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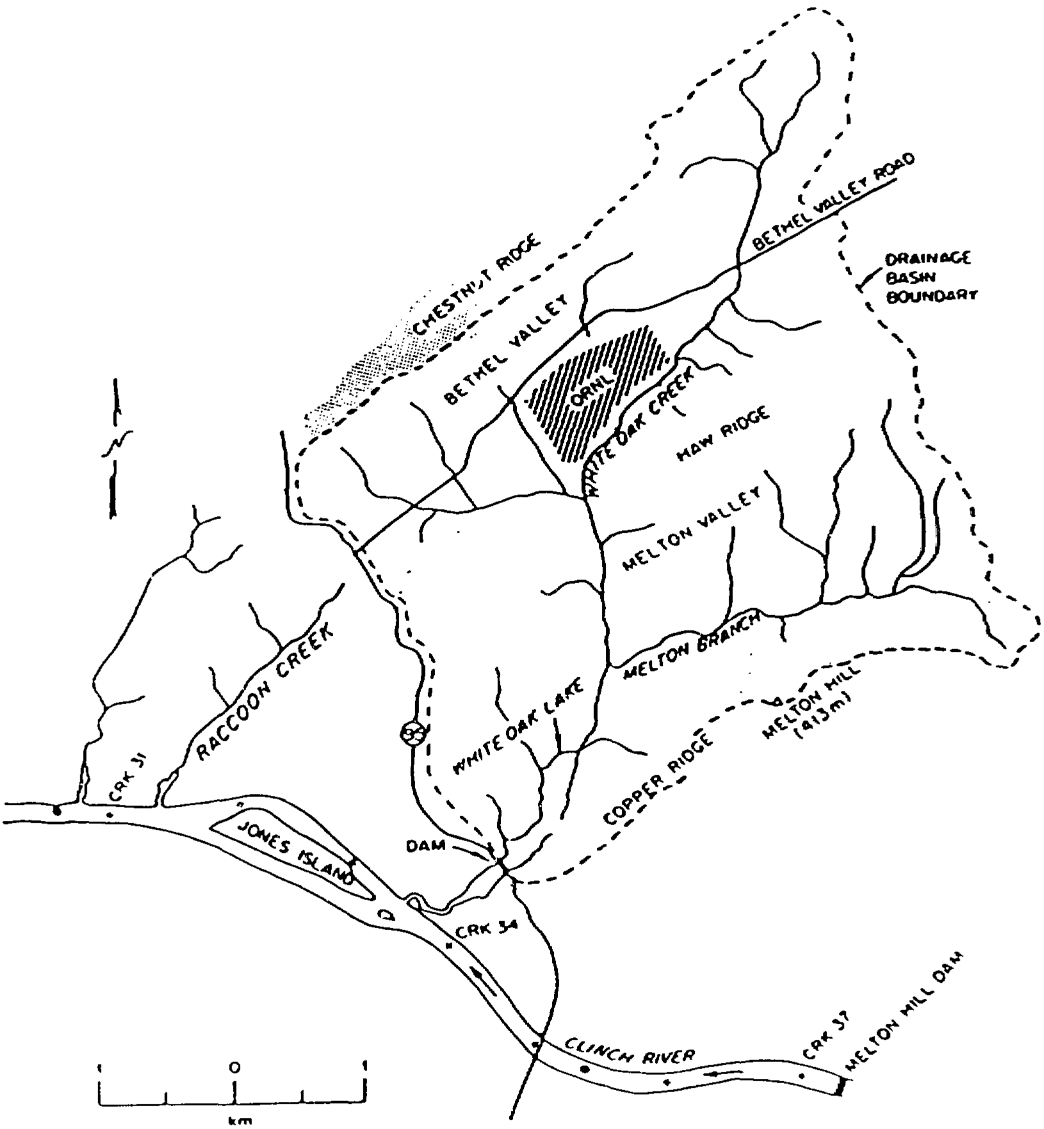
FORECASTING CONTAMINANT CONCENTRATIONS: SPILLS IN THE WHITE OAK CREEK BASIN - Dennis M. Borders, The University of Tennessee, Knoxville, Tennessee; David W. Hyndman, Oak Ridge Associated Universities, Oak Ridge, Tennessee; Dale D. Huff, Environmental Sciences Division, Oak Ridge National Laboratory (operated by Martin Marietta Energy Systems, Inc., under contract DE-AC05-84OR21400 with the U.S. Department of Energy), Oak Ridge, Tennessee.

INTRODUCTION

The Streamflow Synthesis and Reservoir Regulation (SSARR) model has been installed and sufficiently calibrated for use in managing accidental release of contaminants in surface waters of the White Oak Creek (WOC) watershed (Figure 1) at ORNL. The model employs existing watershed conditions, hydrologic parameters representing basin response to precipitation, and a Quantitative Precipitation Forecast (QPF) to predict variable flow conditions throughout the basin. Natural runoff from each of the hydrologically distinct subbasins is simulated and added to specified plant and process water discharges. The resulting flows are then routed through stream reaches and eventually to White Oak Lake (WOL), which is the outlet from the WOC drainage basin. In addition, the SSARR model is being used to simulate change in storage volumes and pool levels in WOL, and most recently, routing characteristics of contaminant spills through WOC and WOL.

The Discharge Forecast Modeling Project originated as a result of the Strontium-90 Action Plan, a response to the abnormal release of radionuclides that occurred from WOC during late November and early December 1985. Excavation activities in the vicinity of the Building 3517 (Fission Products Development Laboratory, FPDL) construction site, combined with heavy rainfall, initiated the release into WOC. The incident occurred when a broken storm drain resulted in contact between ^{90}Sr-contaminated soil and storm runoff, which subsequently entered the storm and sanitary drainage systems. Several notable problems became obvious during ORNL's response to this release: (1) no predetermined criteria existed for the operation of White Oak Dam (WOD) in response to spills, (2) the hydrodynamics of contaminant transport and dispersion within the WOC watershed and downstream were not adequately understood to support requests for modified reservoir releases, and (3) real-time data on streamflow, precipitation, and water quality within the watershed were not readily available in sufficient quantity and usable format. The modeling study was initiated to help address these problems.



ORNL-DWG 86-8445

Figure 1. White Oak Creek drainage basin map.

DATA ACQUISITION AND EVALUATION

ORNL Monitoring Data

Perhaps the most important element involved in hydrologic modeling and discharge forecasting is the data base available to support the calibration and development of hydrologic simulations. The SSARR model has helped to identify limitations in the present data collection process and provide a framework for organizing and using the data that are gathered. Various organizations have been involved in data collection within the ORNL reservation, and historically each organization has dealt with its data according to specific needs. In addition, the projects for which hydrologic data were collected have not had coordinated data management procedures. Because of the diversity of data types needed for discharge forecast modeling and overlapping collection responsibilities, data management was a major task.

The initial forecast modeling required continuous flow records and climatic data at short time intervals for small sub-catchments within the WOC watershed. Several important gaps in WOC hydrologic monitoring were identified in the process of data acquisition. For example, there were no instruments for monitoring the water surface elevation of WOL and there were no gaging stations located upstream from the ORNL main plant area. Most of the problems have been or are being corrected as part of a continuing effort to improve and expand the current basin monitoring network.

