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DISSERTATION

DEVELOPMENT OF A MODEL FOR SIMULATION OF SOLUTE TRANSPORT IN A STREAM-AQUIFER SYSTEM

Submitted by

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In partial fulfillment of the requirements

For the Degree of Doctor of Philosophy

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Spring, 2000

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October 28, 1999

WE HEREBY RECOMMEND THAT THE DISSERTATION PREPARED UNDER OUR SUPERVISION BY HASHEM FAIDI ENTITLED DEVELOPMENT OF A MODEL FOR SIMULATION OF SOLUTE TRANSPORT IN A STREAM-AQUIFER SYSTEM BE ACCEPTED AS FULFILLING IN PART REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY.

Committee on Graduate Work

Advisor

Department Head

ABSTRACT OF DISSERTATION

DEVELOPMENT OF A MODEL FOR SIMULATION OF SOLUTE TRANSPORT IN A STREAM-AQUIFER SYSTEM

A model for simulation of solute transport in a stream-aquifer system is developed. The model is referred to as: Model for Stream-Aquifer Solute Transport or MSAST. The MSAST is developed by coupling four primary models: The groundwater flow model, MODFLOW-96, the coupled groundwater surface water model, MODBRANCH 3.7, the aquifer solute transport model, MT3D 1.11, and a fourth model developed in this study referred to as Stream Solute Transport Model or SSTM 1.0. The flow interaction in a stream-aquifer system is simulated by the MSAST using MODFLOW and MODBRANCH. The solute interaction in a stream-aquifer system is simulated by the MSAST using MT3D and SSTM. An interface is developed between MODFLOW-MODBRANCH and MT3D-SSTM. SSTMLINK Package is added to MODBRANCH to create an interface file containing streamflow hydraulic solution for the stream network. The LKM Package (Zheng, 1990) creates an interface file that contains the output solution of MODFLOW. The SSTMLINK and the LKM Packages interface files are used as input files in the MT3D-SSTM simulation. The Stream Solute Package (SSL1) is added to MT3D to simulate variable stream concentration by calling the SSTM. The SSTM is coded based on the one-dimensional advection dispersion equation. The finite difference method is the numerical technique implemented in the SSTM.

MSAST is used to simulate chloride transport in the stream-aquifer system of the Arkansas River and the Equus Beds Aquifer in south-central Kansas. Previous modeling of the aquifer was conducted by the Bureau of Reclamation using MODFLOW and MT3D to examine groundwater flow and chloride transport in the aquifer. The flow interaction in the MSAST application was simulated using MODFLOW and MODBRANCH. The solute interaction was simulated using MT3D and SSTM. The SSTM requires initial and boundary solute data values. These data are not available in the range of time intervals used by SSTM. The mean concentration of chloride for several disperse measurements in time and space taken for the Arkansas River are used as the initial and boundary values. The simulated mean of chloride concentration in the river matched the observed mean. Chloride concentration in the aquifer decreases in the vicinity of simulated channel for the selected simulation time. Sensitivity analysis showed that the increase in river chloride concentration has a significant effect on chloride concentration in the aquifer.

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Chapter One

INTRODUCTION

1.1 Introduction

For hydraulically connected stream-aquifer systems, contaminated water is usually interchanged between the stream and the adjacent aquifer posing a threat to the water quality of the stream-aquifer system. Many studies of the interaction of groundwater and surface water have been initiated because of problems related to water quality.

Simulation of solute transport in a stream-aquifer system is composed of two main components. These are the simulation of water movement and the simulation of solute movement. The first component incorporates several processes. These processes are groundwater flow in the aquifer, surface flow in the stream, and flow interchange between the aquifer and the stream. The second component incorporates solute transport in the aquifer, solute transport in the stream, and the solute interchange between the stream and the aquifer.

MODFLOW (McDonald and Harbaugh, 1988) is a modular, finite difference model for the simulation of groundwater flow in the aquifer. The model is based on solving the partial differential equation of groundwater flow using finite difference method. The model includes packages that simulate particular hydrologic processes like flow towards wells, through riverbeds, and into drains. Other packages handle evapotranspiration and recharge. The original release of MODFLOW had the River Package that simulates the stream aquifer interaction. The River Package calculates seepage between streambed and aquifer using Darcy's Law. It assumes that the stream stage remained constant over one groundwater stress period.

Prudic (1989) introduced the Stream Package by modifying the River Package so streamflow accounting could be accommodated by the MODFLOW model, but its use is limited to steady flow in rectangular, prismatic channels.

The outstanding difference between surface and groundwater calculations is the disparity in the time scales. Changes in the stream flow occur on a much shorter time scale than changes in the groundwater flow. This variation is not accounted for in the River and Stream Packages of MODFLOW.

Swain and Wexler (1996) noted that groundwater and surface water models have been developed separately. They asserted that in areas with dynamic and hydraulically connected groundwater and surface water systems, stream-aquifer interaction should be simulated using deterministic responses of both systems coupled at the stream aquifer interface. In the situations where transient and the variations in river stage and aquifer heads are rapid the River and Stream Packages are not adequate for the simulation of stream-aquifer interaction.

Swain and Wexler (1996) developed MODBRANCH for the simulation of stream-aquifer interaction. The model links BRANCH (Schaffranek et al, 1981), which is a one-dimensional numerical model designed to simulate unsteady flow in open-channel networks, to MODFLOW. In MODBRANCH, streams are simulated more realistically than in the River and Stream Packages of MODFLOW.

Solute transport in groundwater is simulated using numerical models coded based on the partial differential equation describing solute transport in the aquifer. MT3D is a three-dimensional solute transport model for simulation of advection, dispersion, and chemical reactions of dissolved constituents in groundwater systems. The model uses a modular structure similar to that implemented in MODFLOW. The modular structure makes it possible to independently simulate

advection, dispersion, sink/source mixing, and chemical reactions without reserving computer memory space for unused options. MT3D is used in conjunction with MODFLOW. MT3D retrieves the hydraulic heads and the various flow and source/sink terms saved by MODFLOW, automatically incorporating the specified hydrologic boundary conditions.

The simulation of the stream in MT3D is included in the Sink/Source Package. The stream is considered as a source or a sink with specified flow rate and solute concentration during the model stress period. The concentration in streams is considered constant during the stress period. For the situation of a dynamic, hydraulically connected stream-aquifer system as presented in MODBRANCH, there is usually a variation in the stream concentration due to transport of solute governed by processes like advection, dispersion, and source/sink in the stream. The MT3D in its current format is not adequate for simulation of solute transport interchange for a connected stream-aquifer system.

Development of MODBRANCH as a coupled groundwater surface water simulation model, represent a significant improvement in simulating water movement in stream-aquifer systems. This development could be used as a basic step toward an efficient simulation of solute transport in a stream-aquifer system.

Dietrich et al. (1989) and Jakeman et al. (1989) developed an analytical model for the transport of a conservative solute along a stream connected to an aquifer contaminated by the solute. The model relates downstream concentration to upstream concentrations, stream discharge and piezometric levels in the aquifer. Also, other models for solute travel time in the stream and aquifer inflow to the stream have been developed. They applied the model to a reach of the River Murray in Australia. The analytical solution developed by Dietrich and Jakeman assumes a homogeneous stream-aquifer system. The spatial variation of the properties of the aquifer connected to the stream

is not considered. The model is specific for a situation when the aquifer is contaminating the stream and not the other way around. Other assumptions were considered which are specific to the case study like the solute concentration in the aquifer is high in comparison with that of the stream, advection dominates dispersion in the stream, aquifer properties do not vary along the stream, there is a single valued relationship between wetted cross-sectional areas of the stream and stream discharge, and sources or sinks of water along the river are small enough not to affect significantly the downstream propagation of river flow.

In conclusion, a numerical model that simulates solute transport in a stream-aquifer system is lacking and development of such a model will be a significant step towards better management of water quality in a stream-aquifer system. For this model to be comprehensive and adaptable it is based on existing widely used models describing the individual flow and transport components of the stream-aquifer interaction.

1.2 Research Purpose

The main purpose of this research is to develop a model for simulation of solute transport in a stream-aquifer system. The model will be referred to as Model for Stream-Aquifer Solute Transport.

1.3 Research Specific Objectives

There are several major tasks that need to be taken to develop the primary model for solute transport in a stream-aquifer system, these are:

1. Develop a primary model for solute transport in a stream-aquifer system by integrating several secondary models. The first model will simulate the groundwater flow in the aquifer. The

second model will simulate streamflow in streams and the interaction of flow between the stream and the aquifer. The third model will simulate the solute transport in the aquifer and the fourth model will simulate the solute transport in the stream and the interchange of solute between the stream and the aquifer.

2. The developed model will use MODFLOW for simulation of groundwater flow in the aquifer and MODBRANCH for simulation of streamflow in the stream and the interaction of flow between the stream and the aquifer. The solute transport in the aquifer will be simulated using MT3D. A fourth model will be developed in this study to simulate solute transport in the stream. This model will be coded based on the partial differential equation of one-dimensional solute transport in the stream. This equation accounts for solute concentration variation due to advection, dispersion and interchange of solute with the aquifer.

3. Link or interface packages will be added to integrate the four models. The first link package will be added to MODBRANCH to save the hydraulic solution of stream network which eventually will be used by the stream solute transport model. The second link package will be added to aquifer solute transport model, MT3D. This package will interface with stream solute transport model to get solute concentrations in the stream segments included in the aquifer cells simulated by MT3D

4. Apply the Developed model to a case study and check its performance.

1.4 Research Organization

This Chapter explains the background and the purpose of this study. Chapter Two reviews the literature related to the development of numerical modeling of water flow and solute transport in a stream-aquifer system. Chapter Three describes the mathematical equations and their numerical solutions implemented in the primary models that simulate the movement of water in a stream-aquifer system. Chapter Four describes the mathematical equations and their numerical solutions implemented in the primary models that simulate the movement of solute in a stream-aquifer-system. Chapter Five explains the code structure of the developed model. Chapter Six describes the application of the model to the Arkansas River and the Equus Beds Aquifer in south-central Kansas. Chapters Seven discusses the conclusions from this study and Chapter Eight discusses the recommendations of this study.

Chapter Two

LITERATURE REVIEW

2.1 Introduction

This Chapter describes the literature related to the research study. The studies reviewed fall in two categories. The first category of studies describes the advancement of numerical modeling as a primary tool for analyzing the interaction of groundwater and surface water. Four studies are reviewed under the first category. The first study by Pinder and Sauer (1971) describes the bank storage effects on a stream-aquifer system. The second and third studies describe the packages of the groundwater flow model, MODFLOW (McDonald and Harbaugh, 1988) that simulate the stream-aquifer interaction. The fourth study by Swain and Wexler (1996) describes MODBRANCH, the coupled groundwater-surface water model.

The second category of studies reviewed describes research related to solute transport in a stream-aquifer system. The first study by Squillance et al. (1993) showed how groundwater in the alluvium aquifer adjacent to the stream was the principal source of solute in the stream. The second study by Duffy and Lee (1992) conducted numerical experiments to evaluate the response of baseflow chemistry to nonpoint source contamination in an idealized stream-aquifer system. The third study by Dietrich et al. (1989) is a development of an analytical model for the transport of a conservative solute along a stream connected to a contaminated aquifer.

As noted in Chapter One, numerical modeling of solute transport in stream-aquifer systems is still an open area of research. Studies reviewed in the second category are the closest to the context of this study. The two categories of studies are explained in the next two sections.

2.2 Flow Component of Stream-Aquifer Interaction

Numerical modeling has been the primary tool for analyzing the interaction of groundwater and surface water. Pinder and Sauer (1971) coupled the unsteady river equations with the two-dimensional groundwater flow equations to study bank storage effects.

The purpose of this study was to demonstrate the response of a stream-aquifer system to the propagation of a flood wave along a stream hydraulically connected to a floodplain aquifer using a mathematical model of coupled groundwater and surface water systems. The solution of the differential equations describing open channel flow and groundwater flow is accomplished simultaneously using finite difference schemes. The equation coupling the two systems is Darcy's law, which describes flow through the wetted perimeter of the channel.

The conclusions drawn from the study were:

1. Allowing for leakage into the aquifer (bank storage) attenuates the flood wave, decreasing the peak discharge and extending the hydrograph base time.
2. Increased aquifer width had a minor influence on bank storage.
3. The length of the channel reach and the hydraulic conductivity of the floodplain aquifer have a considerable influence on the modification of the flood wave by bank storage.
4. The response of a floodplain aquifer to the propagation of a flood wave along the channel decreases rapidly with distance from the stream.

The MODFLOW groundwater flow model contains two packages that account for leakage to and from rivers and canals. The River Package simulates rivers assuming a constant stage during MODFLOW stress period and calculates leakage to or from the aquifer. The Stream

Package accounts for leakage but allows flow to be routed through the river system only by a uniform steady state technique (Prudic, 1989).

The purpose of the River Package is to simulate the effects of flow between surface water and groundwater systems. To accomplish this, terms representing seepage to or from the stream or the river are added to the groundwater flow equation simulated in MODFLOW. The stream is divided into reaches so that each reach is completely contained in a single cell. Darcy's Law is used to estimate seepage between the stream and the aquifer. Seepage through the stream bed is simulated between each reach and the model cell based on the head difference between the head in the river reach (stage) and the head in the aquifer and the river bed conductance. The conductance of the riverbed is a function of its hydraulic conductivity and thickness and the area of the reach. The River Package accounts only for leakage between the stream and the aquifer, there is no streamflow routing in it. It does not track the amount of flow in the river nor does it allow the stream to go dry during the stress period.

Prudic (1989) modified the River Package so streamflow tracking could be accommodated by the MODFLOW code, but its use is limited to steady flow in a rectangular, prismatic channel. Streams superimposed on the aquifer are divided into reaches and segments. A segment is a stream or diversion in which streamflow from surface sources and diversions are added or subtracted at the beginning of the segment. A reach is the part of a segment that corresponds to an individual cell in the finite difference grid used to simulate groundwater flow in the aquifer. A segment may consist of one or more reaches.

Streamflow is accounted for by specifying flow for the first reach in each segment that entered the modeled area. Streamflow to adjacent downstream reaches in each segment is equal to inflow in the upstream reach plus or minus leakage from or to the aquifer in the upstream reach.

The accounting scheme used assumes that streamflow entering the modeled layer is instantly available to downstream reaches. Reaches in a segment are permitted to go dry whenever downward leakage to the aquifer exceeds stream inflow into the reach. The downstream reaches can also go dry and leakage into the aquifer is not permitted. Upward leakage from the aquifer is permitted even when there is no streamflow in a reach. This happens when the head in the aquifer exceeds the top of the streambed in a dry reach. Leakage to or from a stream is computed by Darcy's Law as in the River Package. An option is available to compute the stream stage in each reach. Using this option, the discharge in the reach is assumed steady at a constant depth. The stage is computed using Manning Formula.

The Stream Package in MODFLOW (Prudic, 1989) can route flow from more than one tributary into a channel, so it is not limited to single channels as the Pinder Model. However, it is restricted to rectangular cross sections, only route flow downstream and backwater effects cannot be simulated. Flows into diversions must be user defined, and the depth in each reach is calculated as steady uniform flow.

Swain and Wexler (1996) developed the coupled surface water and groundwater flow model termed MODBRANCH. The model links BRANCH, which is a one-dimensional numerical model, designed to simulate unsteady flow in open-channel networks, to MODFLOW. Streams are simulated more realistically than in the River and Stream Packages. Their work involved two main tasks. First, terms that describe leakage between a stream and an aquifer were added to the continuity equation in BRANCH; second, a package was added to MODFLOW to interface with the modified BRANCH. Leakage between the aquifer and the stream can be calculated separately in each model, or leakage calculated in BRANCH can be used in MODFLOW. Total mass in the coupled models is accounted for and conserved.

The MODBRANCH model calculates new stream stages for each time interval in a transient simulation based on upstream boundary conditions, stream properties, and initial estimates of aquifer heads. Next, aquifer heads are calculated in MODFLOW based on stream stages calculated in MODBRANCH, aquifer properties, and stresses. This process is repeated until convergence criteria are met for head and stage. Because time steps used in groundwater modeling can be much longer than time steps used in surface-water simulation, The coupled surface water groundwater model developed by Swain and Wexler can handle multiple surface water flow time steps contained in one groundwater flow time step.

2.3 Solute Transport Component of Stream-Aquifer Interaction

In the first study reviewed about movement of solute in a stream-aquifer system, Squillance et al. (1993) found that groundwater in the alluvium adjacent to the main stem of the Cedar River in Iowa was the principal nonpoint source of atrazine and deethylatrazine to the river after the river had been in baseflow conditions for 5 days. The purpose of the study was to determine the primary source of atrazine and deethylatrazine in the Cedar River during base flow, September 20-22, 1989. The River had been in base flow conditions for 5 days at that time. This was accomplished by presenting data and theoretical calculations that show where these chemicals entered the reach of the Cedar River between September 20 and 22, 1989.

Three hypotheses were tested. Hypothesis one is that groundwater discharge is an important source of atrazine and deethyaltrazine. The second hypothesis is that discharge from tile drains is a significant conrtibutor to these chemicals. In this case, tributary inflow would be expected to be a major source of chemical loads in the main stem of the river. The third hypothesis is that chemical loads in the river are primarily the result of desorption from bed sediment.

Water samples were collected at sites at the main stem of the river, tributaries, and from the alluvial aquifer beneath the riverbed. Results were that tributaries, although they aggregate almost all of the discharge from tile drains within the study area, contributed about 25% of the increase in loads of atrazine and between sampling sites on the main stem of the river, whereas 75% of the increased loads originated along the main stem of the river. Data and theoretical calculations show that the interaction of the river with the bed sediment does not result in substantial increases in the river loads of atrazine. The alluvial aquifer adjacent to the river is the main source of atrazine and deethylatrazine. The evidence for that is the following:

1. Statistically significant increases of atrazine loads were observed only along those reaches of the river where discharge increased substantially because of groundwater discharge
2. Atrazine and deethylatrazine were collected in 15 shallow groundwater samples collected beneath the river
3. Over a period of 9 months atrazine and deethylatrazine were consistently detected in the groundwater at the Palisades site, which provides discharge to the river.

