



## WATER RESOURCES RESEARCH GRANT PROPOSAL

**Title:** A prediction system for transport and fate of toxic substances in surface waters

**Focus Categories:** TS, MOD, WQL

**Keywords:** 274-Water Quality Modeling, 251-Toxic Substances, 48-Contaminant Transport, 206-Rivers, 197-Reservoirs, 272-Water Quality Control

**Duration:** March 1, 1999 to Feb. 28, 2001

**Federal Funds Requested:** \$15,625 (first year)

**Non-federal (matching) Funds Pledged:** \$32,135 (first year) Direct cost \$17,427; Indirect cost \$14,708

**Principal Investigator:** Ruochuan Gu, Assist. Prof., Ph.D., P.E. Dept. of Civil and Construction Engineering Iowa State University, Ames, IA 50011 Phone: (515) 294-4534 FAX: (515) 294-8216 E-Mail: roygu@iastate.edu

**Congressional District:** Iowa 3

### Statement of Critical Regional or State Water Problems

Toxic substances from chemical spills and non-point source runoff into rivers, reservoirs or lakes pose a potential risk to human health and aquatic lives. Accidental spills can be caused by train derailments and truck collisions during ground transportation, leaking from factories and storage tanks, and obsolete navigation (barges in the Midwest waterways and tankers in other regions). More than a thousand toxic spills related to rail alone have been recorded every year in the United States (Elmer-Dewitt 1991). The sites of recent spills were Marshalltown, Iowa, in 1995 and Duluth, Minnesota in 1993. The National Environmental Law Center reported an average of forty-five chemical accidents per month in the Great Lakes States alone. Toxic substances spilled into surface waters are primarily pesticides, herbicides, fungicides, and organic compounds, e.g. sodium methyl dithiocarbamate, methyl isothiocyanate, polychlorinated biphenyls, and polycyclic aromatic hydrocarbons (Gu et al. 1996; Rosario et al. 1994). Toxic contamination in streams and reservoirs may also result from storm events at landfills and superfund (toxic disposal) sites and agricultural runoff as non-point sources (Schnoor et al. 1992; Hayes 1988), especially in the agricultural states such as Iowa and the North Central region.

Toxic contaminants from spills and runoff have a significant impact on the environment and continue to be a serious threat to the Nation's and regional watersheds and water resources. The inevitability of toxic spills and runoff points to the need for a full understanding of the behavior (transport and fate) of toxic chemicals in surface waters

and an effective tool for prediction to assist contamination control, remediation management and watershed protection.

Expected results include (1) an integrated 2-D river and reservoir toxic contaminant simulation model that will be tested and validated with field data for selected watersheds and past spills and (2) a real-time computer prediction and analysis program to provide information on locations and concentrations of spilled or runoff-carried toxic chemicals in a receiving waterbody. The proposed research will advance the understanding of transport and fate of toxic contaminants in surface waters and provide effective prediction techniques for contamination control. Simulations can be performed before, during, and after a spill or a storm event for short-term or long-term predictions and cleanup and postaudit assessment. The real-time prediction and analysis system serves as a tool for quick assessment, emergency response, contamination remediation, and river or reservoir management within the short period after an actual incident. Predicting the location and concentration of toxic chemicals can guide data collection during a spill or runoff event. The integrated real-time computer program can be used by an emergency response and remediation team to make predictions, to warn water plants about closing intake structures, and to notify fisheries and reservoir management personnel. The program can be integrated into a regional or state contingency plan for emergency response and remediation management to minimize the consequences of a toxic runoff or spill, which will benefit the public and the environment.