In order to make timely forecasts for emergency response, it is necessary to access real-time data on streamflow and precipitation at a number of stations within the drainage basin. ORNL's Department of Environmental Monitoring and Compliance (EMC) began acquiring real-time data for WOC, Melton Branch (MB) and WOD in October, 1986. Then, as part of planned improvements, EMC installed a new Data Acquisition System (DAS) and installed more powerful data concentrators at the ambient water monitoring stations in June, 1987. With the application of this system, near real-time data signals are available at the three ambient monitoring stations on the new VAX 11/750 digital computer system. The system is equipped with a means of data verification which flags invalid values as well as system alarms for identifying values which fall outside acceptable ranges. Plans are being made to acquire a dedicated phone line within the Environmental Sciences Division (ESD) for direct access to all needed data available within the system. This will allow a direct link from the EMC computer data base to PCs in ESD where data can be continuously downloaded for input to SSARR modeling.

USGS Hydrologic Data

The U.S. Geological Survey (USGS) continues to work with ORNL to establish and maintain surface-water recording stations in and around the WOC watershed. Data from the following new stations have recently become available: First Creek monitoring station above WOC, the Parshall flume on WOC in the main plant area, and a satellite link (data collection platform, DCP) reporting near real-time flow and precipitation data at the 7500 Bridge monitoring station. A telecommunications link with the USGS data base in Nashville enables direct access of these data for present and future application to SSARR modeling.

The satellite link at 7500 Bridge became operational in April 1987, making flow data available on a near real-time basis. Under normal operating conditions, data are available no later than four hours after values are recorded. At stages of three feet or higher, the signal is reported every 15 minutes, but this situation occurred once in the initial days of site operation, and has not been verified recently. In September, 1987, a precipitation sensor was added to the DCP system, and these data are now available on the same basis as the streamflow records. In the future, an air temperature sensor may be installed at the 7500 Bridge station to supply modelers with near real-time temperature data (required for the new version of the SSARR model). USGS flow data from 7500 Bridge were invaluable as a substitute for WOC data when the record at that station (MS3) was missing.

Quantitative Precipitation Forecasts

ORNL staff have visited the Atmospheric Turbulence and Diffusion Laboratory (ATDL) in Oak Ridge to discuss the status of the emergency response forecast information service. The ATDL can now supply 48-hour (Day 1 and Day 2) QPFs (necessary for SSARR model discharge forecasting) with a breakdown for Knoxville every 6 hours. These forecasts are available as FAX System Products and are updated twice a day (12-h updates). Efforts are also being made to establish a modem link to enable ORNL direct access to the FAX system. In addition, the system is due to be upgraded soon to provide an expanded selection of QPF products. In the event that a QPF cannot be obtained from the ATDL, The National Weather Service (NWS) also maintains a 24 h/d QPF center which can provide 6-h QPFs for two days in advance. In addition, a staff member in the Energy Division, ORNL, obtains QPFs on a daily basis and can provide this information if necessary.

SSARR FORECAST MODELING

Water Quality Modeling

For spill response applications, the model has been adapted to the simulation of ^{90}Sr discharges from a combination of non-point and point-source releases. Strontium-90 has been the primary contaminant studied because it is regarded as one of the most likely candidates to cause an emergency incident by accidental release into WOC. It is also conservative and highly stable. Records of average monthly ^{90}Sr concentrations in WOC for calendar year 1986 as well as records of Solid Waste Storage Area no. 4 (SWSA-4) surface water flows and ^{90}Sr concentration versus flow for November 1985 to March 1987 have been collected. The flow versus ^{90}Sr relationship for SWSA-4 for this period of record has been scaled to represent background contaminant in WOC as a conservative estimate of average observed concentration. Therefore, background concentration is now continuously simulated as a function of flow for the WOC watershed. This relationship will be refined in the future as justified by the collection of samples from WOC at various flows.

Though simulation of background contaminant flux is important to water quality modeling, the major concern lies in forecasting the fate of hazardous substances released into the WOC system. Specific questions which must be addressed include "How long does it take a contaminant released from the main plant area to reach White Oak Dam (WOD)?", "What is the dilution of the contaminant as it travels through WOL?", and "How long will it take before the entire pulse of contaminant has passed through the dam?". Obviously, the answers to these questions vary considerably according to flow conditions and the regulation of the gates at WOD.

In addition, the character of the contaminant has an affect on its residence time within the watershed. Non-conservative (biodegradable) contaminants, such as ethylene glycol, react differently than ^{90}Sr under similar conditions. Modeling the basin response to this type of pollutant will require development of unique parameters for each contaminant considered, including decay coefficients, sediment partition coefficients, etc.

Recently, water quality modeling has been directed toward the development of procedures to simulate basin response to significant contaminant releases (particularly ^{90}Sr) into WOC from the main plant area at ORNL. A basic relationship was developed to route a contaminant spill through WOL assuming constant flow into the lake. According to this scheme, spills are routed coincident to, but independent from, basin model flows with theoretical reach and reservoir routing functions to simulate travel time and dispersion through WOC and WOL to subsequent output at WOD. Contaminant mass flux in WOC and WOL must be simulated as a relationship which is a function of the flows occurring simultaneously within the watershed. The emergency response to a simulated accidental spill (environmental drill) followed this type of procedure for forecasting the release of contaminants from WOD.

Environmental Drill

To test the emergency response of the SSARR modelers to a simulated contaminant release from the main plant area, an environmental drill was planned for June 1987.

To prepare for simulating the response to an actual contaminant release on WOC, a standard procedure was developed to follow each time an incident occurred. A procedure has been established to obtain timely information during emergency conditions on expected flow conditions, time of travel of contaminants, concentrations at key locations, and the consequences of alternative release procedures at WOD. A chart was prepared (Table 1) listing the steps to be taken upon notification of a spill. Included in this chart are the input data necessary for each step as well as all possible sources of this data. This procedure is subject to revision pending further model development and methods of data acquisition. Figure 2 illustrates a more comprehensive view of the

ORNL-DWG 87M 15562

PROCEDURE FOR RESPONSE TO CONTAMINANT RELEASE

STEP	INPUT DATA	SOURCE
1. UPDATE COMPUTER DATA	FLOW (MS3, MS4, MS5, 7500 BRIDGE) PRECIP. (WOD, MELTON VALLEY)	WOCC OPERATOR USGS DATA BASE EMC
2. GATHER FIELD DATA	SAME	FIELD VERIFICATION
3. OBTAIN QPF	QUANTITATIVE PRECIPITATION FORECAST	ATDL OR NWS
4. MAKE INITIAL ESTIMATE OF WOL STORAGE	FLOWS, LAKE ELEVATION	EMC
5. PROCESS DATA SSARR FORMAT		
6. SPILL DESCRIPTION	SPILL (CONTAMINANT DISCHARGE - TIME AND VOLUME)	
7. RUN SSARR MODEL BACKUP	FLOW, PRECIPITATION, UPDATED MODEL RUN	PREVIOUS
8. ENTER SPILL DATA		
9. SIMULATE VARIOUS SCENARIOS (BEST, WORST CASES)	SPILL, QPF LAKE REGULATION	PREVIOUS
10. DETERMINE WOL STRATEGY - PASS INFORMATION TO DISPERSION MODELERS	FORECAST AND DISPERSION GROUPS	

Table 1. Procedure for response to contaminant release.