In the second study reviewed about movement of solute in a stream-aquifer system, Duffy and Lee (1992) conducted numerical experiments to evaluate the response of base flow chemistry to nonpoint source contamination in an idealized stream-aquifer setting. The approach is to evaluate the base flow concentration from a nonpoint source contamination for two-dimensional advective-dispersive transport and steady flow in the vertical plane. The source of contaminants is distributed and arealy recharged to the aquifer. The aquifer is recharging the stream and the base flow was considered to enter the stream along the entire reach. The flow and transport equations were solved using a finite element model. The stream boundary was simulated as a single node maintained at a constant head. The simulation can be described in two parts:

1. The first set of simulations deals with the sensitivity of local transport parameters (dispersivity and equilibrium) and the aspect ratio, L/D of the flow geometry on the time response of the solutes in base flow. The simulations reveal that local dispersion has little effect on base flow concentration. The aspect ratio variation or L/D ratio, which represents length of flow in the aquifer (L) to the saturated depth (D). For small aspect ratio, where the flow penetrates deeper, the impact of flow geometry on the solute response is substantial. When L/D is larger than 10, flow geometry as measured by aspect ratio will have a small effect on base flow concentrations.

2. The second set of simulations examines the impact of stochastic spatial variations of the state variable on base flow solute transport. For these experiments the hydraulic conductivity, nonpoint source concentration, and initial aquifer concentration fields are treated as second-order stationary stochastic processes (constant mean and variance). These variables are considered random variables with probability distribution functions. The results of these simulations suggest that solute response in base flow is insensitive to stationary fluctuation in hydraulic conductivity. The results also revealed that the spatial average source concentration is the important parameter for predicting base flow, while local spatial fluctuation in concentration have no impact at the point of discharge. For the spatial variation of initial aquifer concentration, the simulations shows that the base flow concentration has a strong dependence on the spatial mean initial conditions, while sensitivity to stationary variations in the initial condition is small.

In the third study, Dietrich et al. (1989) and Jakeman et al. (1989) developed a dynamic model for the transport of a conservative solute along a stream connected to an aquifer contaminated by the solute. The model relates downstream concentration to upstream concentrations, stream discharge and piezometric levels in the aquifer. Also, models for solute

travel time in the stream and aquifer inflow to the stream have been developed. They then applied the model to a reach of the River Murray in Australia.

Two objectives were set to achieve: first to provide a daily estimate of stream salinity at a fixed downstream location during periods of low to medium flows in response to upstream flows and upstream salt concentration as well as to lateral inflows from salty aquifers. Second to quantify the salt load discharged from the aquifer into the stream in response to stream flow levels. The first objective stems from the requirement to estimate downstream levels of salt concentration which if too high would be damaging to irrigation activities. Such events usually occur during periods of low to medium flows since in such instances dilution is low and groundwater gradients towards the stream can be high. The second objective results from the need to assess management strategies aimed at reducing the influx of aquifer salinity into the stream. To achieve the previous two objectives the advection dispersion equation of solute transport in a stream was transformed from its differential form to a more global representation that attempts to retain enough physically based structure to be sensitive to relevant variables required by the modeling objectives. The major assumptions were: the solute concentration in the aquifer is high in comparison with that of the stream, advection dominates dispersion in the stream, aquifer properties do not vary along the stream, there is a single-valued relationship between wetted cross-sectional areas of the stream and stream discharge, and sources or sinks of water along the river are small enough not to affect significantly the downstream propagation of river flow. The developed models have been applied to a 207 km reach of the Murray River in Australia. The reach is characterized by a significant amount of salt intrusion from adjacent aquifers. The historical and predicted salinity profiles were compared at a station along the river. The predictions are regarded as quite accurate given the level of error in the data.

2.4 Conclusions from Literature Review

In general, the main conclusion that can be drawn from the literature review conducted is that no model is available for numerical simulation of solute transport in a stream-aquifer system.

Two conclusions can be drawn from the first category of studies which are about flow component in a stream aquifer system, these are:

1. Improved numerical models for simulating the interaction of groundwater and surface water have been developed. With the development of MODBRANCH, two widely accepted models; MODFLOW; and BRANCH representing processes in the aquifer and network of streams respectively were coupled with addition of other processes representing water flow interchange between aquifer and stream.
2. Second, the advancement achieved in groundwater surface water modeling can be used as a base for a better modeling of solute transport in a stream-aquifer system.

The conclusion drawn from the second category of studies which are about solute movement in a stream-aquifer system are:

1. The first study showed that groundwater is the main source of solute detected in the river, so developing a model that quantify the interaction will be very important.
2. The second study showed that stream-aquifer system was modeled in the conventional way used in groundwater models where the stream is assumed a constant head boundary. It is important to consider the actual situation of the stream stage specially when it is variable.
3. The third study introduced an analytical solution for solute transport in a stream-aquifer system with many constraining assumptions usually typical to analytical solutions. Development of a model based on numerical solution will eliminate these constraining assumptions and will consider more realistic situations such as the spatial variability of aquifer properties.

Chapter Three

MATHEMATICAL BACKGROUND

3.1 Introduction

The purpose of this Chapter and the following Chapter (Chapter Four) is to describe the mathematical equations governing the flow and solute transport for an alluvial aquifer connected to a stream. Flow and solute transport in a stream-aquifer system incorporate several main processes: groundwater flow in an aquifer, surface flow in a stream, flow interaction between a stream and an aquifer, solute transport in an aquifer, solute transport in a stream and the solute interchange between a stream and an aquifer. The main model that is developed in this research will simulate these processes. The model is referred to as Model for Stream-Aquifer Solute Transport or MSAST. The model is composed of four primary models; the groundwater flow model (MODFLOW), the coupled groundwater surface water model (MODBRANCH), a modification of the aquifer solute transport model (MT3D), and a fourth model that is developed in this study to simulate the transport of solute in the stream and the interchange of solute between the stream and the aquifer. This model is referred to as Stream Solute Transport Model (SSTM). This Chapter presents a mathematical background that explains the equations that describe the water movement in a stream-aquifer system as represented in the MODFLOW and MODBRANCH models, and the numerical techniques implemented to solve these equations. The following Chapter describes the equations governing the solute transport movement in a stream-aquifer system.

3.2 Groundwater Flow in the Aquifer

The modular three dimensional groundwater flow model referred to as MODFLOW (McDonald and Harbaugh, 1988) is used to simulate groundwater flow in the aquifer. MODFLOW is based on solving the partial differential equation of groundwater flow using a finite difference method. MODFLOW simulates steady and non-steady flow in an irregularly shaped flow system in the aquifer. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow through river beds, and flow to drains can be simulated.

3.2.1 Groundwater Flow in the Aquifer Governing Equation

The three dimensional movement of groundwater of constant density through porous media may be described by the partial differential equation:

$$\frac{\partial}{\partial X}(K_{XX}\frac{\partial h}{\partial X}) + \frac{\partial}{\partial Y}(K_{YY}\frac{\partial h}{\partial Y}) + \frac{\partial}{\partial Z}(K_{ZZ}\frac{\partial h}{\partial Z}) - W = S_s\frac{\partial h}{\partial t} \qquad (3.1)$$

where

K_{XX}, K_{YY}, K_{ZZ} are values of hydraulic conductivity along the X, Y, Z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity (LT^{-1}), hydraulic conductivity is defined as a measure of the ease with which water can be transmitted through porous media;

h is the potentiometric head (L);

W is the volumetric flux per unit volume and represents sources and /or sinks of water (T^{-1}), this term accounts for flow into the system from features or processes external to the aquifer, such as streams, drains, areal recharge, evapotranspiration and wells.

S_s is the specific storage of the porous media, defined as the volume of water released per unit volume of aquifer per unit change of head (L^{-1}); and

t is time (T).

3.2.2 Numerical Solution of the Groundwater Flow in the Aquifer Equation

The finite-difference method is the numerical method used to solve Eq 3.1 in MODFLOW. In the finite difference method the aquifer system is spatially discretized into blocks or cells, the location of these cells are described in terms of rows, columns and layers as shown in Fig. 3.1. The development of the finite-difference form of Eq 3.1 as reported by McDonald and Harbaugh (1988) is described here. Equation 3.1 is transformed into a finite difference formulation for each cell using conservation of mass principle; the sum of all flows into and out of the cell must equal the rate of change in storage within the cell. This is described as:

$$\sum Q_i = S_s \Delta V \frac{\Delta h}{\Delta t} \tag{3.2}$$

where

Q_i is the flow rate into or out of the cell i,j,k (L^3T^{-1});

S_s is the specific storage (L^{-1});

ΔV is the change of volume of cell i,j,k (L^3); and

Δh is the change in head (L) over a time interval of length Δt (T).

Figure 3.2 depicts a cell i,j,k and six adjacent aquifer cells i-1,j,k; i+1,j,k; i,j-1,k; i,j+1,k; i,j,k-1; and i,j,k+1. As shown in Fig. 3.3, flow from cell i,j-1,k into cell i,j,k is estimated using Darcy's Law as:

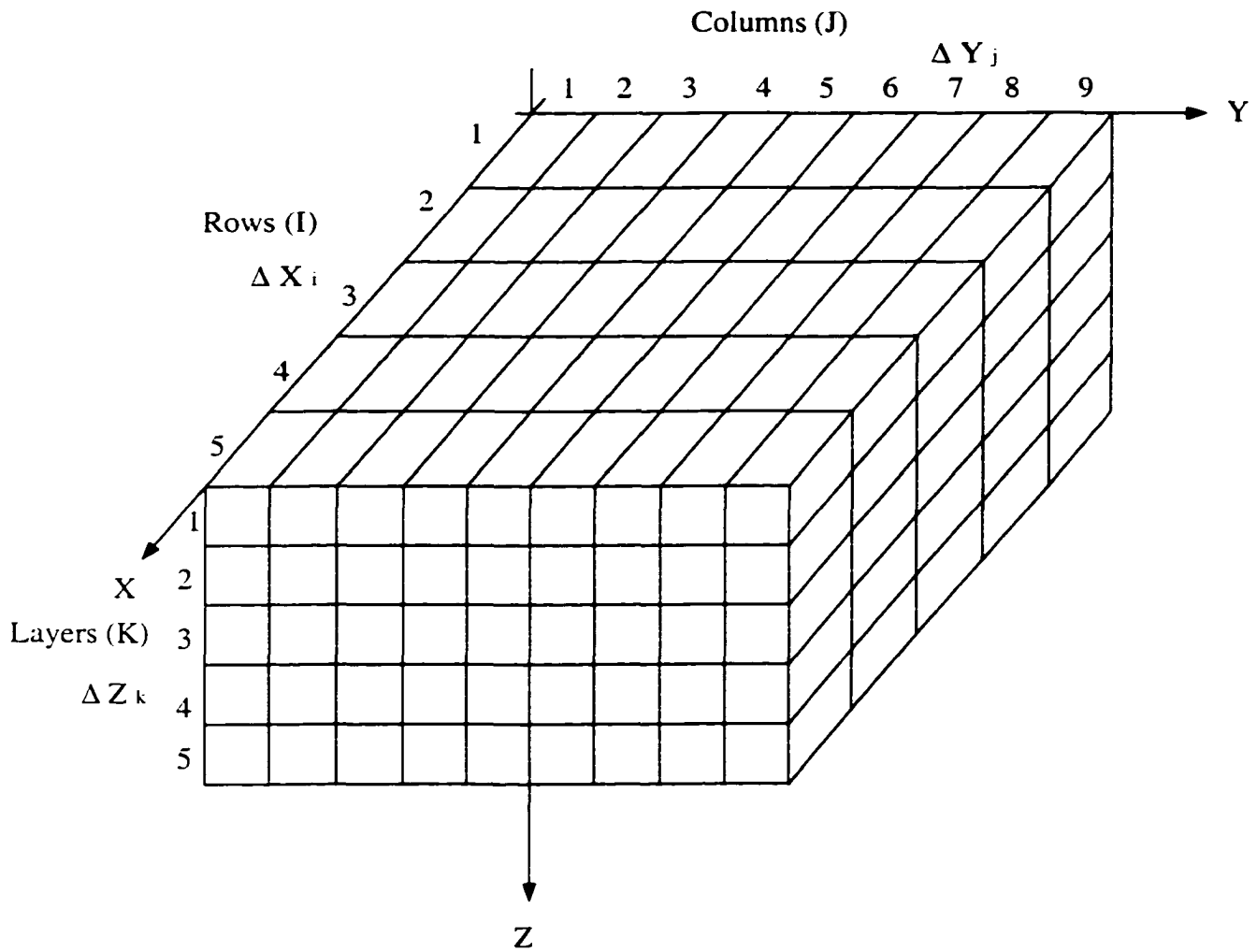


Figure 3.1 A discretized hypothetical aquifer system, McDonald and Harbaugh,1988.

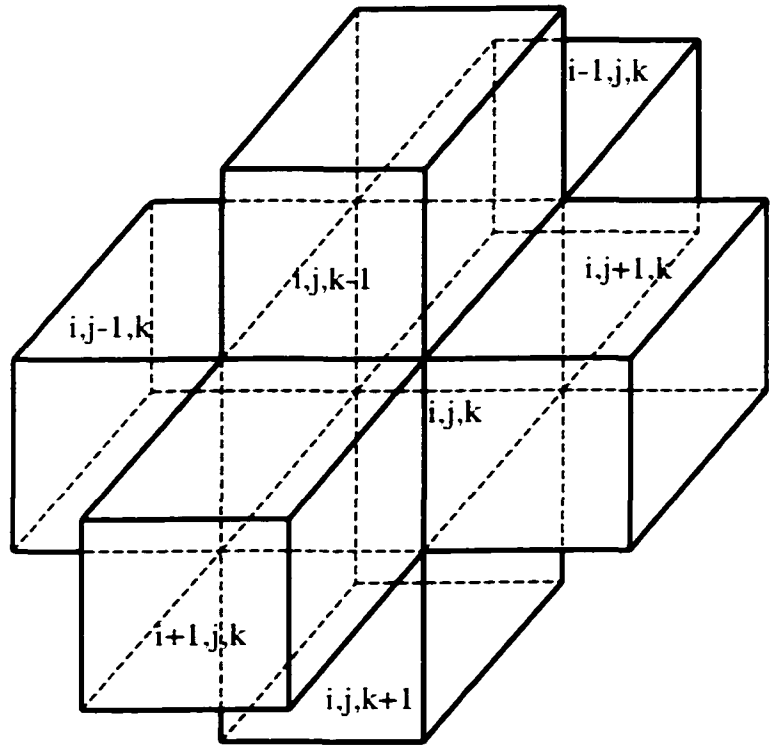


Figure 3.2 Cell i,j,k and indices for the six adjacent cells, McDonald and Harbaugh,1988.

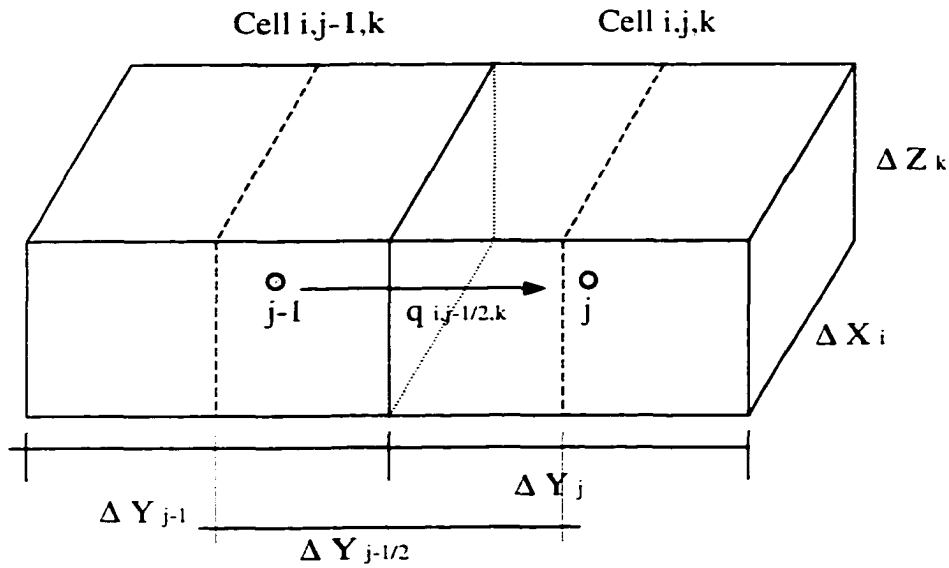


Figure 3.3 Flow into cell i,j,k from cell i,j-1,k , McDonald and Harbaugh (1988)

$$q_{i,j-1/2,k} = K_{y\ i,j-1/2,k}\ \Delta X_i\ \Delta Z_k\ \frac{(h_{i,j-1,k} - h_{i,j,k})}{\Delta Y_{j-1/2}} \tag{3.3}$$

Define $R_{i,j-1/2,k}$ as:

$$R_{i,j-1/2,k} = K_{y\ i,j-1/2,k}\ \frac{\Delta X_i\ \Delta Z_k}{\Delta Y_{j-1/2}} \tag{3.4}$$

then flow to the cell i,j,k in the y-direction is:

$$q_{i,j-1/2,k} = R_{i,j-1/2,k}\ (h_{i,j-1,k} - h_{i,j,k}) \tag{3.5}$$

where $K_{y\ i,j-1/2,k}$ is the effective hydraulic conductivity between nodes i,j,k and i,j-1,k. Flow in row direction out of the cell between i,j,k and i,j+1,k is:

$$q_{i,j+1/2,k} = K_{y\ i,j+1/2,k}\ \Delta X_i\ \Delta Z_k\ \frac{(h_{i,j+1,k} - h_{i,j,k})}{\Delta Y_{j+1/2}} \tag{3.6}$$

