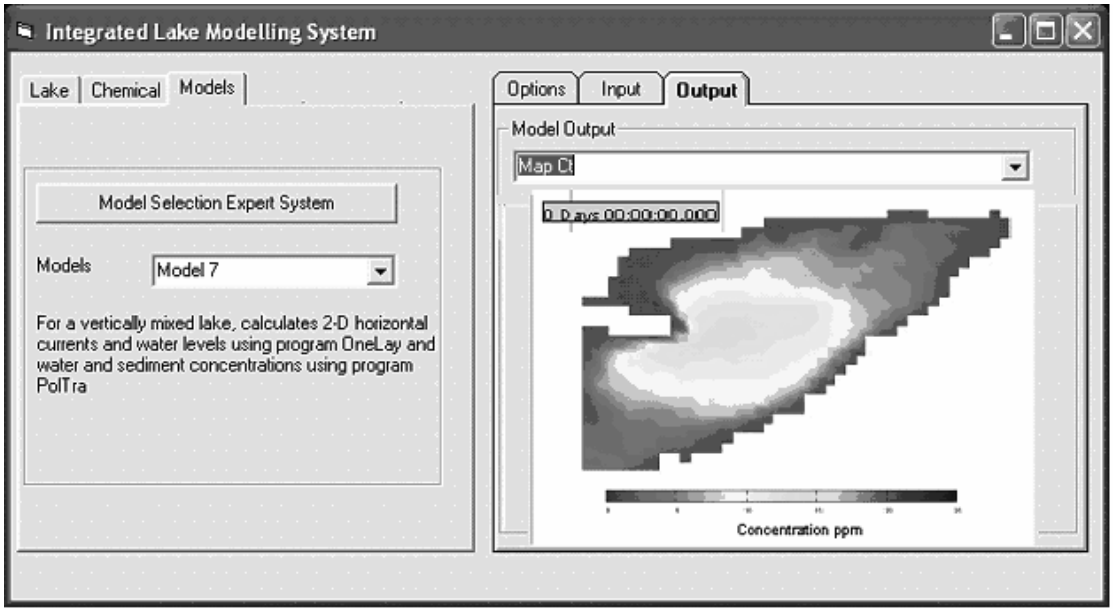

Figure 3 example output from model 7 for the central basin of Lake Erie showing the horizontal total concentration gradients.

4. CONCLUSIONS

Federal government risk assessment evaluators need a tool for characterizing environmental exposure for huge numbers of chemicals over an entire country, often having to rely on various levels of data availability and quality. ChemSim is a suite of tools designed to meet that need. ChemSim has been built to be user-friendly, but rigorous, transparent and flexible. It combines estimated release amounts (e.g. kg) with information from its database to generate aquatic exposure values. Users have the ability to examine both streams and lakes at a wide range of levels of comp lexity. The system allows access to GIS databases that contain information on all of the discharge sites in Canada. The system is now being used routinely by the Risk Assessment Directorate of Environment Canada to evaluate the over 25,000 priority chemicals that are being discharged into watercourses and lakes. The system contains a number of specialized tools that are necessary to be used during an exposure analysis. Without such a system, it would have taken years longer to carry out the mandated research under the Canadian Environmental Protection Act (CEPA).

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