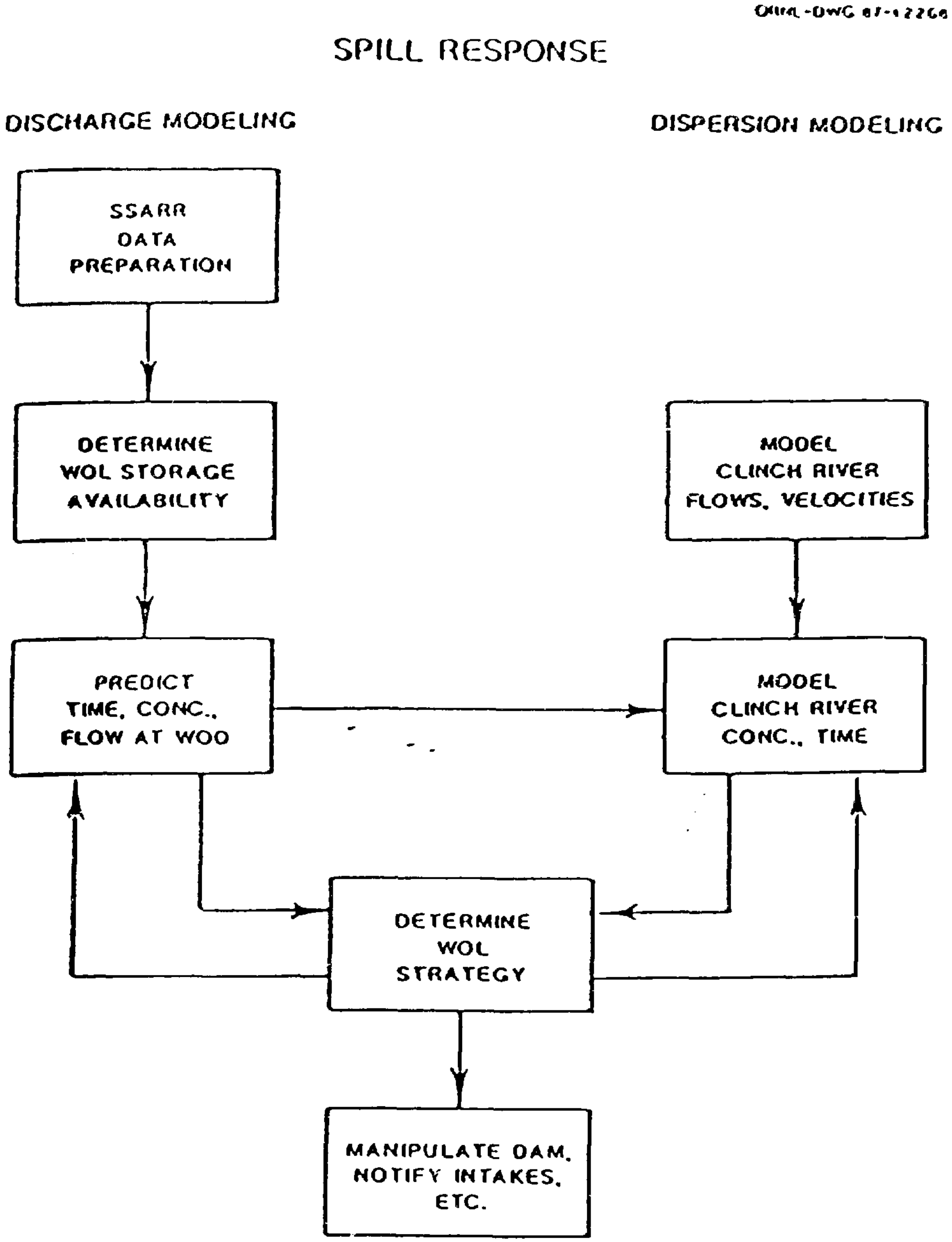


Figure 2. Flowchart of events and interaction between Discharge Forecast and Dispersion modelers.

sequence of events and the interaction which takes place between the discharge forecast and dispersion modeling groups. The dispersion modelers are concerned with the dispersion of contaminants downstream from WOD in the Clinch River system. When a spill is reported, data on flow conditions and lake elevation are needed to make an initial estimate of storage availability on WOL. This initial estimate will inform forecast modelers and management how long the gates on the dam can be closed, under existing conditions, until action is required to avoid overflow conditions at WOD. With the acquisition of all data including a QPF, SSARR model "backup" calculations (a routine which matches model simulations with current conditions), and simulation of the various scenarios (best and worst cases) can begin. At the same time, the dispersion modelers are engaged in modeling Clinch River flows and velocities. After modeling the various possible scenarios to determine timing and concentration of flows at WOD, a transfer of information can take place between the two modeling groups. At this point decisions must be made on the strategy to be employed for the regulation of the gates at WOD and notification of those responsible for the intakes downstream on the Clinch River.

On June 25, Discharge Forecast modelers simulated the following hypothetical spill scenario:

> At 5:30 a.m., assume a waste storage tank ruptured and approximately 30,000 gallons of waste, containing 100,000 Becquerels per liter (Bq/L) was released. By 7:30 am, assume all the waste had entered White Oak Creek near the process waste treatment plant.

The response to this scenario followed the steps set forth in the procedure previously described. The previous day's data was retrieved from the Waste Operation Control Center's operator by phone; however, the flow record at Melton Branch (MB) was incomplete. An ESD data logger, which was placed on MB in May, provided a means to avoid a data gap. A QPF was acquired by phone through the Atmospheric Turbulence and Diffusion Lab in Oak Ridge. The SSARR model backup calculations had been roughly prepared in advance, as part of an effort to test a new version of the model that was not yet operational. The spill data were entered into the model in units of Bq/s. The model forecast was simulated under the best case scenario (no rain over the period of forecast) assuming the gates of WOD were left open. Figure 3 illustrates the simulated basin response to the hypothetical spill through WOL and the contaminant discharge at WOD. A peak waste concentration of 292 Bq/L (59,540 Bq/s at an average flow of 7.2 cfs) was predicted at the dam approximately 48 hours after the assumed spill was released into WOC.