Define $R_{i,j+1/2,k}$ as:

$$R_{i,j+1/2,k} = K_{y\ i,j+1/2,k}\ \frac{\Delta X_i\ \Delta Z_k}{\Delta Y_{j+1/2}} \tag{3.7}$$

then flow out of the cell i,j,k in the y-direction is:

$$q_{i,j+1/2,k} = R_{i,j+1/2,k} \, (h_{i,j+1,k} - h_{i,j,k}) \tag{3.8}$$

Flow in x-direction from i-1,j,k and i,j,k is:

$$q_{i-1/2,j,k} = K_{x\,i-1/2,j,k} \, \Delta Y_j \, \Delta Z_k \, \frac{(h_{i-1,j,k} - h_{i,j,k})}{\Delta X_{i-1/2}} \tag{3.9}$$

Define $U_{i-1/2,j,k}$ as:

$$U_{i-1/2,j,k} = K_{x\,i-1/2,j,k} \, \frac{\Delta Y_j \, \Delta Z_k}{\Delta X_{i-1/2}} \tag{3.10}$$

Then flow into cell i,j,k from the x-direction is:

$$q_{i-1/2,j,k} = U_{i-1/2,j,k} \, (h_{i-1,j,k} - h_{i,j,k}) \tag{3.11}$$

Flow out of the cell i,j,k to i+1,j,k is:

$$q_{i+1/2,j,k} = K_{x\,i+1/2,j,k} \, \Delta Y_j \, \Delta Z_k \, \frac{(h_{i+1,j,k} - h_{i,j,k})}{\Delta X_{i+1/2}} \tag{3.12}$$

Define $U_{i+1/2,j,k}$ as:

$$U_{i+1/2,j,k} = K_{x\,i+1/2,j,k} \frac{\Delta Y_j \, \Delta Z_k}{\Delta X_{i+1/2}} \tag{3.13}$$

Flow out of the cell i,j,k to i+1,j,k is:

$$q_{i+1/2,j,k} = U_{i+1/2,j,k} \, (h_{i+1,j,k} - h_{i,j,k}) \tag{3.14}$$

For vertical direction flow through bottom face in the direction i,j,k-1 to i,j,k is:

$$q_{i,j,k-1/2} = K_{z\,i,j,k-1/2} \Delta X_i \, \Delta Y_j \frac{(h_{i,j,k-1} - h_{i,j,k})}{\Delta Z_{k-1/2}} \tag{3.15}$$

Define $V_{i,j,k-1/2}$ as:

$$V_{i,j,k-1/2} = K_{z\,i,j,k-1/2} \frac{\Delta X_i \, \Delta Y_j}{\Delta Z_{k-1/2}} \tag{3.16}$$

Then flow into the cell in z-direction:

$$q_{i,j,k-1/2} = V_{i,j,k-1/2} (h_{i,j,k-1} - h_{i,j,k}) \tag{3.17}$$

Flow out in the direction i,j,k to i,j,k+1 is :

$$q_{i,j,k+1/2} = K_{z\,i,j,k-1/2} \Delta X_i \Delta Y_i \frac{(h_{i,j,k+1} - h_{i,j,k})}{\Delta Z_{k+1/2}} \tag{3.18}$$

Define $V_{i,j,k+1/2}$ as:

$$V_{i,j,k+1/2} = K_{z\,i,j,k+1/2} \frac{\Delta X_i \, \Delta Y_j}{\Delta Z_{k+1/2}} \tag{3.19}$$

The flow out of the cell in the Z direction is :

$$q_{i,j,k+1/2} = V_{i,j,k+1/2}(h_{i,j,k+1} - h_{i,j,k}) \tag{3.20}$$

The above flows are flows into the cell from adjacent cells, flow from external sources such as streams, drains, areal recharge, evaporation, and wells are represented as:

$$a_{i,j,k,n} = p_{i,j,k,n} h_{i,j,k} + o_{i,j,k,n} \tag{3.21}$$

$a_{i,j,k,n}$ represent flow from the nth external source into cell i,j,k (L^3T^{-1}), $p_{i,j,k,n}$ and $O_{i,j,k,n}$ are constants, (L^2T^{-1}), and (L^3T^{-1}). In general if there are N external sources :

$$QS_{i,j,k} = \sum_{n=1}^{N} a_{i,j,k,n} = \sum_{n=1}^{N} P_{i,j,k,n} h_{i,j,k} + \sum_{n=1}^{N} O_{i,j,k,n} \tag{3.22}$$

Define $P_{i,j,k}$ as:

$$P_{i,j,k} = \sum_{n=1}^{N} p_{i,j,k,n} \tag{3.23}$$

and $O_{i,j,k}$ as :

$$O_{i,j,k} = \sum_{n=1}^{N} o_{i,j,k,n} \tag{3.24}$$

the general external flow term for cell i,j,k is

$$QS_{i,j,k} = P_{i,j,k} h_{i,j,k} + O_{i,j,k} \tag{3.25}$$

putting all the terms back into the continuity equation 3.2 for cell i,j,k yield:

$$\begin{aligned} & R_{i,j-1/2,k}(h_{i,j-1,k} - h_{i,j,k}) + R_{i,j+1/2,k}(h_{i,j+1,k} - h_{i,j,k}) \\ & + U_{i-1/2,j,k}(h_{i-1,j,k} - h_{i,j,k}) + U_{i+1/2,j,k}(h_{i+1,,k} - h_{i,j,k}) \\ & + V_{i,j,k-1/2}(h_{i,j,k-1} - h_{i,j,k}) + V_{i,j,k+1/2}(h_{i,j,k+1} - h_{i,j,k}) \\ & + P_{i,j,k} h_{i,j,k} + O_{i,j,k} = S_{s_{i,j,k}} \Delta X_i \Delta Y_j \Delta Z_k \frac{\Delta h_{i,j,k}}{\Delta t} \end{aligned} \tag{3.26}$$

The time derivative of head is approximated using backward finite difference scheme:

$$\frac{\Delta h_{i,j,k}}{\Delta t_{mf}} = \frac{h_{i,j,k}^{mf} - h_{i,j,k}^{mf-1}}{t_{mf} - t_{mf-1}} \tag{3.27}$$

where:

t_{mf} is time at the end of time step mf

$h^{mf}_{i,j,k}$ head at node i,j, k at time t_{mf}

Equation 3.26 is written in backward difference scheme as:

$$
\begin{aligned}
&R_{i,j-1/2,k}(h^{mf}_{i,j-1,k} - h^{mf}_{i,j,k}) + R_{i,j+1/2,k}(h^{mf}_{i,j+1,k} - h^{mf}_{i,j,k}) \\
&+ U_{i-1/2,j,k}(h^{mf}_{i-1,j,k} - h^{mf}_{i,j,k}) + U_{i+1/2,j,k}(h^{mf}_{i+1,,k} - h^{mf}_{i,j,k}) \\
&+ V_{i,j,k-1/2}(h^{mf}_{i,j,k-1} - h^{mf}_{i,j,k}) + V_{i,j,k+1/2}(h^{mf}_{i,j,k+1} - h^{mf}_{i,j,k}) \\
&+ P_{i,j,k}h^{mf}_{i,j,k} + O_{i,j,k} = S_{s_{i,j,k}}\Delta X_i \Delta Y_j \Delta Z_k \frac{h^{mf}_{i,j,k} - h^{mf-1}_{i,j,k}}{\Delta t_{mf}}
\end{aligned}
\tag{3.28}
$$

Equation 3.28 is rearranged so that all terms containing heads at the end of the current time step are grouped on the left-hand side of the equation, and all terms independent of head at the end of the current time step are on the right-hand side. This yield the form:

$$
\begin{aligned}
&V_{i,j,k-1/2}h^{mf}_{i,j,k-1} + U_{i-1/2,j,k}h^{mf}_{i-1,j,k} + R_{i,j-1/2,k}h^{mf}_{i,j-1,k} \\
&+(-V_{i,j,k-1/2} - U_{i-1/2,j,k} - R_{i,j-1/2,k} - R_{i,j+1/2,k} - U_{i+1/2,j,k} \\
&-V_{i,j,k+1/2} + H_{COEF\,i,j,k})h^{mf}_{i,j,k} + R_{i,j+1/2,k}h^{mf}_{i,j+1,k} + U_{i+1/2,j,k}h^{mf}_{i,j+1,k} \\
&+V_{i,j,k+1/2}h^{mf}_{i,j,k+1} = RHS_{i,j,k}
\end{aligned}
\tag{3.29}
$$

where

$$
H_{COEF\,i,j,k} = P_{i,j,k} - \frac{S_{s\,i,j,k}\Delta X_i \Delta Y_j \Delta Z_k}{\Delta t_{mf}} \tag{3.30}
$$

$$
RHS_{i,j,k} = -O_{i,j,k} - \frac{S_{s\,i,j,k}h^{mf-1}_{i,j,k}\Delta X_i \Delta Y_j \Delta Z_k}{\Delta t_{mf}} \tag{3.31}
$$

The entire system of equations having the form of Eq 3.29 which includes one equation for each variable-head cell in the mesh, is written in matrix form as:

$$[A]\ |h|\ =\ |q| \tag{3.32}$$

where

[A] is a matrix of the coefficients of head, from the left side of the equation;

|h| is a vector of head values at the end of time step mf for all heads in the mesh; and

|q| is a vector of constant terms on the right hand side of the equation.

MODFLOW incorporates several options for iterative solution of the set of finite difference equations defined by Eq 3.32. The Strongly Implicit Procedure (SIP) is one of these techniques. The Strongly Implicit Procedure is described briefly here. The SIP is a method for solving a large system of simultaneous linear equations by iterations. Obtaining a solution for the matrix system of Eq 3.32 by factorizing [A] into [L] , a lower triangular form matrix and [U] an upper triangular form matrix yield a [L] and [U] which are not sparse. This imply a great deal of computer memory. The SIP seeks to find a matrix [B] so that Eq 3.32 is converted into the form:

$$[A\ +\ B]\ |h|\ =\ |q|\ +\ [B]\ |h| \tag{3.33}$$

and matrix [A+B] can be factored easily into two matrices [L] and [U] which are sparse and close to [A] .

Utilizing an iterative process Eq 3.33 may be expressed in the form:

$$[A\ +\ B]\ |h^{L}|\ =\ |q|\ +\ [B]\ |h^{L-1}| \tag{3.34}$$

where

$| h^L |$ is a vector for head values from iteration L ; and

$| h^{L-1} |$ is a vector for head values from iteration L-1 .

the term $[A+B]\,|h^{L-1}|$ is subtracted from each side of Eq 3.34 to yield:

$$[A + B]\,|h^L| - [A + B]|h^{L-1}| = |q| - [A]\,|h^{L-1}| \tag{3.35}$$

Matrix [A+B] is replaced by matrix product [L][U] in Eq 3.35:

$$[L]\,[U]\,|h^L - h^{L-1}| = |q| - [A]\,|h^{L-1}| \tag{3.36}$$

define vector $| R^L |$ as:

$$|R^L| = |q| - [A]\,|h^{L-1}| \tag{3.37}$$

using this notation Eq 3.36 can be written as:

$$[L]\,[U]\,|h^L - h^{L-1}| = |R^L| \tag{3.38}$$

In summary, Eq 3.32 is converted into an iterative process described by Eq 3.38. The solution procedure is :

1. The matrices [L] and [U] are determined

2. the vector $| R^L |$ is calculated using vector $| q |$, the matrix [A] and the heads from the preceding iteration

3. Equation 3.38 is then solved using forward and backward substitution to obtain the vector $| h^L - h^{L-1} |$

4. Vector $|h^{L-1}|$ is added to vector $|h^{L}-h^{L-1}|$ to obtain vector $|h^{L}|$.

For more detail on the SIP technique, refer to MODFLOW Manual, McDonald and Harbaugh (1988) Chapter 12.

3.3 Surface Flow in the Stream

USGS BRANCH (Schaffranek et al., 1981) is a one-dimensional numerical model used to simulate unsteady flow in open channel networks by routing the dynamic water movement in the channel. The BRANCH network flow model is based on the one-dimensional, nonlinear partial differential equations governing unsteady flow in channels for which the dependent variables are flow rate, Q, and water surface elevation, Z. The model is applicable to a channel or a system of channels (network of branches), subject to unsteady flow. A typical network composed of branches is illustrated in Fig. 3.4.

3.3.1 Surface Flow in the Stream Governing Equations

The one-dimensional partial-differential equations governing transient flow in open channels are the continuity equation and the momentum equation, the continuity equation is written as:

$$B\frac{\partial Z}{\partial t}+\frac{\partial Q}{\partial X}=0 \qquad (3.39)$$

where

Z is the water surface elevation (L);

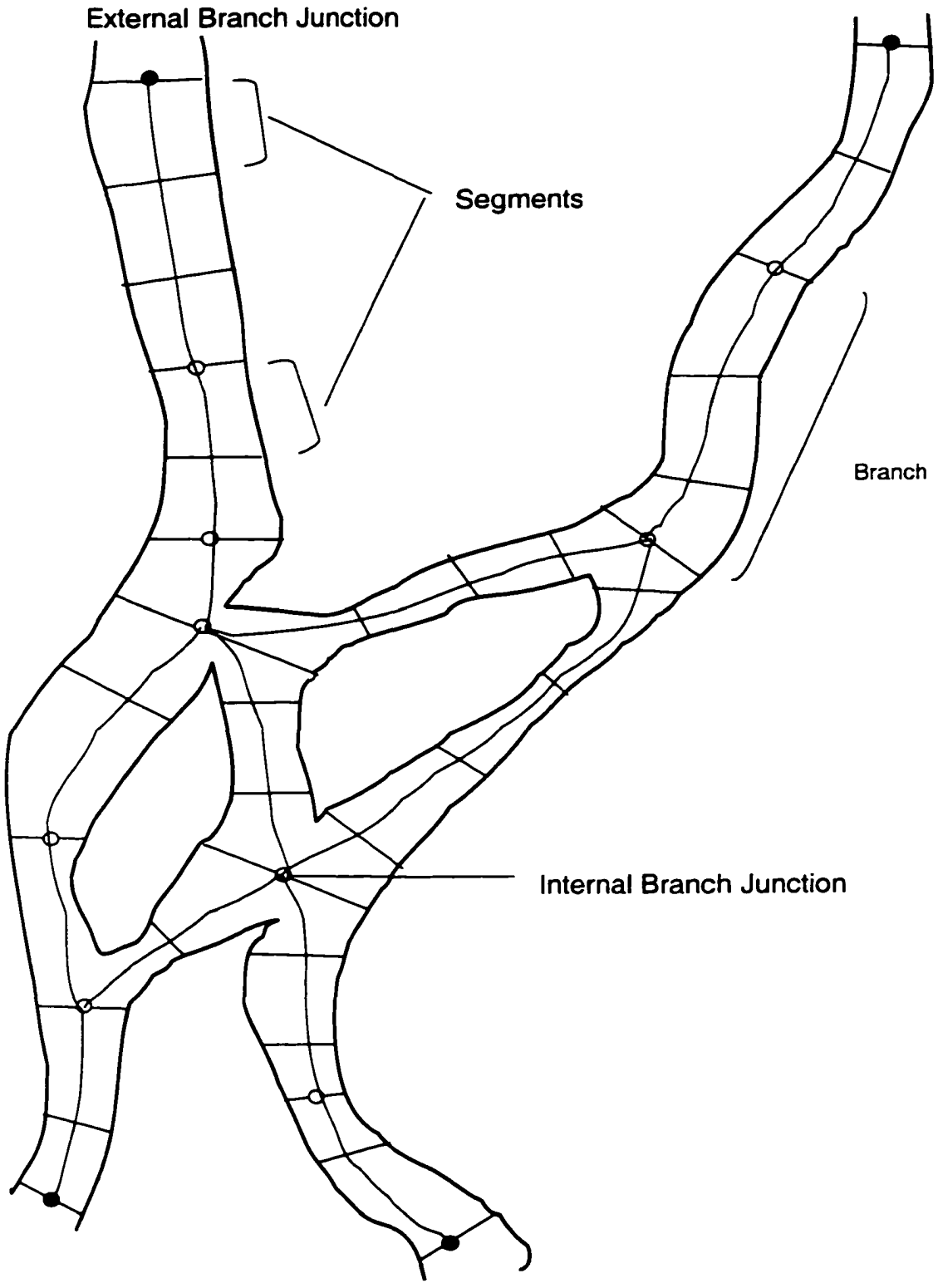


Figure 3.4 Definition schematic of a hypothetical stream network, Schaffranek et al, 1981.

Q is the channel discharge (L^3T^{-1});

B is the channel top width (L);

X is the distance in longitudinal direction (L);

t is time (T).

The continuity equation expresses the idea that if the area is increasing temporally at a point in space, then the flow rate passing this point at that time must be decreasing spatially to account for the water that is stored in the increasing cross section.

The equation of motion or momentum for one dimensional open channel flow is described as:

$$\frac{1}{gA}\frac{\partial Q}{\partial t}+\frac{2\beta Q}{gA^2}\frac{\partial Q}{\partial X}-\frac{\beta Q^2}{gA^3}\frac{\partial A}{\partial X}+\frac{\partial Z}{\partial X}+\frac{\kappa}{A^2R^{4/3}}Q|Q|-\xi\frac{B}{gA}U_a^2\cos\phi = 0 \qquad (3.40)$$

where

g is the acceleration of gravity (L^2T^{-1});

A is the stream cross sectional area (L^2);

R is the hydraulic radius (L);

κ is a function of flow-resistance coefficient, η (similar to Maninng's n), which can be expressed as:

$$\kappa=\left(\frac{\eta}{1.49}\right)^2 \quad \textit{english system}$$
$$\kappa=\eta^2 \quad \textit{metric system} \qquad (3.41)$$

β is the momentum or Boussinesq coefficient; dimensionless

U_a is the wind velocity vector making an angle ϕ with positive x-axis (LT^{-1}) and ξ is a dimensionless wind resistance coefficient

$$\xi = C_d \frac{\rho_a}{\rho} \tag{3.42}$$

C_d is the water surface drag coefficient, dimensionless;

ρ water density (ML^{-3}); and

ρ_a air density (ML^{-3}).

