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Project Summary

Conceptual Development of a Toxic Screening Model

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A project was conducted to determine the utility of a model-based technology for screening the types and concentrations of contaminants that might exist at any point along a stream system. The project was conducted for the lower Mississippi River in the vicinity of New Orleans. A routing and graphical display system (RGDS) was used for the screening process. This system was composed of an analytical reach file and other data bases developed by the U.S. Environmental Protection Agency (EPA). Together these files can be used to route pollutants along the stream system represented in one of the data files. Presently more than 68,000 stream reaches are represented in the data base.

The technology represented by the RGDS was appropriate to the task, but results would have been better if more specific information had been available on the types and quantities of contaminant actually discharged and if specific disappearance rates had been available for the selected contaminants. Pilot-scale tests of this technology are recommended for other locations throughout the United States.

This Project Summary was developed by EPA's Municipal Environmental Research Laboratory, Cincinnati, OH, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

This project examines the utility of a model-based technology for screening the types and concentrations of contaminants that might exist at any point along a stream system. The specific purpose of the project was to conduct this screening process for the lower Mississippi River in the vicinity of the City of New Orleans and to determine the feasibility of further developing it. A routing and graphical display system (RGDS) was selected to carry out the screening process and to demonstrate that this technology could be used for similar purposes at other locations through the United States.

Routing and Graphical Display System

The RGDS is used in conjunction with the analytical reach (AR) file system and other data bases developed by the U.S. Environmental Protection Agency (EPA). Together they form a modular set of computer-based data files and progams that can be used to route pollutants along the stream system represented in one of the data files. At present, more than 68,000 stream reaches are represented in the data base.

The central component in the RGDS is the AR file. Information in the AR file is organized by reach -- that is, a stretch of river uniquely defined by an upstream and downstream point. The AR file contains both base data on stream reaches (length, flow, etc.) and a description of the stream connecting the reaches. In addition, the AR file can save information generated by analysis programs for further analysis and display.

Other information required for analysis is stored in two other data base files: the industrial facilities discharge file (IFD) and the pollutant matrix file. The IFD file contains discharge and discharger information such as discharge flow, the reach to which flow is discharged, and the industrial category or SIC number of the discharger. Information on both industrial and municipal dischargers is included in the IFD. The pollutant matrix file provides information on representative concentrations of selected pollutants under varying treatment conditions for the various industrial discharger categories as stored in the IFD.

Two types of analysis programs are available for estimating the impacts of pollutants on receiving streams: the downstream-directed influence line program, and the upstream-directed influence line program. Both programs use the same general modeling techniques, which incorporate both dilution effects and effects of decay (disappearance)of certain constituents. The effect of dilution is estimated by simple mass balance, as represented by the equation:

Concentration = Load/Flow

A first-order, exponential decay function dependent upon travel time is used to estimate disappearance of constituents because of physical, chemical, and biological processes. This disappearance is represented mathematically as:

$$C_{t_1} = C_{t_0} e^{-(t_1 - t_0)/K}$$

where

C_{t_1} is the concentration of constituent (n) at time t_1,

C_{t_0} is the initial concentration of constituent (n) at time t_0, and

K is the disappearance coefficient (constant).

In the downstream-directed influence line approach, pollutant loadings calculated by information stored in the IFD and pollutant matrix file were applied to a stream and the resulting pollutant concentration at any downstream point was calculated through dilution ratios and first order kinetics. In the upstream-directed influence line approach, the user specified an *in situ* pollutant concentration at any stream point and dilution ratios, and first-order kinetics were used to estimate the maximum pollutant concentrations at upstream points. Both programs store the pollutant concentrations estimated for the downstream end of each reach in the AR file for further analysis or display or both.

The primary display module used in this demonstration project was the profile display software. This software produces computer generated profile (influence line) plots of any information stored in the AR file. For example, it may produce a profile of pollutant concentrations along the Mississipi River from Memphis to New Orleans as calculated by the downstream-directed influence line program.

The overall system is designed to encourage the user to iteratively simulate and display a wide range of alternatives. Used in this context, the system can be a powerful planning tool in the area of water resources and water quality analysis.