Upon obtaining results such as these, the predicted flows and concentrations at WOD would be passed on to the dispersion modelers. Output from dispersion modeling would include time and concentrations at the Oak Ridge Gaseous Diffusion Plant (K-25) water intake and downstream at Kingston. It should be noted that the results from the discharge forecast modeling represent only the best case scenario at constant flow conditions. Additional scenarios include variable flow conditions

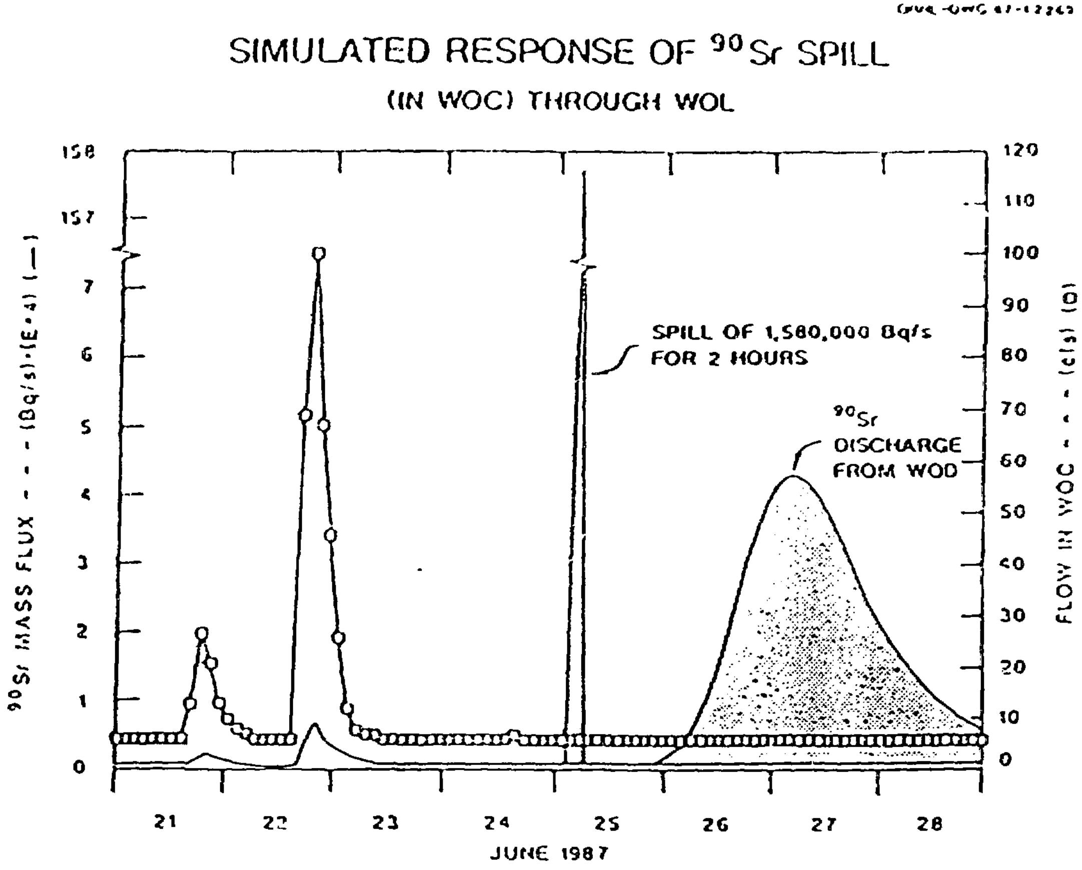


Figure 3. Simulated response of ^{90}Sr spill in White Oak Creek and discharge through White Oak Dam.

(precipitation over the forecast period), as well as all flow conditions with and without regulation of the gates at WOD.

Current Model Applications

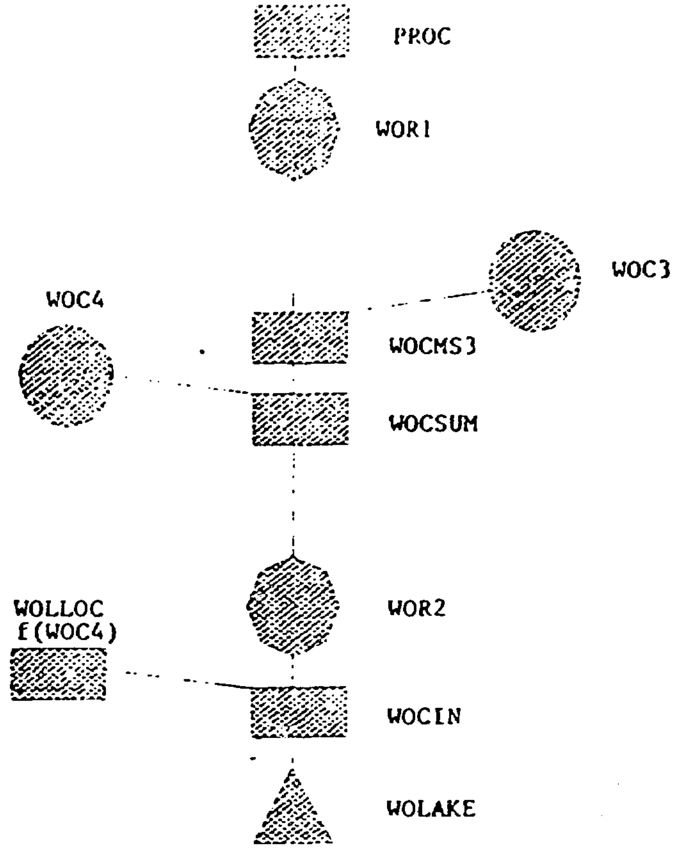
The SSARR model was not developed specifically to simulate and forecast water quality in units of mass flux, only flow in units of volume per increment of time (e.g. ft^3/sec [cfs]). Therefore, contaminant releases must be transformed into units of flow (cfs) and added to surface water in order for the model to recognize them. The current model configuration is made up of two integral components: a flow routing branch (Figure 4) and a contaminant routing branch for modeling background contaminant concentration plus spills released from point or non-point sources. Under this scheme, background from each subbasin is continuously modeled as a function of basin flow while spills are added to model simulations, when they occur, according to their character and point of release to the flow system. The two branches of the model combine (Figure 5) above all routing reaches and reservoirs of the contaminant branch. Basin flows are added to contaminants prior to routing reaches and reservoirs in order for time of travel and dispersion of contaminants to be simulated as a function of the actual flow conditions occurring at that time. After routing flow plus contaminants through a reach or reservoir in the contaminant branch, basin flows are subtracted back out and transformed, leaving routed contaminant mass flux at any given location in the surface water system.

When representing contaminant mass flux in units of flow (cfs) in order to add to basin flows for purposes of routing through stream reaches and reservoirs, it is essential to scale all contaminant values down to a proper level to reduce the impact on natural routing characteristics. For example, given a curve for time of travel versus flow (Q) for a stream reach (Figure 6), a contaminant release of one unit (C = 1) added to each of flows Q_1 and Q_2 results in substantially different impacts to the natural flow routing character of the stream:

$Q_1 = 5$ Travel time = 1.6
$Q_1 + C = 6$ Travel time = 1.8

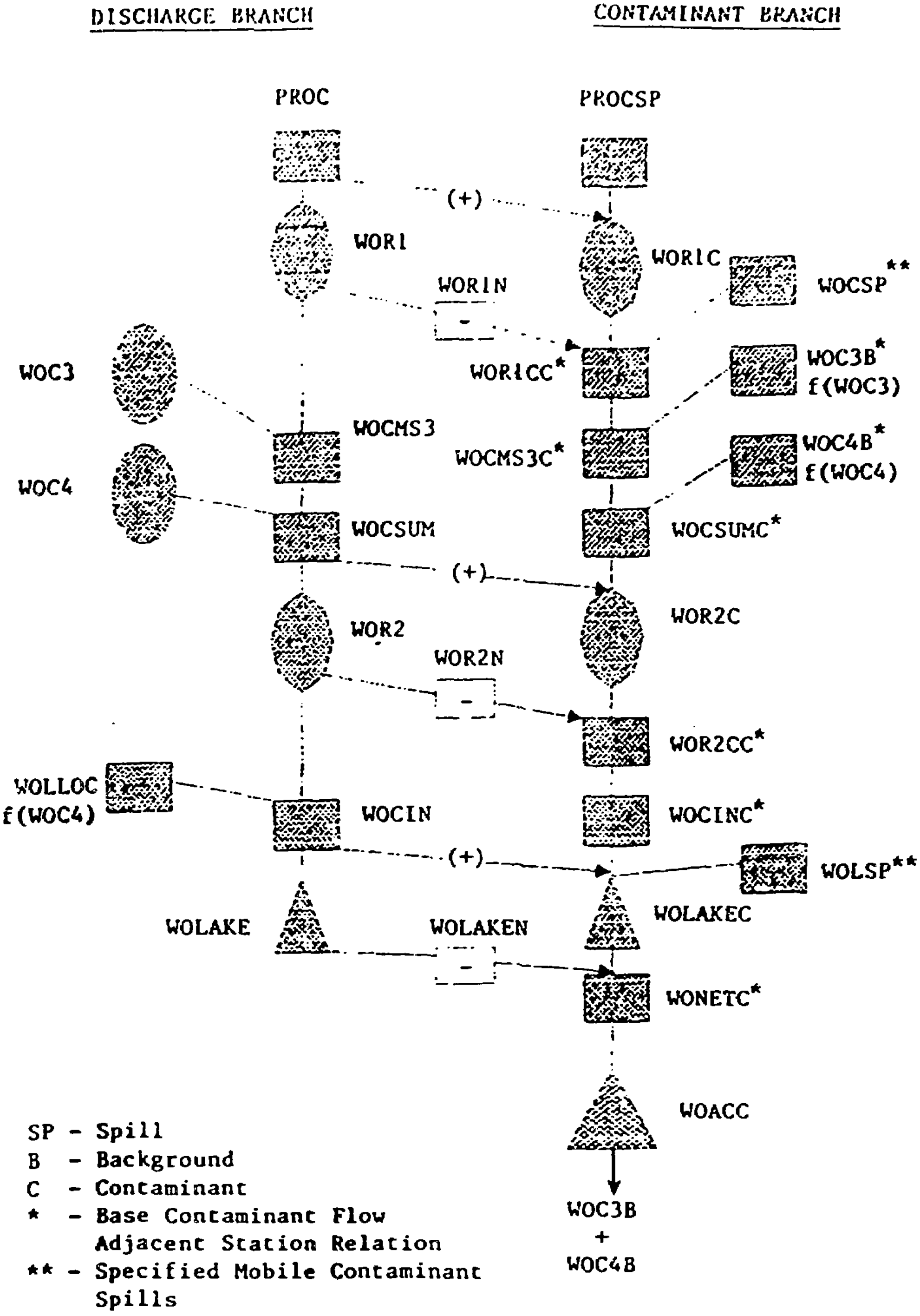
$Q_2 = 1$ Travel time = 4.6
$Q_2 + C = 2$ Travel time = 3.3

The addition of this contaminant release to Q_1 increases the time of travel by 11% while the same value added to Q_2 results in a 28% decrease. Errors of this magnitude could cause gross misrepresentation of basin response as well as loss of model capability to maintain conservation of mass of a contaminant released into the system. Therefore it is necessary to scale contaminant concentrations approximately two orders of magnitude lower than expected basin flows.



PROC = Process inflows to White Oak Creek
WOR1 = White Oak Creek Routing Reach No. 1
WOC3 = Basin runoff from White Oak Creek subbasin
WOC4 = Basin runoff from Melton Branch subbasin
WOCSUM = Summation of flows from Melton Branch and White Oak Creek
WOR2 = White Oak Creek Routing Reach No. 2
WOLLOC = White Oak Lake local inflow
WOCIN = Total inflow to White Oak Lake
WOLAKE = White Oak Lake Reservoir

Fig. 4. White Oak Creek Flow Routing Model Configuration.

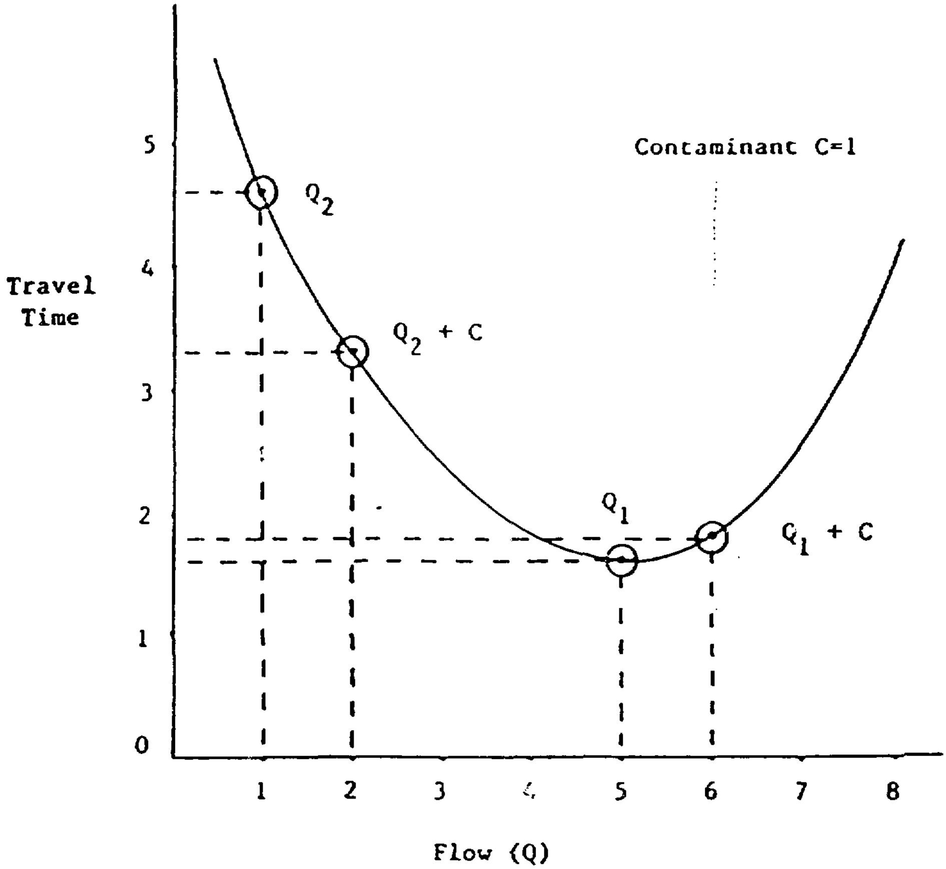


SP - Spill
B - Background
C - Contaminant
* - Base Contaminant Flow Adjacent Station Relation
** - Specified Mobile Contaminant Spills

Fig. 5. White Oak Creek Contaminant Routing Model Configuration.