3.3.2 Numerical Solution of the Surface Flow Equations

The equations of continuity and momentum described previously constitute a system of partial differential equations with two independent variables X and t and two dependent variables Z and Q; the remaining terms are either functions of X, t, Z and / or Q , or they are constants. BRANCH solves the partial differential equations numerically by approximating them with a set of finite-difference algebraic equations; then the system of algebraic equations are solved taking into account the prescribed initial and boundary conditions. The solution technique adopted is the weighted four-point implicit scheme. In this scheme, the continuous x-t plane in which solutions of Z and Q are sought is represented by a rectangular grid of discrete points as shown in Fig. 3.5.

The time derivatives of the dependent variables, stage and discharge are approximated as central both in space and time, as follows:

$$\frac{\partial f(I)}{\partial t} = \frac{f_{i+1}^{nf+1} + f_i^{nf+1} - f_{i+1}^{nf} - f_i^{nf}}{2\Delta t_{nf}} \tag{3.43}$$

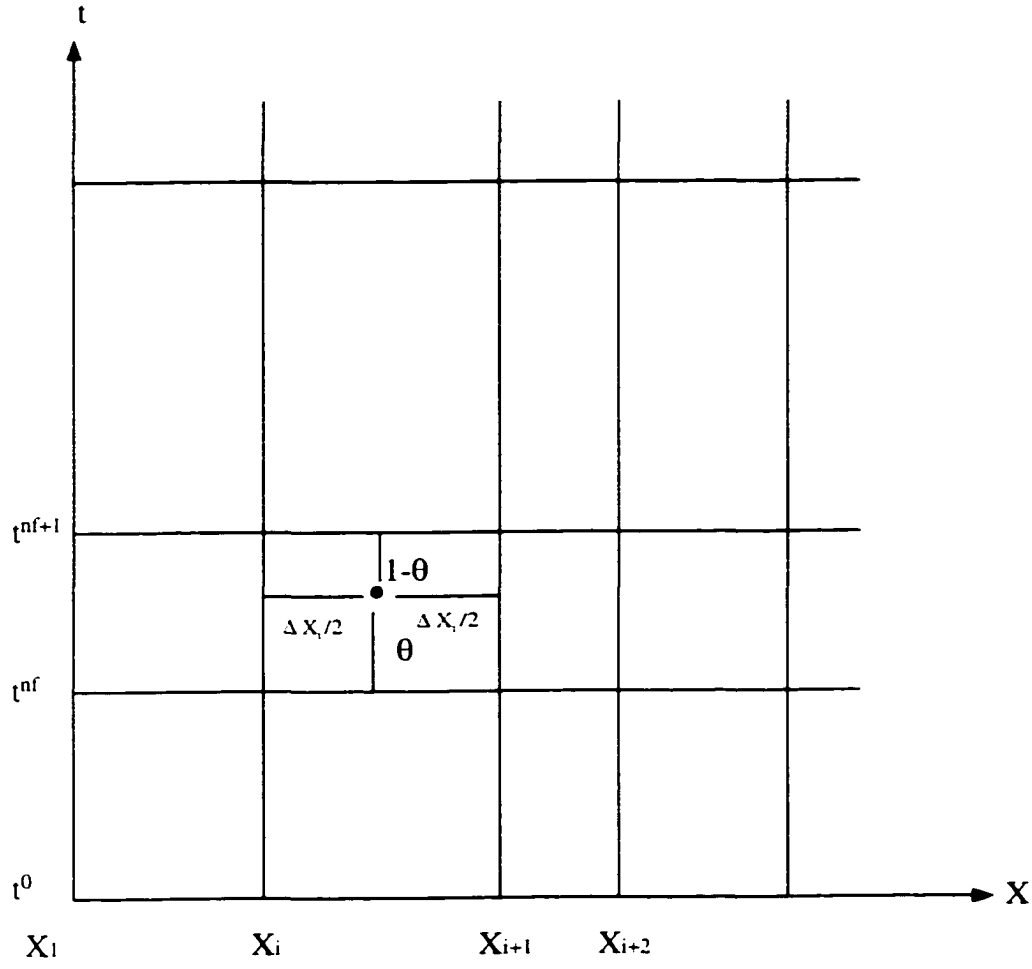


Figure 3.5 Space-time-grid system for finite difference approximation, Schaffranek et al, 1981.

The space derivatives of the dependent variables, stage and discharge, are approximated as centered in space and positioned in time according to a user-defined weighting factor, as follows:

$$\frac{\partial f(I)}{\partial X} \approx \theta \frac{f_{i+1}^{nf+1} - f_i^{nf+1}}{\Delta X_i} + (1-\theta) \frac{f_{i+1}^{nf} - f_i^{nf}}{\Delta X_i} \tag{3.44}$$

The spatial derivative of the cross sectional area in the equation is approximated by a forward difference technique :

$$\frac{\partial A}{\partial X} \approx \frac{A_{i+1}^{nf+1} - A_i^{nf+1}}{\Delta X_i} \tag{3.45}$$

In a manner similar to the treatment of spatial derivatives, quantities such as the cross-sectional area, top width, hydraulic radius, and the discharge in nonderivative form in the equation of motion, represented by f(I) are approximated by:

$$f(I) \approx \chi \frac{f_{i+1}^{nf+1} + f_i^{nf+1}}{2} + (1-\chi) \frac{f_{i+1}^{nf} + f_i^{nf}}{2} \tag{3.46}$$

Utilizing these finite-difference approximations and the notation f(I) to signify function values derived from previous equations, one can transform the partial differential flow equations into the following finite difference expressions for the ith segment:

the continuity equation (Eq 3.39) is written in finite difference form as:

$$\overline{B}\ [\ \frac{Z_{i+1}^{nf+1}+Z_i^{nf+1}}{2\Delta t_{nf}}-\frac{Z_{i+1}^{nf}+Z_i^{nf}}{2\Delta t_{nf}}\ ]+\theta\frac{Q_{i+1}^{nf+1}-Q_i^{nf+1}}{\Delta X_i}+(1-\theta)\frac{Q_{i+1}^{nf}-Q_i^{nf}}{\Delta X_i}\ =\ 0 \qquad (3.47)$$

and for the equation of motion (Eq 3.40),

$$\frac{1}{g\overline{A}}\ [\ \frac{Q_{i+1}^{nf+1}+Q_i^{nf+1}}{2\Delta t_{nf}}-\frac{Q_{i+1}^{nf}+Q_i^{nf}}{2\Delta t_{nf}}\ ]+\frac{2\beta\overline{Q}}{g\overline{A}^2}\ [\ \theta\frac{Q_{i+1}^{nf+1}-Q_i^{nf+1}}{\Delta X_i}+(1-\theta)\frac{Q_{i+1}^{nf}-Q_i^{nf}}{\Delta X_i}\ ]$$

$$-\frac{\beta\overline{Q}^2}{g\overline{A}^3}\ \frac{\overline{A}_{i+1}^{nf+1}-\overline{A}_i^{nf+1}}{\Delta X_i}+[\ \theta\frac{Z_{i+1}^{nf+1}-Z_i^{nf+1}}{\Delta X_i}+(1-\theta)\frac{Z_{i+1}^{nf}-Z_i^{nf}}{\Delta X_i}\ ] \qquad (3.48)$$

$$+\frac{\kappa|\overline{Q}|}{\overline{A}^2\overline{R}^{4/3}}[\ \chi\frac{Q_{i+1}^{nf+1}+Q_i^{nf+1}}{2}+(1-\chi)\frac{Q_{i+1}^{nf}+Q_i^{nf}}{2}\ ]-\frac{\xi\overline{B}}{g\overline{A}}U_a^2\cos\phi\ =\ 0$$

where the average top width is estimated from the previous time interval :

$$\overline{B}\ =\ \chi\frac{B_{i+1}^{nf}+B_i^{nf}}{2}+(1-\chi)\frac{B_{i+1}^{nf-1}+B_i^{nf-1}}{2} \qquad (3.49)$$

the average cross sectional area estimated from the previous iteration:

$$\overline{A}\ =\ \chi\frac{A_{i+1}^{nf}+A_i^{nf}}{2}+(1-\chi)\frac{A_{i+1}^{nf-1}+A_i^{nf-1}}{2} \qquad (3.50)$$

the average discharge Q estimated from the previous iteration:

$$\overline{Q}\ =\ \chi\frac{Q_{i+1}^{nf}+Q_i^{nf}}{2}+(1-\chi)\frac{Q_{i+1}^{nf-1}+Q_i^{nf-1}}{2} \qquad (3.51)$$

and the average hydraulic radius **R** is:

$$\overline{R} = \frac{\overline{A}}{\overline{B}} \tag{3.52}$$

In this solution technique, stage and discharge are computed at the ends of the segment identified by i and i+1 locations. The equations consist of four unknown quantities represented by Z^{nf+1}_{i+1}, Z^{nf+1}_{i}, Q^{nf+1}_{i}, Q^{nf+1}_{i+1} for two equations. With boundary conditions specified, the number of equations can be increased to find the solution.

The solution of the finite difference equations constructed earlier is accomplished by matrix methods after constructing the appropriate coefficient matrices. Rewriting the continuity equation (Eq 3.47) in a finite-difference format as:

$$Q_{i+1}^{nf+1} - Q_i^{nf+1} + \frac{(1-\theta)}{\theta}(Q_{i+1}^{nf} - Q_i^{nf}) + \frac{\overline{B}\Delta X_i}{2\Delta t_{nf}\,\theta}(Z_{i+1}^{nf+1} + Z_i^{nf+1} - Z_{i+1}^{nf} - Z_i^{nf}) = 0 \tag{3.53}$$

Define coefficient γ as :

$$\gamma = \frac{\overline{B}\Delta X_i}{2\Delta t_{nf}\,\theta} \tag{3.54}$$

The coefficient form of the continuity equation in terms of four unknowns for the ith segment, is

$$Q_{i+1}^{nf+1} + \gamma Z_{i+1}^{nf+1} - Q_i^{nf+1} + \gamma Z_i^{nf+1} = \delta \tag{3.55}$$

where

$$\delta = -\frac{(1-\theta)}{\theta}(Q_{i+1}^{nf} - Q_i^{nf}) - \gamma(Z_{i+1}^{nf} + Z_i^{nf}) \tag{3.56}$$

In a like manner, the coefficient form of the equation of motion can be derived from the previously formulated finite difference equation. The equation of motion (Eq 3.48) for the ith segment can be written as:

$$\frac{\Delta X_i}{2\Delta t_{nf}\theta g\overline{A}}[\, Q_{i+1}^{nf+1} + Q_i^{nf+1} - Q_{i+1}^{nf} - Q_i^{nf}\,] + \frac{2\beta\overline{Q}}{g\overline{A}^2}[\, Q_{i+1}^{nf+1} - Q_i^{nf+1} + \frac{(1-\theta)}{\theta}(Q_{i+1}^{nf} - Q_i^{nf})\,]$$

$$+ Z_{i+1}^{nf+1} - Z_i^{nf+1} + \frac{(1-\theta)}{\theta}(Z_{i+1}^{nf} - Z_i^{nf}) + \frac{\chi\Delta x_i \kappa|\overline{Q}|}{2\theta\overline{A}^2\overline{R}^{4/3}}[\, Q_{i+1}^{nf+1} + Q_i^{nf+1} + \tag{3.57}$$

$$\frac{(1-\chi)}{\chi}(Q_{i+1}^{nf} - Q_i^{nf})\,] = \frac{\beta\overline{Q}^2}{\theta g\overline{A}^3}(\overline{A}_{i+1}^{nf+1} - \overline{A}_i^{nf+1}) + \frac{\xi\Delta X_i\overline{B}}{\theta g\overline{A}}U_a^2\cos\phi$$

with the definitions of the coefficients,

$$\lambda = \frac{\Delta X_i}{2\Delta t_{nf}\theta gA} \tag{3.58a}$$

$$\mu = \frac{2\beta Q}{gA^2} \tag{3.58b}$$

$$\sigma = \frac{\chi \Delta X_i \kappa |\overline{Q}|}{2\theta \overline{A}^2 \overline{R}^{4/3}} \tag{3.58c}$$

the equation of motion, after substitution and collection of terms, becomes:

$$(\lambda+\sigma)[Q_{i+1}^{nf+1} + Q_i^{nf+1}] + \mu[Q_{i+1}^{nf+1} - Q_i^{nf+1}] + [Z_{i+1}^{nf+1} - Z_i^{nf+1}] = \epsilon \tag{3.59}$$

wherein

$$\begin{aligned} \epsilon = {} & (\lambda - \sigma\frac{(1-\chi)}{\chi}[Q_{i+1}^{nf} + Q_i^{nf}] \\ & - \mu\frac{(1-\theta)}{\theta}[Q_{i+1}^{nf} - Q_i^{nf}] - \frac{(1-\theta)}{\theta}[Z_{i+1}^{nf} - Z_i^{nf}] \\ & + \frac{\beta\overline{Q}^2}{\theta g\overline{A}^3}[\overline{A}_{i+1}^{nf+1} - \overline{A}_i^{nf+1}] + \frac{\xi\Delta X_i \overline{B}}{\theta g\overline{A}} U_a^2 \cos\phi \end{aligned} \tag{3.60}$$

let $\nu = \lambda+\sigma+\mu$, and $\omega = \lambda+\sigma-\mu$, the coefficient form of the equation of motion in the four unknown quantities for the ith segment can be written as:

$$\nu Q_{i+1}^{nf+1} + Z_{i+1}^{nf+1} + \omega Q_i^{nf+1} - Z_i^{nf+1} = \epsilon \tag{3.61}$$

the flow equations (Eq 3.55 and Eq 3.61) for the ith segment can be expressed in the following matrix form:

$$\begin{pmatrix} 1 & \nu \\ \gamma & 1 \end{pmatrix} \begin{pmatrix} Z_{i+1}^{nf+1} \\ Q_{i+1}^{nf+1} \end{pmatrix} - \begin{pmatrix} 1 & -\omega \\ -\gamma & 1 \end{pmatrix} \begin{pmatrix} Z_i^{nf+1} \\ Q_i^{nf+1} \end{pmatrix} = \begin{pmatrix} \epsilon \\ \delta \end{pmatrix} \tag{3.62}$$

Using appropriate internal and external boundary conditions and initial values, the solution could be obtained for the set of equations of all the segments within the network. The resultant solution set would consist of computed values of stage and discharge at all the cross sections delineating the segments. However, the equation set of a network consisting of M segments would form a coefficient matrix of minimum order M+2 requiring solution at each time step. Since this could consume a lot of computer time and memory, a transformation equation can be obtained that defines the relationship between the unknowns at consecutive cross sections that delimit a branch segment. By coupling all segment transformation equations for a branch, a transformation equation results that relates the unknown at the edges of the branch. By using these branch transformation equations instead of segment flow equations, the size of the coefficient matrix is reduced to order 4N for a network on N branches.

Defining a two-component vector state at the ith cross section,

$$S_i^{nf+1} = \begin{pmatrix} Z_i^{nf+1} \\ Q_i^{nf+1} \end{pmatrix} \tag{3.63}$$

The transformation equation for the state vector at i+1 is:

$$S_{i+1}^{nf+1} = U_{(i)} S_i^{nf+1} + u_{(i)} \tag{3.64}$$

The transformation matrices of the ith segment, U(i) and u(i), follow from the previously defined coefficient matrices thus:

$$U_{(i)} = \begin{pmatrix} 1 & \nu_{(i)} \\ \gamma_{(i)} & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 & -\omega_{(i)} \\ -\gamma_{(i)} & 1 \end{pmatrix} \tag{3.65}$$

and

$$u_{(i)} = \begin{pmatrix} 1 & \nu_{(i)} \\ \gamma_{(i)} & 1 \end{pmatrix}^{-1} \begin{pmatrix} \epsilon_{(i)} \\ \delta_{(i)} \end{pmatrix} \tag{3.66}$$

A branch-transformation equation can now be obtained through successive application of the segment transformation equation. The resulting equation that relates the unknown at cross section 1 and m of the nth branch that is composed of m cross sections could be written as:

$$S_m^{nf+1} = U_n S_1^{nf+1} + u_n \tag{3.67}$$

Wherein the transformation matrices of the nth branch, U_n and u_n, are obtained through successive substitution of the segment-transformation equation from m-1 down to the first segment. These branch transformation matrices,

$$U_n = U_{(m-1)}U_{(m-2)}\cdots U_1 \tag{3.68}$$

and

$$u_n = u_{(m-1)} + U_{(m-1)}[\, u_{(m-2)} + U_{(m-2)}(u_{(m-3)}\cdots + U_{(3)}(u_{(2)} + U_{(2)}u_{(1)})\cdots\,] \tag{3.69}$$

describe the relationship between the vectors of state, S_1^{nf+1} and S_m^{nf+1}, at the ends of the branch, that is at the junctions. If the n branch has five segments then:

$$S_5^{nf+1} = U_n S_1^{nf+1} + u_n \tag{3.70}$$

where

$$U_n = U_4 U_3 U_2 U_1 \tag{3.71}$$

and

$$u_n = u_4 + U_4[u_3 + U_3(u_2 + U_2 u_1)] \tag{3.72}$$

After a matrix solution is executed producing the stages and discharges at junctions, intermediate values of the unknowns at additional cross sections that delimit the branch segments are successively computed using the segment transformation equation for the particular branch.

For a network of N branches, the branch transformation equations, internal boundary conditions, and external boundary conditions form a linear system of 4N equations with 4N

unknowns. Branch transformation equations appear first in the matrix followed immediately by internal boundary equations and finally by the external boundary conditions expressed in equation form. The system of equations may be expressed in matrix notation as AX=B, where the coefficient matrix A is 4N x 4N , X is the vector of 4N unknowns, and B is the right hand column vector of 4N constants. The system of equations is solved by Gaussian elimination.

3.4 Flow Interchange between the Stream and the Aquifer

Streams contribute water to the aquifer or take water from it depending on the head gradient between the stream and the aquifer. Swain and Wexler (1996) developed MODBRANCH , which is a model that links BRANCH, which is a one-dimensional numerical model designated to simulate unsteady flow in an open-channel network, to MODFLOW. MODBRANCH simulates the interaction between the aquifer and the stream. A description of MODBRANCH mathematical procedure is presented here.