Study Area

The study area is composed of Hydrologic Region 8, the Lower Mississippi River, as defined by the Water Resources Council. This area encompasses the mainstream of the Mississippi River, from its confluence with the Ohio River to the Gulf of Mexico and all the tributaries in between that are represented in the AR file data base. Hydrologic Region 8 is represented by approximately 1800 reaches or stream segments in the AR file data base. Primary emphasis is placed on the highly industrialized mainstem of the Mississippi River from the Baton Rouge area to New Orleans.

Streamflow and suspended solids time series data are available from the U.S. Geological Survey (USGS) for a gaging station at Tarbert Landing, Mississippi. This gaging station is approximately 200 miles upstream of New Orleans and 8.2 miles downstream of the Old River control structure, through which approximately 30 percent of the streamflow is diverted to the Atchafalaya River Basin. Based on the gage data for the period of record (water years 1973-79), the average flow at this point on the mainstem Mississippi River is approximately 540,000 cfs, and the range flow is 129,000 to 1.5 million cfs. Time-of-travel (velocity) information based on dye studies by USGS are available in the RGDS. Average velocities for the mainstem Lower Mississippi River are 2.6 fps and 1.5 fps for average and low flows respectively.

Water Quality

Water quality data for the Lower Mississippi River are extensive and available from several sources. This study used sampling data collected and analyzed at the Jefferson Parish Water Treatment Plant just upstream of New Orleans. This data base covered a 3-year period and included analyses of nonspecific organics, volatile organics, semivolatile organics, physical and chemical constituents, and microbiological parameters.

Various statistical and graphical analyses were performed on the data set, and the following observations were made.

- Because the concentration and loading of most contaminants vary greatly, it is presumed that streamflow influences pollutant concentration and that the discharge of the mass of contaminants varies greatly

- Because streamflow and contami nant concentration or load do no correlate for most contaminants very little relationship exist between river flow and the presenc of contaminants.

- A few contaminants appeared t have a strong negative correlatio with streamflow (i.e., as streamflo increased, contaminant concentra tion decreased). This result suggest that the contaminant mas discharged is reasonably constan for these contaminants.

- A strong positive correlation appea to exist between streamflow an contaminant concentration for a fe contaminants. This result is not easy to interpret, but it may caused by increased discharges contaminants at higher flow including contaminants contained runoff or groundwater inflow.

- Very little correlation appears to exi between the concentration contaminants and suspended solid This result is interpreted to mea that sediments do not appear to a as a significant reservoir or transpo mechanism for the contaminan (assuming the analytical procedur extract contaminants attached to t sediments). A few contaminants a negatively correlated wi suspended solids concentration; b these may be spurious correlatio given the apparent lack of correlati between flow and contamina concentration and the stro correlation between streamflow a suspended solids. This result is to expected given the severe eros problems of the central Uni States.

EPA has expressed an interest in the contaminants listed in Table 1 beca they were consistently present in water quality samples and because there is relatively more known about the character of upstream discharges of these contaminants. The means and standard deviations of these contaminants are presented in Table 1 together with the concentrations defining the lower and upper 10 percent of the distribution of values (i.e., limits within which 80 percent of values were observed).

Technology Application

The RGDS was applied to Hydrologic Region 8 under varying hydrologic conditions Both the downstream-directed and upstream-directed methods were used

The downstream-directed influence line approach was applied for 12 different contaminants at two different streamflow regimes for three assumed disappearance rates. The contaminants were selected on the basis of the *in situ* water quality data base at Jefferson Parish and the availability of discharger data in the pollutant/contaminant loading matrices. The contaminants selected were those given in Table 1 and phenol. The flow regimes used for the analyses were average and low streamflows contained in the AR file data base. Low flow, as defined in the file, is an estimate of the minimum weekly flow that is expected to occur once every 10 years (i e , the lowest 7-day flow in 10 years). The three assumed disappearance rate coefficients were 0, 0 05, and 0.2 days^{-1}. A value of zero was selected to demonstrate the effect of a conservative contaminant The disappearance rate coefficient of 0.2 day^{-1} results in a half-life of approximately $3^1/_2$ days, which corresponds with the upper end of decay rates and was selected to demonstrate the effect of rapidly decaying contaminants. In all cases, the concentration of pollutants in water flowing into the study area boundaries was assumed to be zero