### **Nature, Scope, and Objectives of the Research**

Concern has been growing over accidental chemical spills into streams, reservoirs, or lakes because of the potential risk to human and aquatic lives, threat to downstream drinking and industrial waters, and damage to the ecosystem and the environment. Toxic substances into surface waters resulting from instream shipping, railroad, ground transport, and distributed sources, e.g., agricultural runoff, are primarily pesticides, herbicides, fungicides, organic compounds, and other chemical contaminants (Hayes 1988; Jasen 1988; Schnoor et al. 1992; Rosario et al. 1994). More than 1,000 toxic spill incidents related to rail alone are recorded every year in the United States (Elmer-Dewitt 1991). The inevitability of toxic spills points to the need for a full understanding of spill behavior in surface waters, including physical processes, chemical reactions, and biodegradation. An effective tool for fate and transport prediction of spilled chemicals and contamination levels is needed to assist contamination remediation and to minimize the consequences of a toxic spill and runoff. On the other hand, lack of understanding of toxic substance behavior in a reservoir can hamper effective implementation of spill control measures.

An integrated two-dimensional (2-D) mathematical model is needed to simulate the variations of flow, sediments, and contaminants with time and in the vertical and longitudinal directions in a stream and reservoir system. A real-time computer prediction and analysis program, which has been lacking, is necessary for serving as a tool for quick assessment, emergency response, contamination control, and river or reservoir management within the short period after a spill and runoff. The model is expected to

easily and quickly predict the fate and transport of spilled toxicants and pollutants in a river or reservoir system before a spill and runoff or during an actual emergency response. The model may also be used for post-audit simulations. The computer program is expected to be user friendly and, as a part of the toxic spill response program, assist (1) contingency planning before a possible spill and runoff, (2) data collection and contamination control during the emergency response to a reported accident, and (3) cleanup and post-audit assessment of the environmental impact of a past event. The program should be operational on a microcomputer or personal computer. In the event of a toxic spill or runoff, the model can be used on a real-time basis to forecast the location and distribution of the spilled materials.

Numerical models were first developed in 1970s for the fate and transport of toxic chemicals in surface waters (Thomann 1978; Smith et al. 1977). The screening-level EXAMS model for the premanufacture testing of toxic chemicals in site-specific water quality problems (Burns and Cline 1985) does not include a simultaneous mass balance equation for suspended sediment. The existing analytical models by Richardson et al. (1983) and by van Gils (1988), which does not capture kinetics of physio-chemical reactions, are simple and descriptive or conceptual and suitable only for first approximation. Gu et al. (1996) developed and applied a longitudinal 1-D simulation model for contaminated density currents in the Shasta Reservoir during and following the 1991 Sacramento River toxic spill. The model was intended to describe the gross flow behavior and to analyze the dilution mechanism of the contaminant plume in different flow regimes and under stratified reservoir conditions. However, the model treated the spilled chemicals as a conservative tracer, excluding the kinetics of physical and chemical processes. Other existing 1-D models (Schnoor et al. 1992), including WASP5/TOXIC5 (Ambrose et al. 1987, 1993), are not capable of providing insight into mixing processes and depicting the fate and transport of toxic substances under various flow regimes in a river/reservoir system. Therefore, a 2-D model capable of simulating toxicant concentration levels at various times and locations in a river and reservoir system has been lacking, in addition to the needed real-time prediction and analysis program for emergency response and remediation management.

The objectives of the proposed research are (1) to develop and validate an integrated 2-D mathematical model that simulates and predicts the fate and transport of toxic chemical spills and runoff in rivers and reservoirs or lakes, (2) to develop a real-time prediction and analysis computer program for emergency responses and remediation management, and (3) to incorporate the prediction system into an existing regional contingency plan or a toxic contamination control program at the state level. Real-time modeling must be fast or by the time that analysis and results are received the priorities for contamination control may have changed. To meet the requirements, the following special features of the model will be considered: (a) interactive, (b) operable on a personal computer or microcomputer, (c) directly accessible to input data, (d) automatically linked to the hydrologic and hydrodynamic database, and (e) short prediction time compared to actual spill travel time. The menu-driven computer simulation and analysis program to be developed will include a data entry module, an integrated spill model, and a visualization/output data presentation module. The program can yield travel times and

concentration curves versus time at various locations and provide timely information by forecasting the location and distribution of toxicants in the event of a toxic spill or runoff.