The network of channels is imposed on the aquifer discretitization. A typical arrangement of aquifer model cells and river segments is shown in Fig. 3.6. The head in each aquifer cell is assumed to be the same throughout the entire cell. Each stream segment is assigned to an aquifer cell; thus, no segment can span more than one cell, and a channel cross section is defined at each point where a river enters or leaves an aquifer cell. The transfer of water occurs through the stream sediments or bed. The cross-section of Fig. 3.7a shows a situation in which the open water of a stream is separated from the aquifer by a layer of low permeability streambed material. Figure 3.7b shows a conceptual representation of stream-aquifer interconnection in simulation.

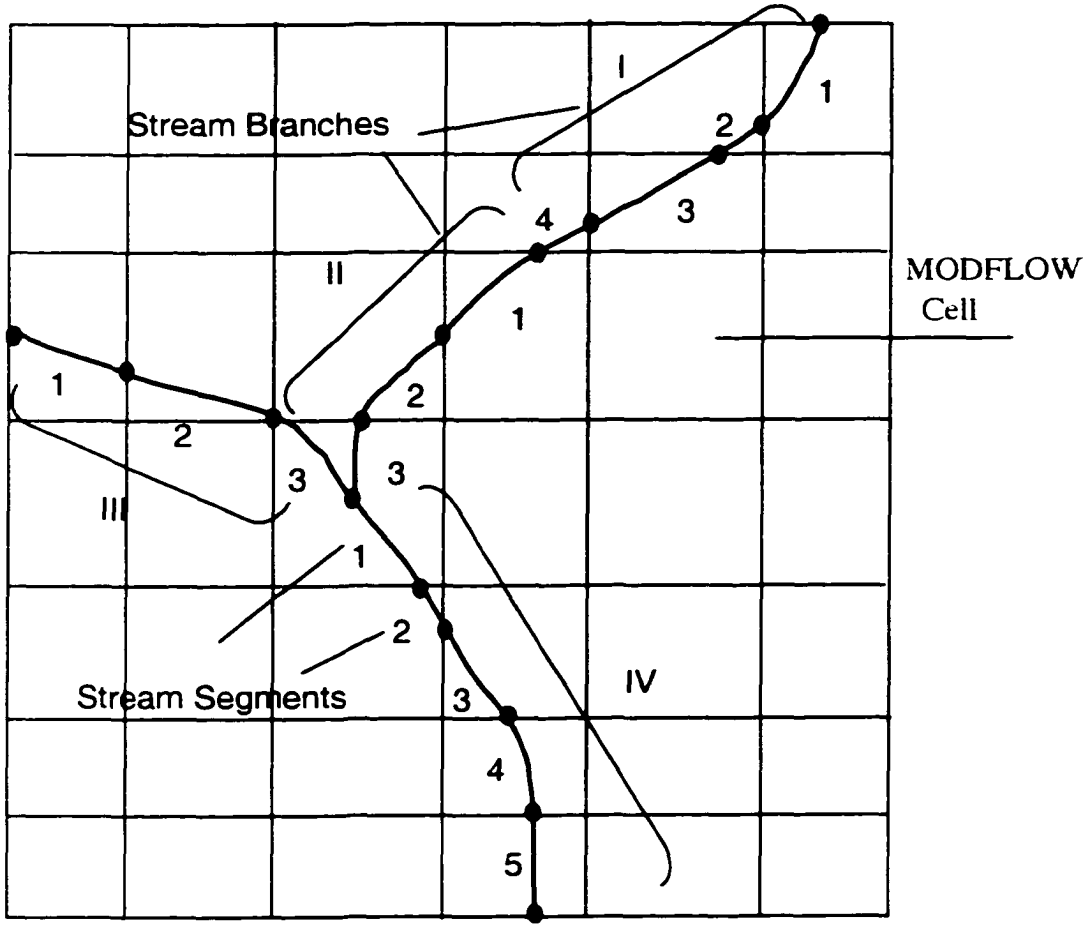


Figure 3.6 Arrangement of MODFLOW model cells and BRANCH stream reaches, Swain and Wexler,1996.

3.4.1 Flow Interchange between the Stream and the Aquifer Governing Equations

The leakage between the stream and the aquifer is simulated using Darcy's Law as:

$$q_L = \frac{K'}{b'} B(Z - h_{i,j,k}) \tag{3.73}$$

where

q_L is the flow leakage between the stream and the aquifer per unit length of the channel ($L^3T^{-1}L^{-1}$);

b' is streambed thickness (L);

K' riverbed hydraulic conductivity (LT^{-1});

B is the top width of the stream segment (L);

$h_{i,j,k}$ head in the aquifer cell underlying the stream (L); and

Z Surface water elevation (L).

q_L is taken positive if it is directed into the aquifer. Figure 3.8a shows the situation described by Eq 3.73; water level in the aquifer is above the bottom of the streambed layer, and flow through that layer is proportional to the head difference between the stream and the aquifer. In Fig. 3.8b, water level in the aquifer has fallen below the bottom of the streambed layer, leaving an unsaturated interval beneath that layer; if it is assumed that the streambed layer itself remains saturated, the head at its base will simply be the elevation at that point. If this elevation is designated Z_{bot}, the flow through the streambed layer is given by:

$$q_L = \frac{K'}{b'} B(Z - Z_{bot}) \tag{3.74}$$

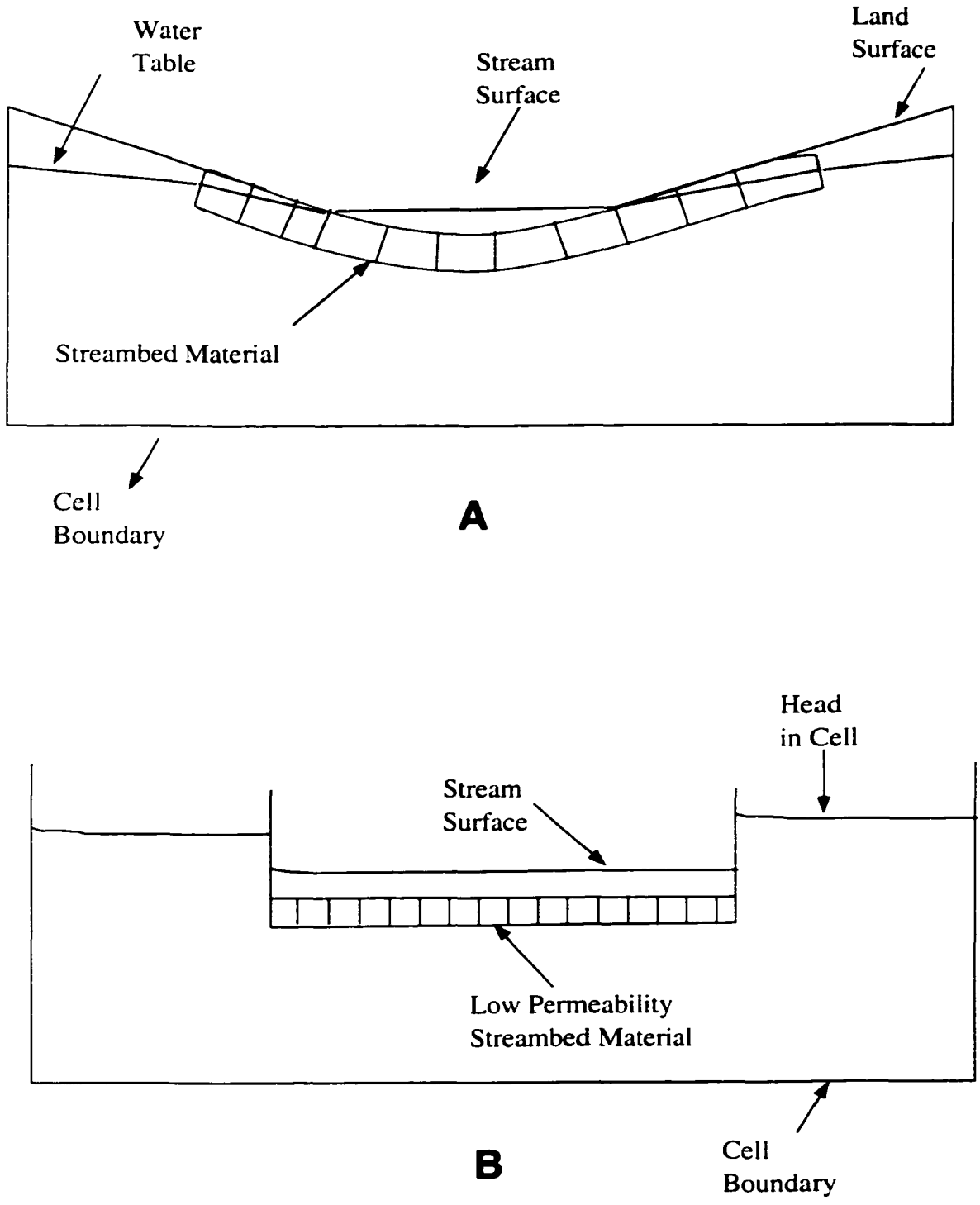


Figure 3.7 (a) Cross section of an aquifer containing a stream and (b) Conceptual representation of stream-aquifer interconnection in simulation, McDonald and Harbaugh (1988).

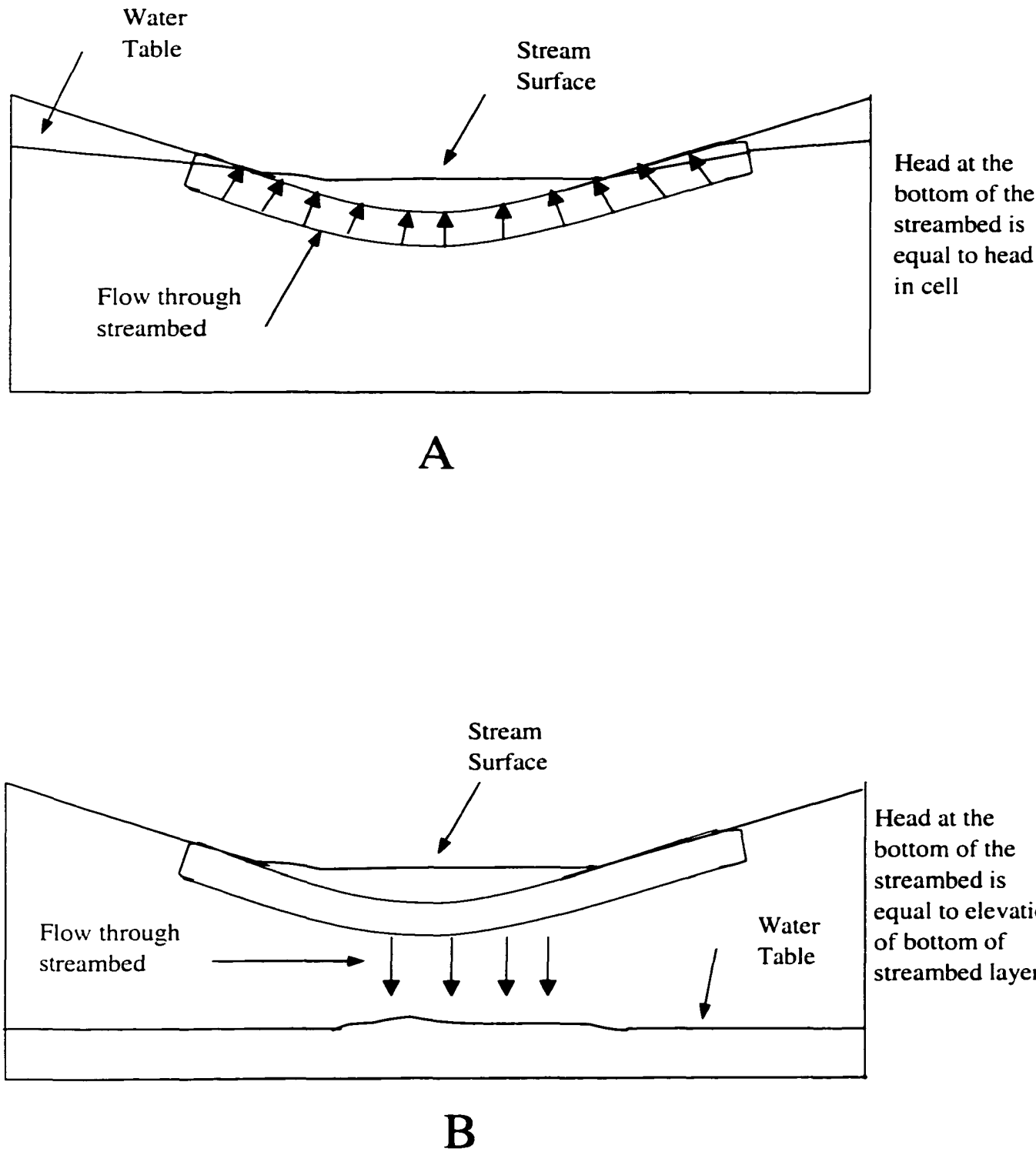


Figure 3.8 Cross sections showing the relation between head at the bottom of the streambed layer and head in the cell. Head in the cell is equal to the water table elevation, adapted from McDonald and Harbaugh (1988).

leakage between the stream and cell i,j,k is simulated according to the equation set

$$q_L = \frac{K'}{b'} B(Z - h_{i,j,k}) \qquad h_{i,j,k} > Z_{bot}$$
$$q_L = \frac{K'}{b'} B(Z - Z_{bot}) \qquad h_{i,j,k} \le Z_{bot} \tag{3.75}$$

Figure 3.9 shows a graph of flow between the stream and cell i,j,k as a function of the head, $h_{i,j,k}$ as calculated using Eq 3.75. Flow is zero when $h_{i,j,k}$ is equal to the water level in the stream, Z, for higher values of $h_{i,j,k}$ flow is negative that is, into the stream; for lower values of $h_{i,j,k}$ flow is positive, that is, into the aquifer. This positive flow increases linearly as $h_{i,j,k}$ decreases, until $h_{i,j,k}$ reaches Z_{bot}; thereafter the flow remains constant. In the following equations, it will be assumed that if the aquifer head is below the stream bottom, the value of h in the streamflow equation will be replaced by Z_{bot}.

3.4.2 Coupled groundwater surface water Governing Equations

The leakage term q_L described above is incorporated in the MODBRANCH formulation. Equation 3.39 described in Section 3.3.1 is modified to include lateral inflows or outflows represented by q_L. After that the equation has the form:

$$B\frac{\partial Z}{\partial t} + \frac{\partial Q}{\partial X} + q_L = 0 \tag{3.76}$$

Equation 3.76 is written in finite-difference form with similar format to that used in Section 3.3.2 of Eq 3.47:

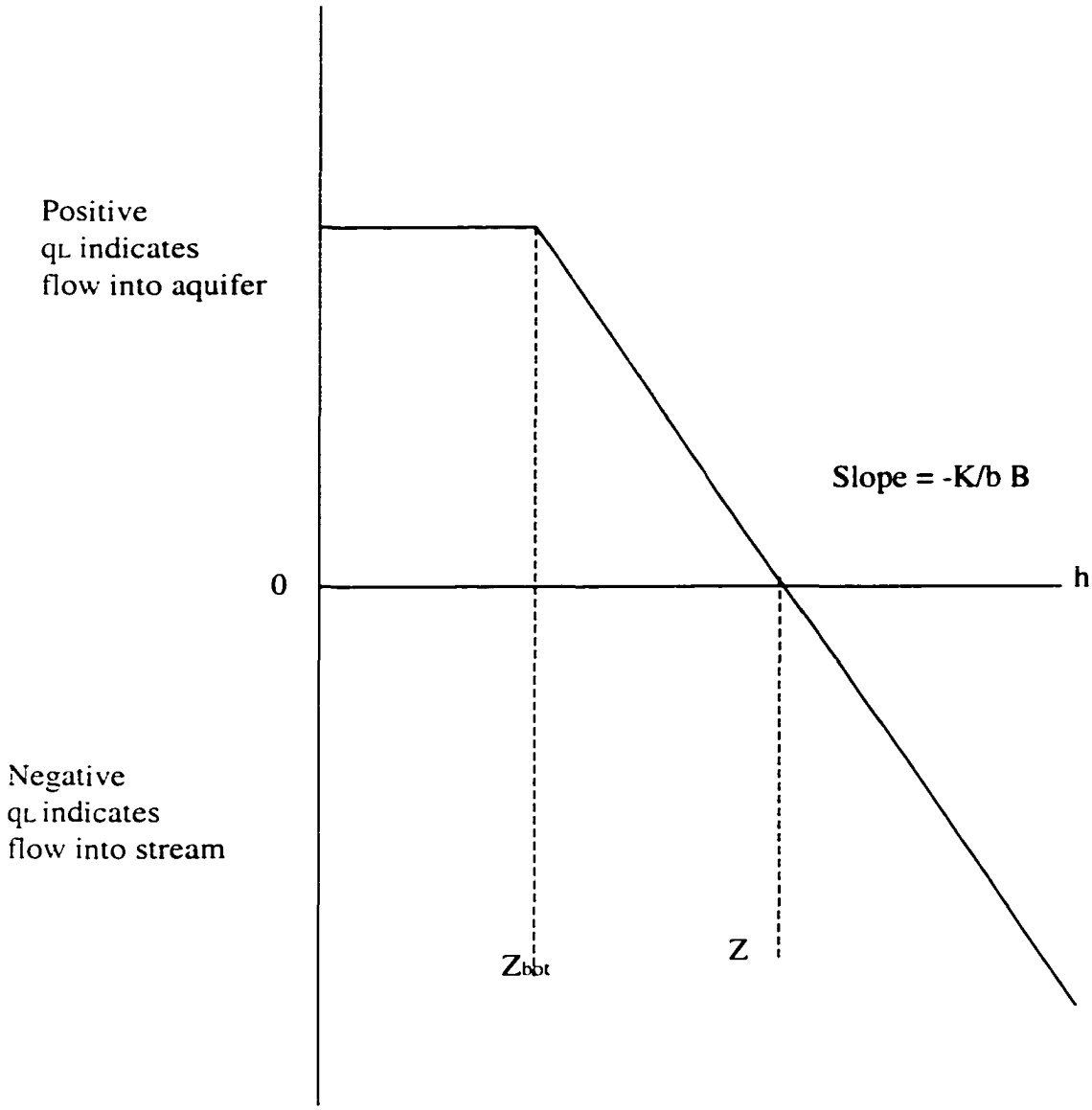


Figure 3.9- Plot of leakage q_L, from s stream into a cell as a function of head, h in the cell where Z_{bot} is the elevation of the bottom of the streambed and Z is the stage in the stream, McDonald and Harbaugh (1988).

$$\overline{B}\left[\frac{Z_{i+1}^{nf+1}+Z_i^{nf+1}}{2\Delta t_{nf}}-\frac{Z_{i+1}^{nf}+Z_i^{nf}}{2\Delta t_{nf}}\right]+\theta\frac{Q_{i+1}^{nf+1}-Q_i^{nf+1}}{\Delta X_i}+(1-\theta)\frac{Q_{i+1}^{nf}-Q_i^{nf}}{\Delta X_i}$$

$$\frac{\chi}{2}\left[CN_{i+1}B_{i+1}(Z_{i+1}^{nf+1}-h^{nf+1})+CN_iB_i(Z_{i+1}^{nf+1}-h^{nf+1})\right] \qquad (3.77)$$

$$\frac{(1-\chi)}{2}\left[CN_{i+1}B_{i+1}^{nf}(Z_{i+1}^{nf}-h^{nf})+CN_iB_i^{nf}(Z_i^{nf}-h^{nf})\right]=0$$

where

CN is hydraulic conductivity of stream bed divided by its thickness, K`/b` (T^{-1});

ΔX_i is length of channel segment from points i to i+1 (L);

θ is weighting factor for spatial derivatives, dimensionless;

χ is a weighting factor for averaged quantities, dimensionless;

B is average channel top width from the previous time interval (L).