Discharges of pollutants to the river were estimated by using the IFD file and a supplementary pollutant matrix file for the selected organic constituents provided by EPA This matrix used a combination of (1) specific representative information for industries on the Lower Mississippi River, and (2) industry-wide representative discharger data

The upstream-directed influence line approach was applied under the same streamflow and decay characteristics assumed for the downstream-directed influence line approach. For example, the *in situ* concentration was fixed at 10 μg/L at the end of the reach immediately upstream of New Orleans for all flow and decay conditions

Results

Based on the downstream-directed approach, contaminant profiles were produced for each of the selected constituents for the selected streamflows and decay rates The simulated concentrations and actual *in situ* values at Jefferson Parish are presented in Table 2 Except for nitrobenzene, bis (2 ethyl hexyl) phthalate, and toluene, the simulated values reasonably approximate the range of *in situ* concentrations The correspondence is best at average flow The simulated concentrations at low flow exceed the range of actual values for some contaminants (e g , benzene) This result might be expected because actual streamflows during the monitoring program were never as low as the low flow used for simulation. An anomaly is apparent in the case of carbon tetrachloride. For this pollutant, the low flow simulated values are within the range of actual values, but the average-flow concentrations are not. This result could indicate an under loading of carbon tetrachloride in the simulation compared with actual quantities discharged to river.

Conclusions

The technology represented by the RGDS was appropriate to the task, but the quality and specificity of the results would have been considerably enhanced if (1) more specific information had been available on the types and quantities of contaminants actually discharged upstream, and (2) specific disappearance rate had been available for the selected contaminants

Results of downstream-directed and upstream-directed analyses used in conjunction with the results of a water quality monitoring program, the IFD, and the pollutant loading matrix provide a method for comparing simulated and observed concentrations. Thus, the types and concentrations of contaminants actually being discharge (as defined by IFD and pollutant matrix) could be compared with those that would have to be discharged upstream to produce the observed types and concentrations of contaminants

Contaminant contributions from runoff leachate, from contaminant disposal sites, and from spills were not considered in this project. If the contaminant

Table 1 *Statistical Characteristics of Selected Pollutants in the Mississippi River at Jefferson Parish*

Pollutant No	*Pollutant*	*No of Samples*	*Mean Conc (μg/L)*	*Standard Deviation*	*Conc Defining Lower 10% of Distr Values (μg/L)*	*Conc. Defining Upper 10% of Distr Values (μg/L)*	*Mean Conc. (μg/L)*	*Standard Deviation*
47	*Dichloromethane*	*209*	*712*	*1824*	*0*	*1900*	*1.34*	*3.17*
7	*Chloroform*	*209*	*800*	*633*	*200*	*1660*	*1 80*	*1.54*
43	*Carbon Tetrachloride*	*209*	*248*	*1006*	*0*	*250*	*0.50*	*1.63*
23	*1,2-Dichloroethane*	*209*	*3585*	*4889*	*480*	*8600*	*7 30*	*8.46*
35	*Trichloroethane*	*209*	*188*	*396*	*0*	*390*	*0.53*	*1.47*
126	*Tetrachloroethane*	*156*	*74 6*	*170*	*0*	*140*	*0.20*	*0.52*
27	*Benzene*	*103*	*299*	*526*	*0*	*720*	*0.56*	*1.25*
31	*Toluene*	*103*	*45 5*	*100*	*0*	*210*	*0.11*	*0.29*
91	*Bis (2-ethyl hexyl) phthalate*	*306*	*16 8*	*97*	*1 1*	*18.7*	*0 05*	*0.29*
104	*Fluorene*	*263*	*1 72*	*4 6*	*0*	*4 8*	*0.006*	*0.018*
98	*Nibrobenzene*	*263*	*28 2*	*37 7*	*0*	*70*	*0.06*	*0.17*

contribution from such sources can be quantified, however, the RGDS technology can be used to simulate the resulting downstream concentrations.