ROUTING REACH - TRAVEL TIME

VERSUS FLOW RATE



$Q_1 = 5$	Travel Time = 1.6
$Q_1 + C = 6$	Travel Time = 1.8
$Q_2 = 1$	Travel Time = 4.6
$Q_2 + C = 2$	Travel Time = 3.3

Fig. 6. Stream Reach Time of Travel Versus Flow.

DYE TRACER STUDY

In September 1987, staff at ORNL performed a dye tracer study to further characterize surface waters of the WOC basin and to modify the SSARR model calibration. The present calibration of the flow model is based on the estimation of time of travel versus flow for various reaches in the watershed under varying conditions of flow. The dye study supplied real values for travel times under a base flow (low flow) condition. These values will enable the modification of both the flow and contaminant branches of model calibration. Real travel time will enable the flow model to more accurately represent the basin response to rainfall. At the same time, travel times and dispersion characteristics will enable the calibration of the contaminant portion of the model and begin to answer the questions previously asked concerning the fate and consequences of hazardous contaminants released into the WOC system. In addition, the knowledge of defined flow paths through WOL could help to expedite sampling and cleanup efforts in the event of a contaminant spill.

Prior to releasing dye into WOC above WOL, drogues (plastic milk jugs nearly full of water) were released below WOC into the headwaters of WOL. This was done to determine flow paths of water entering the lake and to facilitate calculations for quantity of dye to release upstream. The drogues proved to be an excellent indicator of flow paths through WOL.

On September 14, at 11:45 a.m., approximately 1.25 gallons of a 20% solution of Rhodamine WT dye were instantaneously injected into WOC just below the water monitoring station (MS3) above the confluence with Melton Branch, 1.02 miles upstream of WOD. Automatic samplers were placed along WOC below the dye injection point and just above the lake, on the North and South banks of WOL about half the distance to the dam, and at WOD (Figure 7). This sampling was done to develop an understanding of flow paths, time of travel, and dispersion characteristics through WOL. The dye was also visually tracked and timed at various points to verify results.

Visual observation indicated that the dye reached the upper portion of the lake at about 1:15 p.m. Initially, the dye appeared to stay in a fairly concentrated plume as it traveled over the shallow sediment bar which extends through the upper reaches of the lake. As it reached the deeper water of the lake, which is warmer than the WOC water, the dye appeared to sink and disappear from sight. Upon returning to the lake on the morning of Sept. 15 (day 2), the dye had reappeared along the south bank and had followed a distinct flow path to the old dam outlet structure, and then along the face of the dam (northward along highway 95) to the new outlet structure. At the same time, waters along the north bank of the lake appeared to be relatively free of dye. However, by the morning of the 16th (day 3), the dye appeared to be evenly dispersed throughout the lower reaches of the lake.

From the time of injection, it took approximately 90 minutes for the leading edge of the plume to reach the headwaters of WOL and another 45 minutes for the peak concentration to be reached at this site. Measured peak to peak, travel time for this section of the creek is 2 hours and 15 minutes. A dilution factor of 2.9 was calculated between these two

ORNL-DWG 86-9445

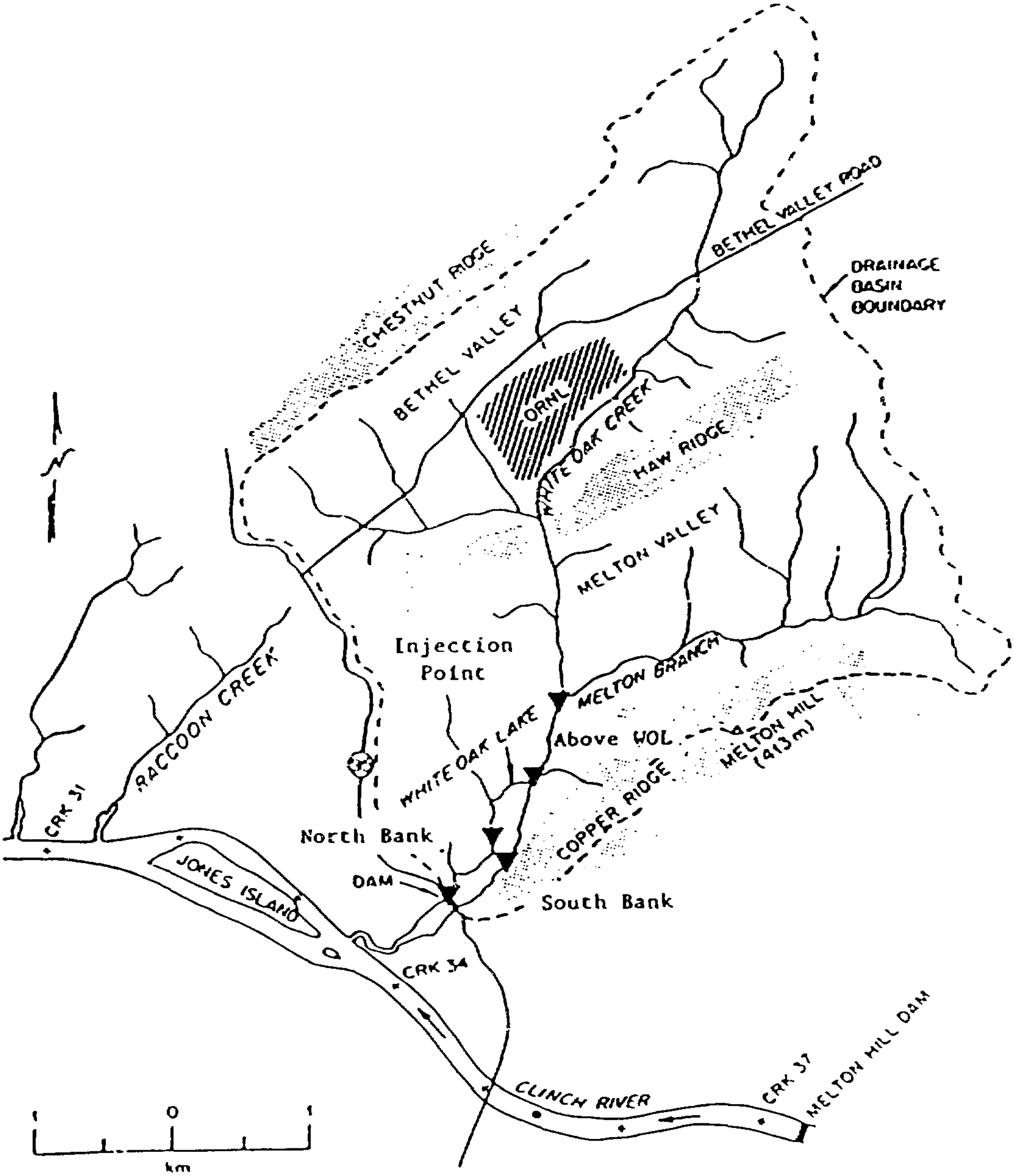


Figure 7. Location of automatic samplers during dye tracer study.

sites by comparing the peak of 4673 parts per billion (ppb) observed just below MS3 to the peak of 1613 ppb observed at the headwaters of the lake (Figure 8). From the time of injection, the leading edge of the dye plume (detectable concentrations) reached the dam in approximately 6 hours but less than 0.5 ppb of dye was recorded until approximately 12 hours after injection. The peak concentration measured at the dam was 22.5 ppb and was recorded 29 hours after the initial dye injection. Therefore, the time of travel through the lake is approximately 27 hours measured peak to peak under a low flow condition (Figure 9). A dilution of 72 times was calculated between the headwaters of the lake and the dam.