Equation 3.77 is solved simultaneously for all segments with Eq 3.57 which represent the finite difference form of the momentum equation used in Section 3.3.2. Coefficients for a matrix solution were developed to use the same matrix solution that was already implemented in BRANCH, writing Eq 3.77 in the form similar to Eq 3.55 described in Section 3.3.2 :

$$Q_{i+1}^{nf+1}+\gamma Z_{i+1}^{nf+1}-Q_i^{nf+1}+\alpha Z_i^{nf+1}=\delta \qquad (3.78)$$

where

$$\gamma = \frac{\overline{B}\Delta X_i}{2\Delta t_{nf}\theta} + \frac{\chi CN_{i+1}B_{i+1}^{nf+1}}{2\theta} \tag{3.79a}$$

$$\alpha = \frac{\overline{B}\Delta X_i}{2\Delta t_{nf}\theta} + \frac{\chi CN_i B_i^{nf+1}\Delta X_i}{2\theta} \tag{3.79b}$$

and

$$\begin{aligned}\delta = & -\frac{1-\theta}{\theta}(Q_{i+1}^{nf} - Q_i^{nf}) + [\frac{\overline{B}\Delta X}{2\Delta t_{nf}\theta} - (1-\chi)(CN_{i+1}B_{i+1}^{nf}\frac{\Delta X_i}{2\theta}]Z_{i+1}^{nf} \\ & + [\frac{\overline{B}\Delta X}{2\Delta t_{nf}\theta} - (1-\chi)(CN_i B_i^{nf}\frac{\Delta X_i}{2\theta}]Z_i^{nf} \\ & + \frac{\Delta X_i}{2\theta}[\chi(CN_{i+1}B_{i+1}^{nf+1}h^{nf+1} + CN_i B_i^{nf+1}h^{nf+1} \\ & + (1-\chi)(CN_{i+1}B_{i+1}^{nf}h^{nf} + CN_i B_i^{nf}h^{nf})]\end{aligned} \tag{3.79c}$$

a similar matrix form of the flow equations in the ith segment is written as Eq 3.62 :

$$\begin{pmatrix} 1 & \nu \\ \gamma & 1 \end{pmatrix}\begin{pmatrix} Z_{i+1}^{nf+1} \\ Q_{i+1}^{nf+1} \end{pmatrix} - \begin{pmatrix} 1 & -\omega \\ -\alpha & 1 \end{pmatrix}\begin{pmatrix} Z_i^{nf+1} \\ Q_i^{nf+1} \end{pmatrix} = \begin{pmatrix} \epsilon \\ \delta \end{pmatrix} \tag{3.80}$$

MODBRANCH is a modification of BRANCH in which channel bed leakage is incorporated to and from the aquifer. The only variable in the computation scheme upon which leakage depends is the stage Z. The only input needed from the ground-water model is the aquifer head h, which are fixed values for the solution of Eq 3.80. The leakage quantities for all the MODBRANCH time

intervals during one MODFLOW time step must be calculated and averaged in MODBRANCH. This averaging process is accomplished using:

$$\overline{q_L \Delta X_i} = \frac{\Delta X_i}{nonf} \sum_{nf=T_s}^{T_s+nonf} \frac{\chi}{2}[\ CN_{i+1} B_{i+1}^{nf+1}(Z_{i+1}^{nf+1} - h^{nf+1}) + CN_i B_i^{nf+1}(Z_i^{nf+1} - h^{nf+1})\ ] \quad (3.81)$$
$$\frac{1-\chi}{2}[\ CN_{i+1} B_{i+1}^{nf}(Z_{i+1}^{nf}(Z_{i=1}^{nf} - h^{nf}) + CN_i B_i^{nf}(Z_i^{nf} - h^{nf})\ ]$$

where

Ts is the starting time interval when MODBRANCH is entered from MODFLOW

nonf is equal to the ratio mf/nf which is the number of MODBRANCH time intervals in one MODFLOW time step

The quantity derived in Eq 3.81 is the average leakage flow rate into or out of reach i of the stream during the MODFLOW time step (nonf MODBRANCH time intervals). This quantity is transferred back to MODFLOW and added to the term $O_{i,j,k}$ of Eq 3.31 for the aquifer model cell which contains reach i.

If there is only one MODBRANCH time interval in the MODFLOW time step (same-scale lengths nf =mf), leakage can be calculated implicitly in MODFLOW instead of passing $q_L \Delta X$ from MODBRANCH. This is achieved by setting the terms in Eq 3.29 as follows:

$$P_{i,j,k} = -(CN_{i+1} B_{i+1}^{nf+1} + CN_i B_i^{nf+1}) \frac{\Delta X_i}{2} \quad (3.82)$$

$$O_{i,j,k} = (CN_{i+1} B_{i+1}^{j+1} Z_{i+1}^{j+1} + C_i B_i^{j+1} Z_i^{j+1}) \frac{\Delta X_i}{2} \tag{3.83}$$

3.4.3 Surface flow Steady State Simulation

Steady state streamflow can be simulated in MODBRANCH. This is achieved by removing the time dependent terms in the continuity and momentum equations.

The continuity equation is written as:

$$\frac{\partial Q}{\partial X} + q_L = 0 \tag{3.84}$$

and the equation of motion is written as:

$$\frac{2\beta Q}{gA^2}\frac{\partial Q}{\partial X} - \frac{\beta Q^2}{gA^3}\frac{\partial A}{\partial X} + \frac{\partial Z}{\partial X} + \frac{\kappa}{A^2 R^{4/3}} Q|Q| - \xi \frac{B}{gA} U_a^2 \cos\phi = 0 \tag{3.85}$$

The coefficients γ and α of describing Eqs 3.79a and 3.79b are modified as:

$$\gamma = \frac{\chi CN_{i+1} B_{i+1}^{nf+1}}{2\theta} \tag{3.86}$$

$$\alpha = \frac{\chi CN_i B_i^{nf+1} \Delta X_i}{2\theta} \tag{3.87}$$

coefficient δ of Eq 3.79c is modified as:

$$\delta = -\frac{1-\theta}{\theta}(Q_{i+1}^{nf} - Q_i^{nf}) + [\ -(1-\chi)(CN_{i+1}B_{i+1}^{nf}\frac{\Delta X_i}{2\theta}\ ]Z_{i+1}^{nf}$$

$$+ [\ -(1-\chi)(CN_iB_i^{nf}\frac{\Delta X_i}{2\theta}\ ]Z_i^{nf} \qquad (3.88)$$

$$+ \frac{\Delta X_i}{2\theta}[\ \chi(CN_{i+1}B_{i+1}^{nf+1}h^{nf+1} + CN_iB_i^{nf+1}h^{nf+1}$$

$$+(1-\chi)(CN_{i+1}B_{i+1}^{nf}h^{nf} + CN_iB_i^{nf}h^{nf})\ ]$$

and λ of Eq 3.58a is set to zero. The equations are solved by the previously described method and the leakage effects are retained.

Chapter Four

MATHEMATICAL DEVELOPMENT

4.1 Introduction

This Chapter completes the mathematical description of the processes that occur during solute transport in a stream-aquifer system. It describes the mathematical development used to establish the main model. This includes modification of the solute transport equations in the aquifer as presented in the MT3D Model, and the development of the solute transport equations in the stream as presented in the SSTM Model. The numerical techniques implemented to solve these equations are explained. The mathematical terms required for the solute transport movement are identified from several equations described in Chapter Three.

4.2 Solute Transport in the Aquifer

The Modular Three Dimensional Solute Transport Model referred to as MT3D (Zheng, 1990) is used to simulate the solute transport in the aquifer. MT3D is a model for simulation of advection, dispersion and chemical reactions of dissolved constituents in the aquifer. MT3D uses a numerical technique to solve the advection dispersion that describes the transport of solutes in the aquifer. The numerical solution implemented in MT3D is a mixed Eulerian-Lagrangian method. The Lagrangian part of the method, used for solving the advection term, employs the forward tracking method of characteristics (MOC), the backward-tracking modified method of characteristics (MMOC), or hybrid of these two methods. The Eulerian part of the method, used for solving the dispersion, source/sink, and chemical reaction terms, utilizes a conventional block-centered finite difference method.

4.2.1 Solute Transport in the Aquifer Governing Equations

The three-dimensional partial differential equation describing transport of contaminants in the aquifer can be written as follows:

$$\begin{aligned}\frac{\partial C_a}{\partial t} &= -V_X\frac{\partial C_a}{\partial X} - V_Y\frac{\partial C_a}{\partial Y} - V_Z\frac{\partial C_a}{\partial Z} \\ &+ \frac{\partial}{\partial X}(D_{XX}\frac{\partial C_a}{\partial X}) + \frac{\partial}{\partial X}(D_{XY}\frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial X}(D_{XZ}\frac{\partial C_a}{\partial Z}) \\ &+ \frac{\partial}{\partial Y}(D_{YX}\frac{\partial C_a}{\partial X}) + \frac{\partial}{\partial Y}(D_{YY}\frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial Y}(D_{YZ}\frac{\partial C_a}{\partial Z}) \\ &+ \frac{\partial}{\partial Z}(D_{ZX}\frac{\partial C_a}{\partial X} + \frac{\partial}{\partial Z}(D_{ZY}\frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial Z}(D_{ZZ}\frac{\partial C_a}{\partial Z}) \\ &- \frac{q_{ss}}{\rho}(C_a - C_{ss}) + \sum_{kk=1}^{N} R_{kk}\end{aligned} \tag{4.1}$$

where

C_a is the concentration of dissolved solutes in the aquifer, ML^{-3};

t is time, T;

X,Y,Z is the distance along the respective Cartesian coordinate, L:

V_x, V_y, V_z are seepage velocities along x,y,z respectively (LT^{-1});

D_{xx}, D_{yy}, D_{zz},

$D_{xy} = D_{yx}$, $D_{xz} = D_{zx}$,

and $D_{yz} = D_{zy}$ are hydrodynamic dispersion coefficients in x,y,z (L^2T^{-1});

q_{ss} is the volumetric flux of water per unit volume of aquifer representing sources

(positive) and sinks (negative), T^{-1};

C_{ss} is the concentration of the sources or sinks, ML^{-3};

ρ is the porosity of the porous medium, dimensionless; and

$\sum R_k$ is a chemical reaction term, $ML^{-3}T^{-1}$.

The terms on the right hand side of Eq 4.1 are composed of the advection term, the dispersion term, the source/sink term, and the chemical reaction term. The terms representing advection are:

$$\textit{Advection Terms} = -V_X\frac{\partial C_a}{\partial X} - V_Y\frac{\partial C_a}{\partial Y} - V_Z\frac{\partial C_a}{\partial Z} \tag{4.2}$$

The advection term describes the transport of solute at the same velocity of groundwater flow. The dispersion terms are:

$$\begin{aligned}\textit{Dispersion Terms} = {} & \frac{\partial}{\partial X}(D_{XX}\frac{\partial C_a}{\partial X}) + \frac{\partial}{\partial X}(D_{XY}\frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial X}(D_{XZ}\frac{\partial C_a}{\partial Z}) \\ & + \frac{\partial}{\partial Y}(D_{YX}\frac{\partial C_a}{\partial X}) + \frac{\partial}{\partial Y}(D_{YY}\frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial Y}(D_{YZ}\frac{\partial C_a}{\partial Z}) \\ & + \frac{\partial}{\partial Z}(D_{ZX}\frac{\partial C_a}{\partial X} + \frac{\partial}{\partial Z}(D_{ZY}\frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial Z}(D_{ZZ}\frac{\partial C_a}{\partial Z})\end{aligned} \tag{4.3}$$

Dispersion in porous media refers to spreading of contaminant. Dispersion is caused by mechanical dispersion, a result of deviation of actual velocity on a micro scale from the average groundwater velocity, and molecular diffusion, a result of concentration variations. The sum of the mechanical dispersion and molecular diffusion is termed hydrodynamic dispersion. The hydrodynamic dispersion tensor for isotropic porous media is defined in the following component forms (Zheng,

1990):

$$
\begin{aligned}
D_{xx} &= \alpha_L \frac{V_x^2}{|V|} + \alpha_T \frac{V_y^2}{|V|} + \alpha_T \frac{V_z^2}{|V|} + D^* \\
D_{yy} &= \alpha_L \frac{V_y^2}{|V|} + \alpha_T \frac{V_x^2}{|V|} + \alpha_T \frac{V_z^2}{|V|} + D^* \\
D_{zz} &= \alpha_L \frac{V_z^2}{|V|} + \alpha_T \frac{V_x^2}{|V|} + \alpha_T \frac{V_y^2}{|V|} + D^* \\
D_{xy} &= D_{yx} = (\alpha_L - \alpha_T) \frac{V_x V_y}{|V|} \\
D_{xz} &= D_{zx} = (\alpha_L - \alpha_T) \frac{V_x V_z}{|V|} \\
D_{yz} &= D_{zy} = (\alpha_L - \alpha_T) \frac{V_y V_z}{|V|}
\end{aligned}
\tag{4.4}
$$

where

α_L is the longitudinal dispersivity (L);

α_L is the transverse dispersivity, (L);

D^* is the effective molecular diffusion coefficient (L^2T^{-1});

V_x, V_y, V_z are components of the velocity vector along the x, y, and z axes (LT^{-1});

$|V|=(V_x^2+V_y^2+V_z^2)^{1/2}$ is the magnitude of the velocity vector (LT^{-1}).

The source / sink term of Eq 4.1 is:

$$
Source/Sink\ Term = -\frac{q_{ss}}{\rho}(C_a - C_{ss}) \tag{4.5}
$$

the source/sink term represents solute mass dissolved in water entering the aquifer through sources, or solute mass dissolved in water leaving the aquifer through sinks. Sources/sinks are of two types:

point sources like wells, drains, rivers and areally distributed sinks and sources like recharge and evapotranspiration. MT3D treats rivers or streams as constant concentration sources or sinks and as a constant head boundary. The rate of water entering the aquifer or leaving it is obtained from the link to the ground water flow model. The concentration of solute source is set to be constant during the simulation stress period. In this study the solute is routed in the stream and the concentration is varied for each time step. To model that, the source/sink term is divided into two terms, one represents the stream source/sink term and the other term represents other sources and sinks considered by the model like wells, drains, recharge, evapotranspiration. The q_{ss} term of Eq 4.5 is reformed as:

$$q_{ss} = q_{LV} + q_{SO} \tag{4.6}$$

where

q_{LV} is the leakage from the stream to the aquifer or from the aquifer to the stream (T^{-1}); and

q_{SO} sources or sinks other than streams such as: wells, drains, recharge, evapotranspiration (T^{-1}).

The source/sink term is updated to:

$$\textit{Source/Sink Term} = -\frac{q_{LV}}{\rho}(C_a - C_s) - \frac{q_{SO}}{\rho}(C_a - C_{so}) \tag{4.7}$$

where

C_s is the solute concentration from stream inflow (ML^{-3}); and

C_{so} is the solute concentration from other sources (ML^{-3}).

q_{LV} is obtained from Eq 3.81 after dividing by aquifer cell volume as presented in the equation:

$$q_{LV} = \frac{q_L \Delta X}{\Delta X \Delta Y \Delta Z} \tag{4.8}$$

The last term on the right hand side of Eq 4.1 is the chemical reaction term. This term is dropped here since the assumption is made that the solute is conservative. After these adjustments Eq 4.1 is written as:

$$\begin{aligned}
\frac{\partial C_a}{\partial t} &= -V_X \frac{\partial C_a}{\partial X} - V_Y \frac{\partial C_a}{\partial Y} - V_Z \frac{\partial C_a}{\partial Z} \\
&+ \frac{\partial}{\partial X}(D_{XX} \frac{\partial C_a}{\partial X}) + \frac{\partial}{\partial X}(D_{XY} \frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial X}(D_{XZ} \frac{\partial C_a}{\partial Z}) \\
&+ \frac{\partial}{\partial Y}(D_{YX} \frac{\partial C_a}{\partial X}) + \frac{\partial}{\partial Y}(D_{YY} \frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial Y}(D_{YZ} \frac{\partial C_a}{\partial Z}) \\
&+ \frac{\partial}{\partial Z}(D_{ZX} \frac{\partial C_a}{\partial X} + \frac{\partial}{\partial Z}(D_{ZY} \frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial Z}(D_{ZZ} \frac{\partial C_a}{\partial Z}) \\
&- \frac{q_{LV}}{\rho}(C_a - C_s) - \frac{q_{SO}}{\rho}(C_a - C_{so})
\end{aligned} \tag{4.9}$$

4.2.2 Numerical Solution of the Solute Transport Equation in the Aquifer

The MT3D transport model follows the same spatial dsicretization convention as used by the MODFLOW model. An aquifer system is discretized into a mesh of blocks, or cells, the location of which are described in terms of rows (i), columns (j), and layers (k) as illustrated in Fig 3.1.