In summary, the RGDS is useful for conducting model-based screening to estimate the types and concentrations of contaminants that might be expected to occur at a specified location downstream of discharges containing the contaminants. Of course, the stream reaches involved must be part of the AR file system data base. The quality of the screening results will be largely determined by the quality of the input data on the types and quantities of contaminants being discharged and the specificity with which the disappearance rate can be defined for each contaminant.

The user's objectives would determine which, of the dozens of available models, would be selected. Models such as EXAMS and TOXIWASP use a sophisticated kinetic structure that allows the study of different ionic forms of a chemical, several ways to calculate photolysis, etc. Although the EXAMS fate module formulates a total transformation rate, the extensive data requirements could be too costly and time-consuming for preliminary water resource planning strategies. As research advances on the fate of chemicals in local environments, it seems feasible that a refined overall disappearance rate for the priority pollutants will be available without having to determine the individual data necessary to operate EXAMS. If the user requires different hydraulics or chemical processes, other models should be considered; but for this analysis, the simple model presented can provide the results desired given the resources available.

Recommendations

To improve the quality of screening results, users must understand the limitations of the approach and be aware of the latest discoveries about relationships between contaminants and the environment. Before implementing the RGDS, or any model, the following recommendations should be considered:

- Reasonable, accurate disappearance coefficients should be developed for either specific contaminants or specific classes of contaminants.
- More specific and detailed discharge contaminant loading data should be incorporated into the pollutant loading matrix (e.g., those available from NPDES permit applications, operating reports, and compliance monitoring).
- The technology should be applied on a pilot scale to other situations throughout the United States where data similar to those from Jefferson Parish are available.

The full report was submitted in fulfillment of a purchase order contract by W. E. Gates and Associates under the sponsorship of the U.S. Environmental Protection Agency.

Table 2. *Comparison of Simulated and Observed Concentrations at Jefferson Parish*

			Simulated Concentrations (µg/L)					
			Average Flows			*Low Flows*		
Pollutant	*Pollutant No.*	*Average Conc. (µg/L)*	*K=0*	*K=0.05*	*K=0.2*	*K=0*	*K=0.05*	*K=0.2*
Dichloromethane	*47*	*0.712*	*0.093*	*0.076*	*0.044*	*0.408*	*0.291*	*0.113*
Chloroform	*7*	*0.800*	*0.562*	*0.445*	*0.242*	*2.541*	*1.656*	*0.604*
Carbon tetrachloride	*43*	*0.248*	*0.007*	*0.006*	*0.004*	*0.033*	*0.023*	*0.009*
1,2-Dichloroethane	*23*	*3.585*	*7.412*	*6.116*	*3.507*	*33.635*	*23.318*	*9.080*
Trichloroethane	*35*	*0.188*	*1.061*	*0.846*	*0.464*	*4.781*	*3.150*	*1.159*
Tetrachloroethane	*126*	*0.075*	*0.065*	*0.045*	*0.024*	*0.454*	*0.189*	*0.069*
Benzene	*27*	*0.229*	*1.764*	*1.456*	*0.835*	*7.767*	*5.550*	*2.161*
Toluene	*31*	*0.046*	*1.417*	*1.169*	*0.670*	*6.238*	*4.459*	*1.736*
Bis (2-ethyl hexyl) phthalate	*91*	*0.017*	*0.066*	*0.048*	*0.028*	*0.472*	*0.213*	*0.094*
Fluorene	*104*	*0.002*	*0.009*	*0.007*	*0.004*	*0.038*	*0.028*	*0.011*
Phenol	*NA*	*NA*	*7 135*	*5.708*	*3.140*	*31.581*	*21.196*	*7.804*
Nitrobenzene	*98*	*0.028*	*5.631*	*4.649*	*2.664*	*24.794*	*17.716*	*6.899*

NA = Not Available

*USGPO: 1984-759-102-10679

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The complete report, entitled "Conceptual Development of a Toxic Screening Model," (Order No. PB 84-223 494; Cost: $13.00, subject to change) will be available only from:

National Technical Information Service
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