A second portion of the dye study is planned for further characterization of WOC above MS3. It will involve the injection of dye into WOC near the main plant area because this is the most likely area for an accidental release of contaminants to occur. Melton Branch (MB) will also be studied with dye tracer tests because of its effect on WOC and the possibility of a contaminant release from the High Flux Isotope Reactor (HFIR) located 0.95 miles upstream from WOC.

ETHYLENE GLYCOL SPILL

Some useful information on the time of travel in WOC has been obtained from data collected during a spill of ethylene glycol which occurred on August 7, 1987 (Figure 10). Ethylene glycol, a coolant fluid, contains fluorescein dye to facilitate tracing in the event of a spill. Samplers were placed along the creek approximately 2 hours after the spill. However, the leading edge and peak of the spill had already passed the main plant area (spill site) and the 7500 Bridge water monitoring station in this interval. There were better results at MS3. Sample analyses at this location exhibit a well defined peak and recession of fluorescein dye concentrations. Additional data and information on the spill obtained by EMC staff should enable SSARR modelers to further characterize travel time and dispersion through the upper reaches of WOC for the conditions which existed during this event.

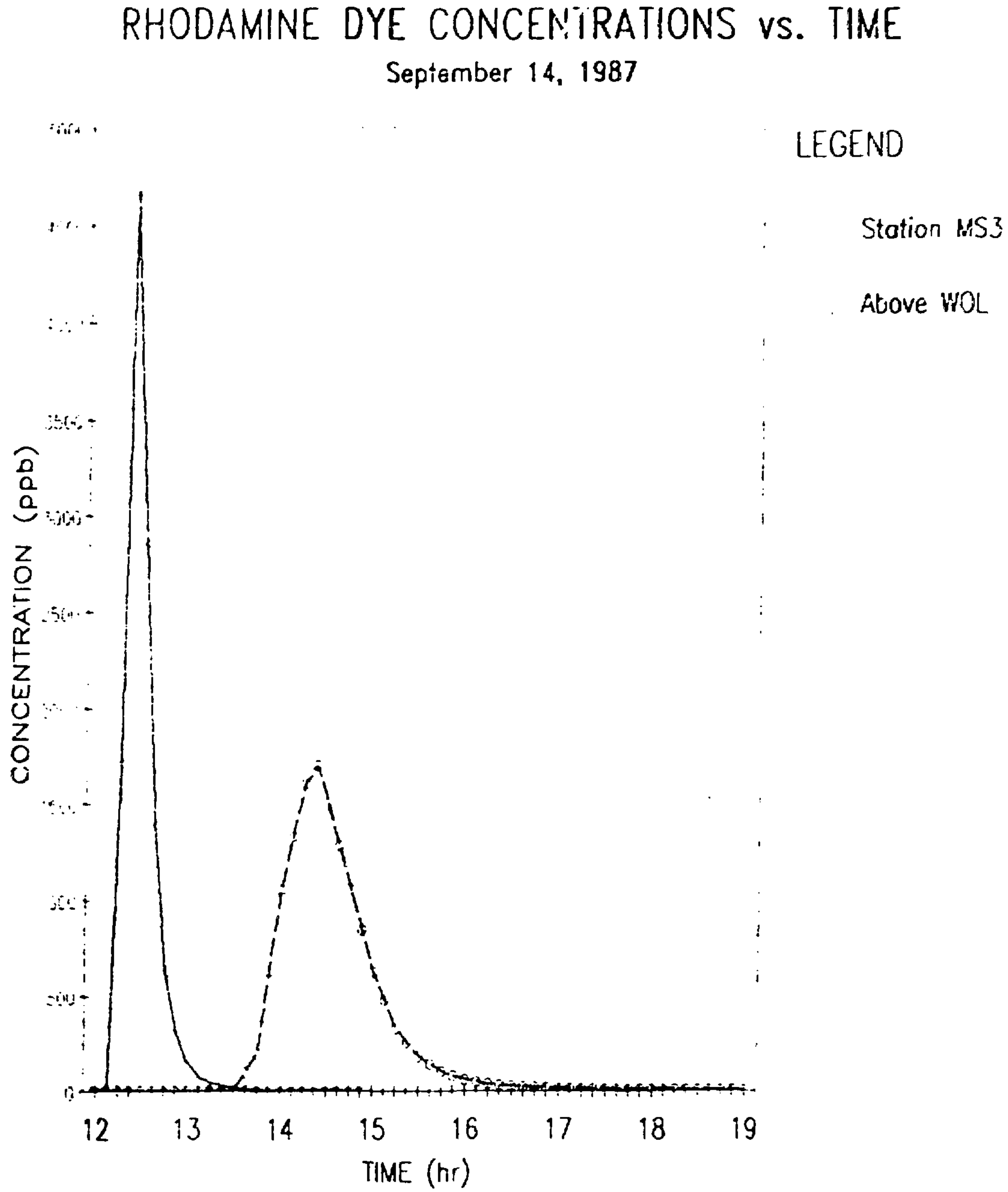


Figure 8. Observed Rhodamine concentrations in White Oak Creek.