The numerical solution implemented in MT3D is a mixed Eulerian-Lagrangian method. Equation 4.9 is an Eulerian expression in which the partial derivative $\partial C_a/\partial t$, indicates the rate of change in solute concentration (C_a) at a fixed point in space. Equation 4.9 can be expressed in Lagrangian form as:

$$\frac{dC_a}{dt} = \frac{\partial}{\partial X}(D_{XX}\frac{\partial C_a}{\partial X}) + \frac{\partial}{\partial X}(D_{XY}\frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial X}(D_{XZ}\frac{\partial C_a}{\partial Z})$$
$$+ \frac{\partial}{\partial Y}(D_{YX}\frac{\partial C_a}{\partial X}) + \frac{\partial}{\partial Y}(D_{YY}\frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial Y}(D_{YZ}\frac{\partial C_a}{\partial Z})$$
$$+ \frac{\partial}{\partial Z}(D_{ZX}\frac{\partial C_a}{\partial X} + \frac{\partial}{\partial Z}(D_{ZY}\frac{\partial C_a}{\partial Y}) + \frac{\partial}{\partial Z}(D_{ZZ}\frac{\partial C_a}{\partial Z}) \qquad (4.10)$$
$$- \frac{q_{LV}}{\rho}(C_a - C_s) - \frac{q_{SO}}{\rho}(C_a - C_{so})$$

where the substantial derivative, dC_a/dt is expressed as:

$$\frac{dC_a}{dt} = \frac{\partial C_a}{\partial t} + V_X\frac{\partial C_a}{\partial X} + V_Y\frac{\partial C_a}{\partial Y} + V_Z\frac{\partial C_a}{\partial Z} \qquad (4.11)$$

Equation 4.11 indicates the rate of change in solute concentration C_a along the pathline of a contaminant particle or the curve of the characteristics of the velocity field.

Using Eqs 4.10 and 4.11 dC_a/dt is approximated in the finite difference form as:

$$\frac{dC_a}{dt} = \frac{C_{a\,i,j,k}^{nt+1} - C_{a\,i,j,k}^{nt}}{\Delta t_{nt}} \qquad (4.12)$$

where

$C_{a\,i,j,k}^{nt+1}$ is the average solute concentration for cell i,j,k at the new time step nt+1;

$C_{a\,i,j,k}^{nt}$ is the average solute concentration for cell i,j,k at the old time level nt;

Δt_{nt} is the time step between time nt and nt+1;

The solute concentration at the new time step is estimated in MT3D using the mixed Eulerian-

Lagrangian method. In this method, Eq 4.11, which accounts for the effect of advection, is solved with a lagrangian method on a moving coordinate, while Eq 4.10, which accounts for the effect of dispersion, sink/source mixing, is solved with the finite-difference method on the fixed Eulerian grid. Equation 4.12 is written as:

$$\frac{\Delta C_{a\ i,j,k}}{\Delta t_{nf}} = \frac{\Delta C_{a\ i,j,kADV}}{\Delta t_{nf}} + \frac{\Delta C_{a\ i,j,kDSP}}{\Delta t_{nf}} + \frac{\Delta C_{a\ i,j,kSSM}}{\Delta t_{nf}} \qquad (4.13)$$

The first term on the right hand side of Eq 4.13 is estimated using the method of characteristics or the modified method of characteristics which use a particle tracking technique. The particle tracking technique requires the evaluation of velocity at an arbitrary point from hydraulic heads calculated at the cells using MODFLOW. The details of this technique are presented in the MT3D manual (Zheng, 1990). The second term on the right hand side of Eq. 4.13 which represents the change of concentration due to dispersion estimated using a fully explicit finite difference scheme. Details are in MT3D Manual (Zheng, 1990).

The third term on the right hand side of Eq 4.13 which represents concentration change due to fluid sink and/or source mixing and written as :

$$\frac{dC_{a\ SSM}}{dt} = -\frac{q_{LV}}{\rho}(C_a - C_s) - \frac{q_{so}}{\rho}(C_a - C_{so}) \qquad (4.14)$$

will be modified in this study so that the concentration of the solute in the stream referred to as: C_s will be obtained from the link to the Stream Solute Transport Model, SSTM.

Equation 4.14 is solved with the fully explicit finite-difference scheme,

$$\frac{dC_{a\ SSM}}{dt} = \frac{\Delta C_{a\ SSM\ i,j,k}}{\Delta t_{nf}} = \frac{q^{nt}_{LV\ i,j,k}}{\rho_{i,j,k}}(C^{nt'}_{a\ i,j,k} - C^{nt}_{s\ i,j,k}) - \frac{q^{n}_{SO\ i,j,k}}{\rho_{i,j,k}}(C^{nt'}_{a\ i,j,k} - C^{nt}_{so\ i,j,k}) \qquad (4.15)$$

where

$\Delta C_{a\ SSM\ ijk}$ is the concentration change due to sink/source mixing from old time level (nt) to new time level (nt+1) at sink or source cell (i,j,k).

$C_{a\ i,j,k}^{nt'}$ is the average solute concentration in cell i,j,k due to advection alone.

$C_{s\ i,j,k}^{nt}$ is the stream inflow/outflow concentration at old time level nt,

$C_{so\ i,j,k}^{nt}$ is the other sources/sinks concentration like wells, drains, evapotranspiration, and recharge. The value of $C_{s\ i,j,k}^{nt}$ will be obtained from the link to SSTM. The MT3D Transport step (nt) is set equal to SSTM time steps (ns). $C_{s\ i,j,k}^{nt}$ is obtained from SSTM for time step nt.

A new package referred to as Stream Solute Package, (SSL1) is added MT3D to link to SSTM. The structure of the modified MT3D is explained in Chapter 5. Value of $C_{so\ i,j,k}^{nt}$ representing concentration of other sources or sinks will be constant for the stress period and is read from MT3D input file designated for sources and sinks.

4.3 Solute Transport in the Stream

A model is developed to route solutes in the stream connected to the aquifer. This is a primary part of the MSAST and referred to as Stream Solute Transport Model, SSTM. The model is coded based on the one-dimensional advection dispersion equation in the stream. The details of the structure of the model are explained in Chapter 5. The governing equations of solute transport in the stream and the numerical solution that is used to solve them are explained below.

4.3.1 Solute Transport in the Stream Governing Equations

Solute transport in the stream is routed using the conservation of solute mass equation:

$$\frac{\partial(C_s A)}{\partial t} = -\frac{\partial}{\partial X}(C_s Q) + \frac{\partial}{\partial X}(AD\frac{\partial C_s}{\partial X}) + C_a q_{lin} \qquad (4.17a)$$

$$\frac{\partial(C_s A)}{\partial t} = -\frac{\partial}{\partial X}(C_s Q) + \frac{\partial}{\partial X}(AD\frac{\partial C_s}{\partial X}) - C_s q_{lout} \qquad (4.17b)$$

where

A is the stream channel cross-sectional area (L^2);

C_s is the solute concentration in the stream (ML^{-3});

C_a is solute concentration in leakage to the stream from the aquifer (ML^{-3});

D is stream longitudinal dispersion coefficient (L^2T^{-1});

q_{lin} lateral leakage rate from the aquifer into the stream per unit length of stream($L^3T^{-1}L^{-1}$);

q_{lout} lateral outflow rate from the stream to the aquifer ($L^3T^{-1}L^{-1}$);

t time (T); and

X distance along X-direction (L).

The terms on the left-hand side of Eqs 4.17a, 4.17b represent accumulation of solute mass; the terms on the right-hand side represent change in solute mass due to advection, dispersion, and inflow/outflow to the stream.

Fisher et al. (1979) have developed the following formula for a longitudinal dispersion

coefficient:

$$D = 0.011 \frac{U^2 B_m^2}{ZU*} \quad (4.18)$$

where

U is mean velocity (LT^{-1});

B_m is stream mean width (L);

Z is mean depth (L); and

U* is shear velocity (L).

Shear velocity U* is obtained using the formula:

$$U* = \sqrt{gZS} \quad (4.19)$$

where

g is acceleration due to gravity (LT^{-2}); and

S is channel slope, dimensionless.

4.3.2 Numerical Solution of the Solute Transport Equation in the Stream

The finite difference technique will be used to solve the above equations. The time and spatial derivatives are approximated using backward in time backward in space finite difference approximations. The stream channel network will be discretized based on MODBRANCH scheme, see Fig. 3.6. The parameters of the hydraulic solution of the flow filed obtained from MODBRANCH is utilized in the solution. For each stream segment values of discharge ; cross sectional area; mean depth; mean width; slope; and leakage to or from the aquifer are utilized. Using this, Eq 4.17a is approximated as:

$$\frac{(C_sA)_i^{ns+1}-(C_sA)_i^{ns}}{\Delta t_{ns}} = -\frac{(C_sQ)_i^{ns+1}-(C_sQ)_{i-1}^{ns+1}}{\Delta X}$$

$$+\frac{1}{\Delta X}\left[\frac{(AD)_i^{ns+1}(C_{s\,i+1}^{ns+1}-C_{s\,i}^{ns+1})}{\Delta X}-\frac{(AD)_{i-1}^{ns+1}(C_{s\,i}^{ns+1}-C_{s\,i-1}^{ns+1})}{\Delta X}\right] \qquad (4.20a)$$

$$+C_{ai}^{ns+1}q_{lini}^{ns+1}$$

for the case of outflow to the aquifer Eq 4.17b is approximated as:

$$\frac{(C_sA)_i^{ns+1}-(C_sA)_i^{ns}}{\Delta t} = -\frac{(C_sQ)_i^{ns+1}-(C_sQ)_{i-1}^{ns+1}}{\Delta X}$$

$$+\frac{1}{\Delta X}\left[\frac{(AD)_i^{ns+1}(C_{s\,i+1}^{ns+1}-C_{s\,i}^{ns+1})}{\Delta X}-\frac{(AD)_{i-1}^{ns+1}(C_{s\,i}^{ns+1}-C_{s\,i-1}^{ns+1})}{\Delta X}\right] \qquad (4.20b)$$

$$-C_{si}^{ns+1}q_{louti}^{ns+1}$$

Equations 4.20a, 4.20b are rearranged so that all of the known quantities (solute concentration at previous time step, ns) appear on the right-hand side, and all of the unknown quantities (solute transport at time step ns) appear on the left-hand side. One exception to this rearrangement is that an unknown quantity C_a^{ns+1}, which is the concentration in the aquifer at time step ns remains on the right-hand side. Equations 4.20a, 4.20b are coupled with the aquifer solute transport equation (Eq 4.15). The value of C_a in equation 4.20a is obtained from Eq 4.15. The value of C_a in equation 4.15 is obtained from Eq 4.20b. After rearrangement, Eq 4.20a is written as:

$$\begin{aligned}
&\left[-Q_{i-1}^{ns+1}\frac{\Delta t_{ns}}{\Delta X} - (AD)_{i-1}^{ns+1}\frac{\Delta t_{ns}}{(\Delta X)^2} \right] C_{s\,i-1}^{ns+1} \\
&+ \left[A_i^{ns+1} + Q_i^{ns+1}\frac{\Delta t_{ns}}{\Delta X} + (AD)_i^{ns+1}\frac{\Delta t_{ns}}{(\Delta X)^2} + (AD)_{i-1}^{ns+1}\frac{\Delta t_{ns}}{(\Delta X)^2} \right] C_{s\,i}^{ns+1} \\
&-\left[(AD)_i^{ns+1}\frac{\Delta t_{ns}}{(\Delta X)^2} \right] C_{s\,i+1}^{ns+1} = C_{s\,i}^{ns} A_i^{ns} + C_{a\,i}^{ns+1} q_{lin\,i}^{ns+1} \Delta t_{ns}
\end{aligned} \tag{4.21a}$$

and Eq 4.20b is written as:

$$\begin{aligned}
&\left[-Q_{i-1}^{ns+1}\frac{\Delta t_{ns}}{\Delta X} - (AD)_{i-1}^{ns+1}\frac{\Delta t_{ns}}{(\Delta X)^2} \right] C_{s\,i-1}^{ns+1} \\
&+ \left[A_i^{ns+1} + Q_i^{ns+1}\frac{\Delta t_{ns}}{\Delta X} + (AD)_i^{ns+1}\frac{\Delta t_{ns}}{(\Delta X)^2} + (AD)_{i-1}^{ns+1}\frac{\Delta t_{ns}}{(\Delta X)^2} + q_{lout\,i}^{ns+1} \right] C_{s\,i}^{ns+1} \\
&-\left[(AD)_i^{ns+1}\frac{\Delta t_{ns}}{(\Delta X)^2} \right] C_{s\,i+1}^{ns+1} = C_{s\,i}^{ns} A_i^{ns}
\end{aligned} \tag{4.21b}$$

The equations are rearranged in terms of the coefficients of $C_{s\,i-1}$, $C_{s\,i}$, $C_{s\,i+1}$ for the time step ns+1:

$$e_i C_{s\,i-1}^{ns+1} + f_i C_{s\,i}^{ns+1} + g_i C_{s\,i+1}^{ns+1} = r_i \tag{4.22}$$

where

$$e_i = [-Q_{i-1}^{ns+1} \frac{\Delta t_{ns}}{\Delta X} - (AD)_{i-1}^{ns+1} \frac{\Delta t_{ns}}{(\Delta X)^2}] \tag{4.23}$$

e_i is the same for both inflow and outflow equations, now f_i for inflow is written as:

$$f_i = [A_i^{ns+1} + Q_i^{ns+1} \frac{\Delta t_{ns}}{\Delta X} + (AD)_i^{ns+1} \frac{\Delta t_{ns}}{(\Delta X)^2} + (AD)_{i-1}^{ns+1} \frac{\Delta t_{ns}}{(\Delta X)^2}] \tag{4.24a}$$

and f_i for outflow:

$$f_i = [A_i^{ns+1} + Q_i^{ns+1} \frac{\Delta t_{ns}}{\Delta X} + (AD)_i^{ns+1} \frac{\Delta t_{ns}}{(\Delta X)^2} + (AD)_{i-1}^{ns+1} \frac{\Delta t_{ns}}{(\Delta X)^2} + q_{lout\,i}^{ns+1}] \tag{4.24b}$$

and g_i for both inflow and outflow:

$$g_i = -[(AD)_i^{ns+1} \frac{\Delta t_{ns}}{(\Delta X)^2}] \tag{4.25}$$

r_i for inflow and outflow are written respectively:

$$r_i = C_{s\,i}^{ns} A_i^{ns} + C_{a\,i}^{ns+1} q_{lin\,i}^{ns+1} \Delta t_{ns} \tag{4.26a}$$

in the case of a junction element with a tributary upstream element, the basic equation becomes:

$$r_i = C_{s\,i}^{ns} A_i^{ns} \tag{4.26b}$$

$$e_i C_{s\,i+1}^{ns+1} + f_i C_{s\,i}^{ns+1} + g_i C_{s\,i-1}^{ns+1} + l_{ju} C_{s\,ju}^{ns+1} = r_i \tag{4.27}$$

where

$$l_{ju} = [-Q_{ju}^{ns+1} \frac{\Delta t_{ns}}{\Delta X} - (AD)_{ju}^{ns+1} \frac{\Delta t_{ns}}{(\Delta X)^2}] \tag{4.28}$$

ju the segment upstream of segment i

$C^{ns+1}{}_{s\,ju}$ concentration of solute in element ju at time step ns+1

Equation 4.22 is established for each segment i in the stream network. For all segments, the equations represent a set of simultaneous linear equations whose solution provides the values of $C^{ns+1}{}_{s\,i}$ at time step ns+1 for all i's. Expressed in matrix form, it appears as shown in Eq. 4.29.

$$\begin{bmatrix} f_1 & g_1 & & & & & \\ e_2 & f_2 & g_2 & & & & \\ & e_3 & f_3 & g_3 & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & e_i & f_i & g_i & \\ & & & & \cdot & \cdot & \cdot \\ & & & & & e_{N-1} & f_{N-1} & g_{N-1} \\ & & & & & & e_N & f_N \end{bmatrix} X \begin{bmatrix} C_{s1}^{ns+1} \\ C_{s2}^{ns+1} \\ C_{s3}^{ns+1} \\ \cdot \\ C_{si}^{ns+1} \\ \cdot \\ C_{sN-1}^{ns+1} \\ C_{sN}^{ns+1} \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ \cdot \\ r_i \\ \cdot \\ r_{N-1} \\ r_N \end{bmatrix} \qquad (4.29)$$

the left matrix is a tri-diagonal matrix, the solution algorithm is obtained using the following steps:

1. Divide the first equation in the set of matrix Eqs 4.29 by f_1 to obtain:

$$C_{s1}^{ns+1} + W_1 C_{s2}^{ns+1} = G_1 \qquad (4.30)$$

where

$$W_1 = \frac{g_1}{f_1} \tag{4.31}$$

$$G_1 = \frac{r_1}{f_1} \tag{4.32}$$

2. Eliminate e_2 of the equation represented by the second row of the set of Eqs 4.29 by substituting the value of C^{ns+1}_{s1} the result is :

$$C_{s2}^{ns+1} + W_2 C_{s3}^{ns+1} = G_2 \tag{4.33}$$

where

$$W_2 = \frac{g_2}{f_2 - e_2 W_1} \tag{4.34}$$

$$G_2 = \frac{r_2 - e_2 G_1}{f_2 - e_2 W_1} \tag{4.35}$$

3. Combine Eq 4.33 and the third equation in the matrix set 4.29 to eliminate e_3 and the result is:

$$C_{s3}^{ns+1} + W_3 C_{s4}^{ns+1} = G_3 \tag{4.36}$$

where

$$W_3 = \frac{g_3}{f_3 - e_3 W_2} \tag{4.37}$$

$$G_3 = \frac{r_3 - e_3 G_2}{f_3 - e_3 W_2} \tag{4.38}$$

4. Proceed through the equations, eliminating e_i and storing values of W_i and G_i given by:

$$W_i = \frac{g_i}{f_i - e_i W_{i-1}}, \quad i = 2, 3, \ldots, N \tag{4.39}$$

$$G_i = \frac{r_i - e_i G_{i-1}}{f_i - e_i W_{i-1}}, \quad i = 2, 3, \ldots, N \tag{4.40}$$

The last equation is solved for C_{sN}^{ns+1} by :

$$C_{sN}^{ns+1} = G_N \tag{4.41}$$

5- Solve for $C^{ns+1}_{s\,i-1}$, $C^{ns+1}_{s\,i-2}$, ... , $C^{ns+1}_{s\,1}$ by back substitution.

$$C_{si}^{ns+1} = G_i - W_i C_{si+1}^{ns+1}, \quad i=N-1, N-2, \ldots, 1 \tag{4.42}$$

Solving the system of equations, the values of C_S at the new time step ns+1 are obtained. This modification obtains the stream concentrations C_s, appeared in Eq 4.15 of the MT3D from the link to the SSTM instead of reading that from the MT3D input file designated for sources and sinks.