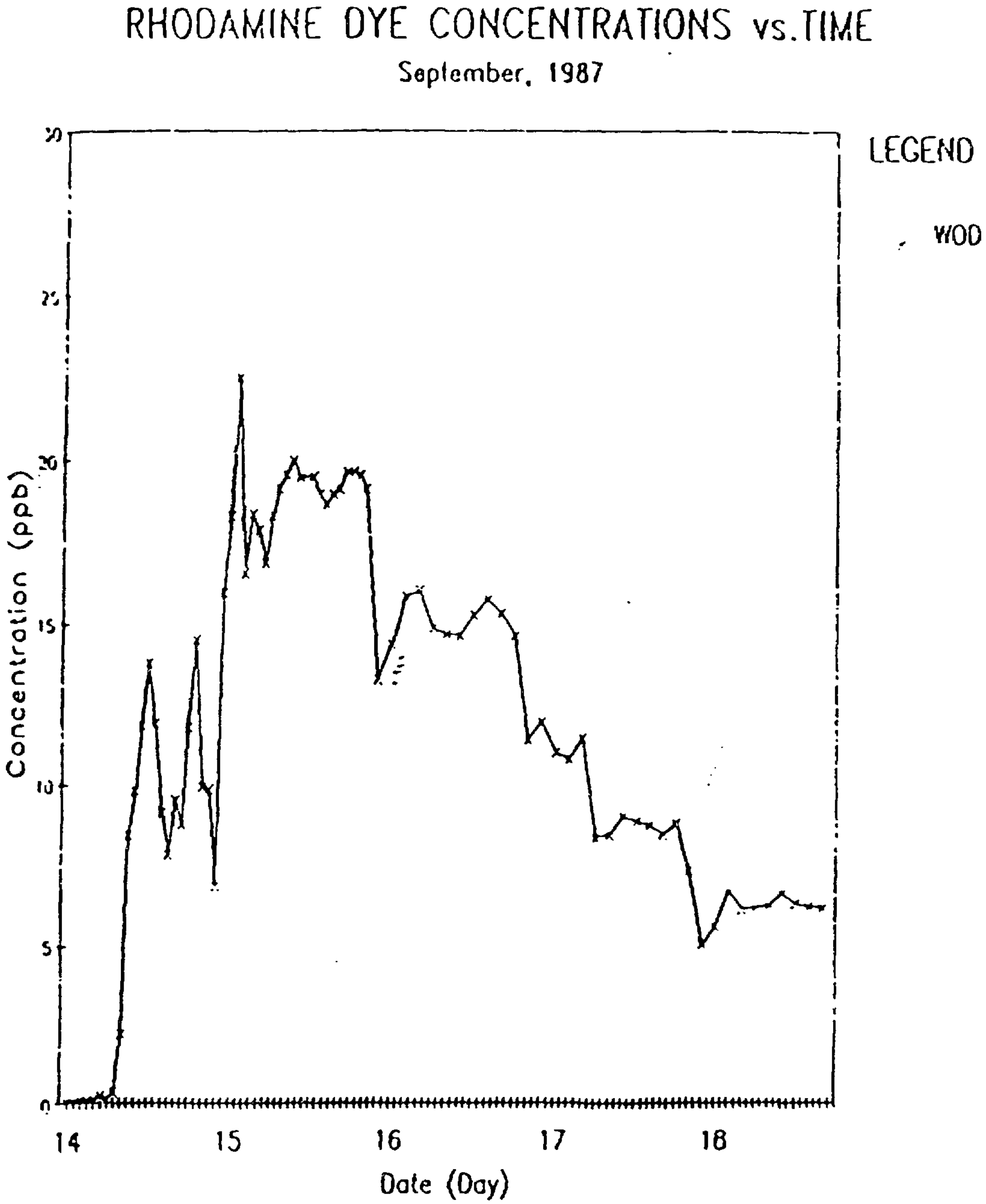


Figure 9. Observed Rhodamine concentrations at White Oak Dam.

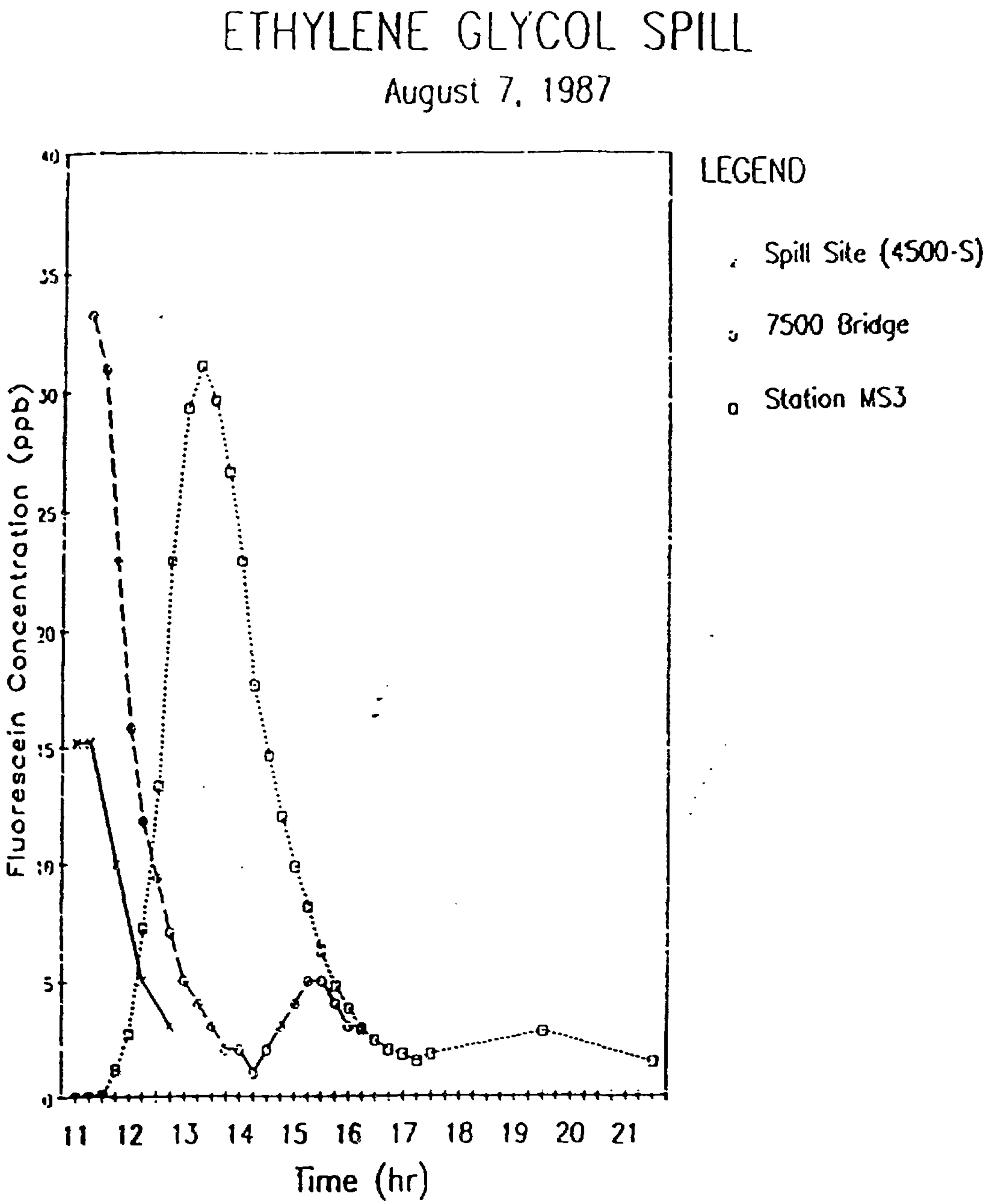


Figure 10. Ethylene glycol spill data for August 7, 1987.

CONCLUSIONS

The most important and timely task for contaminant and discharge forecast modeling within the WOC watershed is the development and implementation of a method for representation of contaminant dispersion and travel through WOL as a function of WOC and MB flows (inflow to WOL) as well as the travel time from the main plant area to WOL through WOC. The first in a series of dye tracer studies has been performed to initiate this representation; however, experiments of this type must be performed under a variety of hydrologic conditions to properly calibrate the model for forecasting operations. In addition, procedures must be developed to characterize basin response to non-conservative contaminants and the effects of regulation on the fate of contaminants in the WOC system and downstream in the Clinch River.

The prospective future of the discharge forecast modeling project involves the establishment of a continuously operational model to achieve and maintain a high level of operational emergency response preparedness. Current goals include dynamic simulation of spills of conservative and non-conservative contaminants, the investigation of alternate operating rules for WOD, and the development of more refined data for improving model calibration. The model will also be utilized to generate response procedures for various types and magnitudes of emergency events. Using real-time flow data and a quantitative precipitation forecast, the SSARR model results can be combined with a dispersion model to predict expected contaminant concentrations at downstream locations.