Chapter Five

MODEL STRUCTURE

5.1 Introduction

This Chapter illustrates the structure of the developed model. The main model is referred to as Model for Stream-Aquifer Solute Transport or MSAST and its main purpose is to simulate conservative solute transport in a stream-aquifer system. This involves simulation of flow and solute transport in the aquifer, flow and solute transport in the stream, and the interchange of flow and solute between the stream and the aquifer. The MSAST is composed of four primary models. MODFLOW, the aquifer flow model, MODBRANCH, the coupled groundwater surface water flow model, a modification of MT3D, the aquifer solute transport model, and a model that is developed in this study to simulate the interchange of solute between the stream and the aquifer and the transport of solute in the stream. This model is referred to as Stream Solute Transport Model, SSTM. The structure of the MSAST is shown in Fig. 5.1. The structure of the primary models and how they interact with each other will be described here.

MODFLOW code is designed having a modular structure. The model consists of a main program and a large number of independent modules. MT3D and MODBRANCH program structure and design are similar to MODFLOW. This structure makes it possible to simulate model processes independently and save computer space. Also this allows new packages to be added without having to modify the existing code. SSTM is designed utilizing similar structural design.

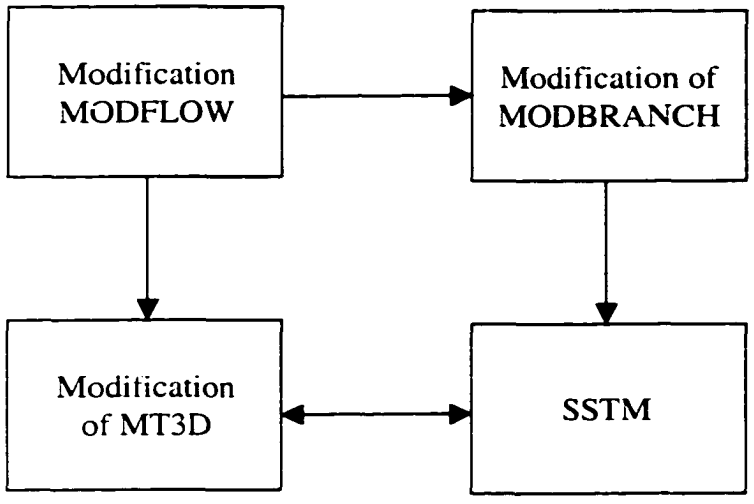


Figure 5.1 Model for Stream-Aquifer Solute Transport, MSAST main model structure showing primary models and their interfaces

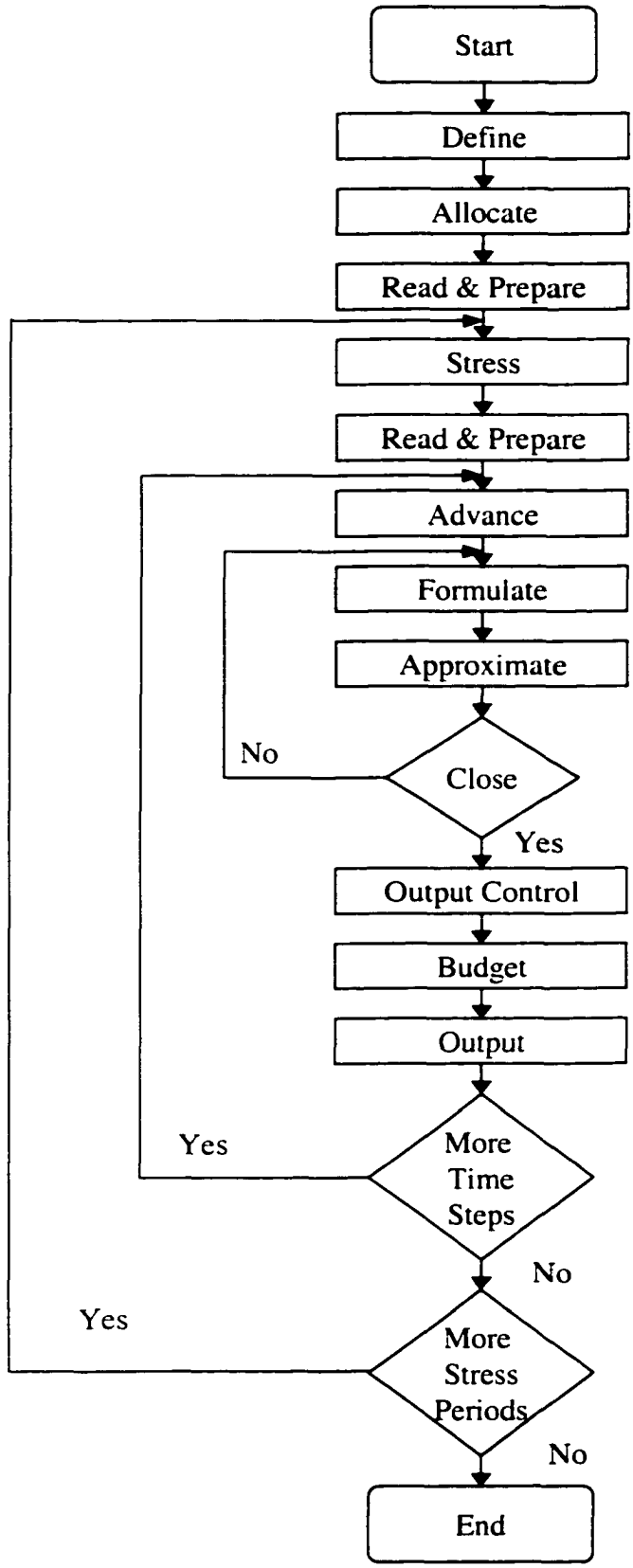
Two main interfaces are already established. The interface between MODFLOW and MT3D through the LKM Package and the interface between MODFLOW and MODBRANCH through the BRC2 Package. There are three major tasks that are taken to develop the MSAST, these are:

1. Development of SSTM having a similar structural design to MODFLOW, MODBRANCH and MT3D
2. Including the SSTMLINK Package in MODBRANCH that interfaces with SSTM and saves the stream variables needed by SSTM
3. Including the SSL1 Package in MT3D that interface with SSTM. These tasks are explained while describing each primary model of the MSAST in the following sections.

5.2 MODFLOW Structure

The current version of MODFLOW, referred to as MODFLOW-96 is described here. MODFLOW-96 is based on the old version of MODFLOW with many new capabilities added to it. A brief description is provided here, for a complete description of the MODFLOW structure refer to McDonald and Harbaugh, 1988, Harbaugh and McDonald, 1996a, and Harbaugh and McDonald, 1996b.

MODFLOW consists of a main program and a large number of highly independent subroutines called modules. A package in MODFLOW is a combination of subroutines required to incorporate a particular hydrologic process or solution algorithm into the simulation. For example the River Package, or the Well Package. Procedures in MODFLOW are subroutines that need to be performed for a typical simulation like allocating space or reading data. These procedures are shown in Fig. 5.2. Procedures are grouped into packages. Figure 5.3 illustrates MODFLOW



DEFINE-Read data specifying number of rows, columns, layers, stress periods, and major program options

ALLOCATE - Allocate space in the computer to store data

READ AND PREPARE - Read data which are constant throughout the simulation. Prepare the data by performing whatever calculations can be made at this stage.

ADVANCE - Calculate length of time step and set heads at beginning of a new time step equal to heads calculated for the end of the previous time step.

FORMULATE - Calculate the coefficients of the finite difference equations for each cell.

APROXIMATE - Make one cut at approximating a solution to the system of finite difference equations.

OUTPUT CONTROL - Determine whether results should be written or saved on disk for this time step. Send signals to the BUDGET and OUTPUT procedures to indicate exactly what information should be put out.

BUDGET - Calculate terms for the overall volumetric budget and calculate and save cell by cell flow terms for each component of flow.

OUTPUT - Print and save heads, drawdown and overall volumetric budgets in accordance with signals from OUTPUT CONTROL procedure.

Figure 5.2 MODFLOW overall program structure, McDonald and Harbaugh, 1988.

packages and their procedures. Rows in Fig. 5.3 correspond to procedures, while columns correspond to packages.

Table 5.1 lists the various packages available in MODFLOW-96 version 3.2, gives three characters abbreviation used in the package designation scheme, and provides documentation reference of each package. Figure 5.4 shows a detailed flow chart of the main program, indicating all of the primary modules together with the tests that determine whether each module is to be called.

5.3 MODBRANCH Structure

MODBRANCH (Swain and Wexler, 1996) was developed by combining MODFLOW and BRANCH. MODBRANCH version 3.7 will be used here. MODBRANCH interface of MODFLOW and BRANCH is similar to any other independent package interface to MODFLOW. The main purpose of MODBRANCH is to simulate flow in a stream-aquifer system. Two main tasks were taken in the coupling of MODFLOW and BRANCH. First, BRANCH was modified where the leakage to or from the aquifer was included in the formulation as explained in Chapter 3 Section 3.3. Modified BRANCH is referred to as MODBRANCH. Second, an additional package referred to as BRC2 Package was added to MODFLOW. The purpose of this package is to interface with MODBRANCH and get the values of leakage in stream cells and incorporate those values in the solution of the groundwater equation. BRC2 modules or subroutines are added to MODFLOW as shown in Fig. 5.5. BRC2 Package is composed of four modules:

1. BRC2AL: allocates space for data arrays used by MODBRANCH

Packages

Procedures	BAS	BCF	WEL	DRN	RIV	EVT	TLK	GHB	RCH	GFD	HFB	RES	STR	IBS	CHD	FHB	SIP	SOR	DE4	PCG
Define (DF)	BAS5DF													IBS1AL	CHD1AL	FHB1AL	SIP5AL	SOR5AL	DE45AL	
Allocate (AL)	BAS5AL	BCF5AL	WEL5AL	DRN5AL	RIV5AL	EVT5AL	TLK1AL	GHB5AL	RCH5AL	GFD1AL	HFB1AL	RES1AL	STR1AL							
Read & Prepare (RP)	BAS5RP	BCF5RP																		
Sterss (ST)	BAS5ST																			
Read & Prepare (RP)			WEL5RP	DRN5RP	RIV5RP	EVT5RP	TLK1RP	GHB5RP	RCH5RP	GFD1RP	HFB1RP	RES1RP	STR1RP	IBS1RP	CHD1RP	FHB1RP	SIP5RP	SOR5RP	DE45RP	PCG2RP
Advance (AD)	BAS5AD						TLK1AD													
Formulate (FM)	BAS5FM	BCF5FM	WEL5FM	DRN5FM	RIV5FM	EVT5FM	TLK1FM	GHB5FM	RCH5FM	GFD1FM	HFB1FM	RES1FM	STR1FM	IBS1FM	CHD1FM	FHB1FM				
Approximate (AP)																	SIP5AD	SORAD	DE45AD	PCG2AP
Output Control (OC)	BAS5OC													IBS1OC						
Budget (BD)		BCF5BD	WEL5BD	DRN5BD	RIV5BD	EVT5BD		GHB5BD	RCH5BD	GFD1BD		RES1BD	STR1BD			FHB1BD				
Output (OT)	BAS5OT																			

Figure 5.3 MODFLOW-96 primary modules organized by packages and procedures.

Table 5.1 List of main packages of MODFLOW-96 with their abbreviations and documentation.

Package Name	Abbreviation	Documentation
Basic	BAS	McDonald and Harbaugh, 1988
Block Centered Flow	BCF	McDonald and Harbaugh, 1988
Well	WEL	McDonald and Harbaugh, 1988
Recharge	RCH	McDonald and Harbaugh, 1988
River	RIV	McDonald and Harbaugh, 1988
Drain	DRN	McDonald and Harbaugh, 1988
Evapotranspiration	EVT	McDonald and Harbaugh, 1988
General Head Boundaries	GHB	McDonald and Harbaugh, 1988
Strongly Implicit Procedure	SIP	McDonald and Harbaugh, 1988
Slice-Successive Overrelaxation	SOR	McDonald and Harbaugh, 1988
Preconditional Conjugate Gradient	PCG	Hill, 1990
Stream	STR	Prudic, 1989
Interbed Storage	IBS	Leake and Prudic, 1991
Time Variant Specified Head	CHD	Leake and Prudic, 1991
General Finite Difference Flow	GFD	Harbaugh, 1992
Horizontal Flow Barriers	HFB	Hsieh and Freckleton, 1993
Transient Leakage	TLK	Leake, Leahy, and Navoy, 1994
Direct Solver	DE4	Harbaugh, 1995
Reservoir	RES	Fenske, Leake, and Prudic, 1996
Flow and Head Boundary	FHB	Leake and Lilly, 1997

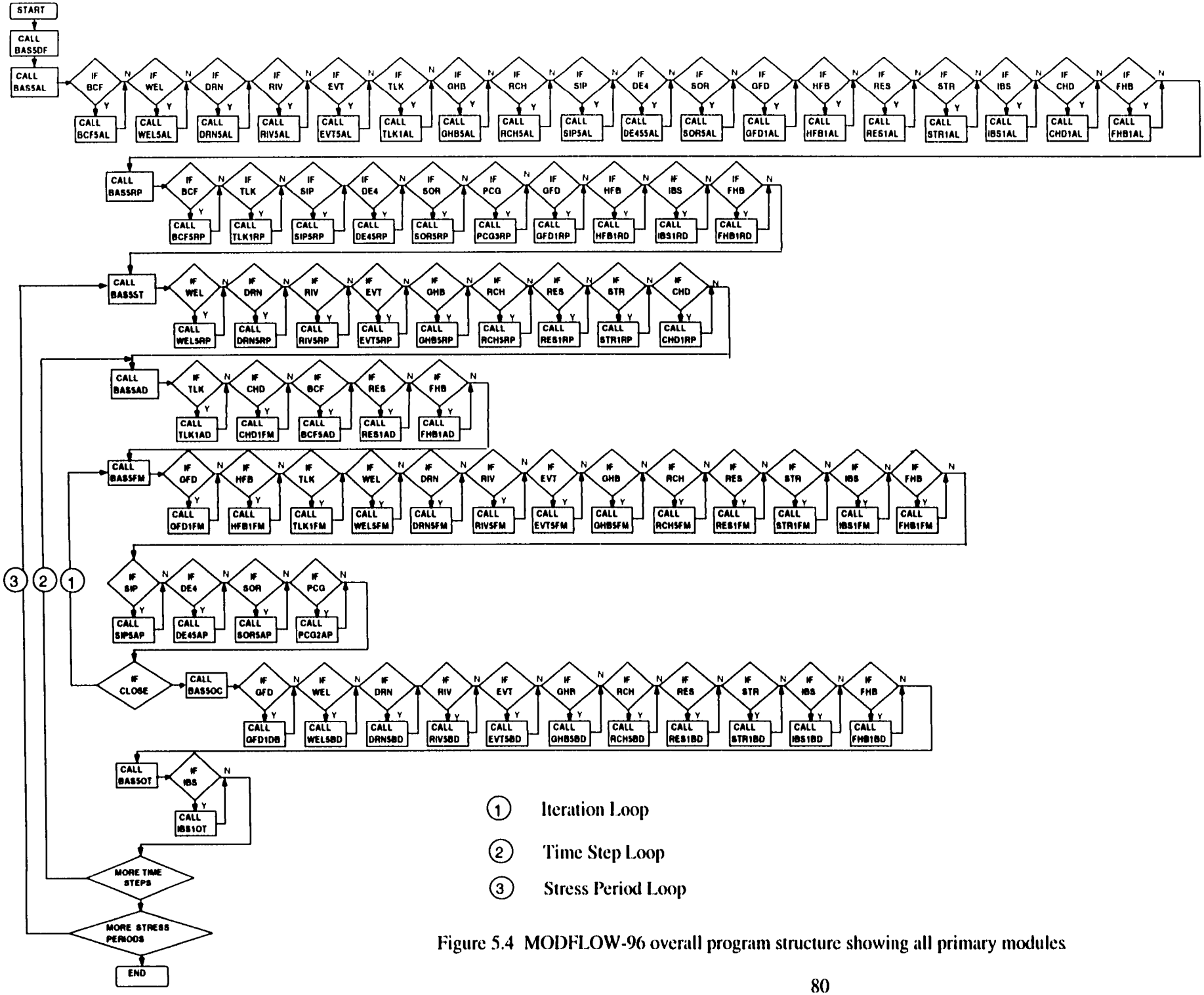


Figure 5.4 MODFLOW-96 overall program structure showing all primary modules

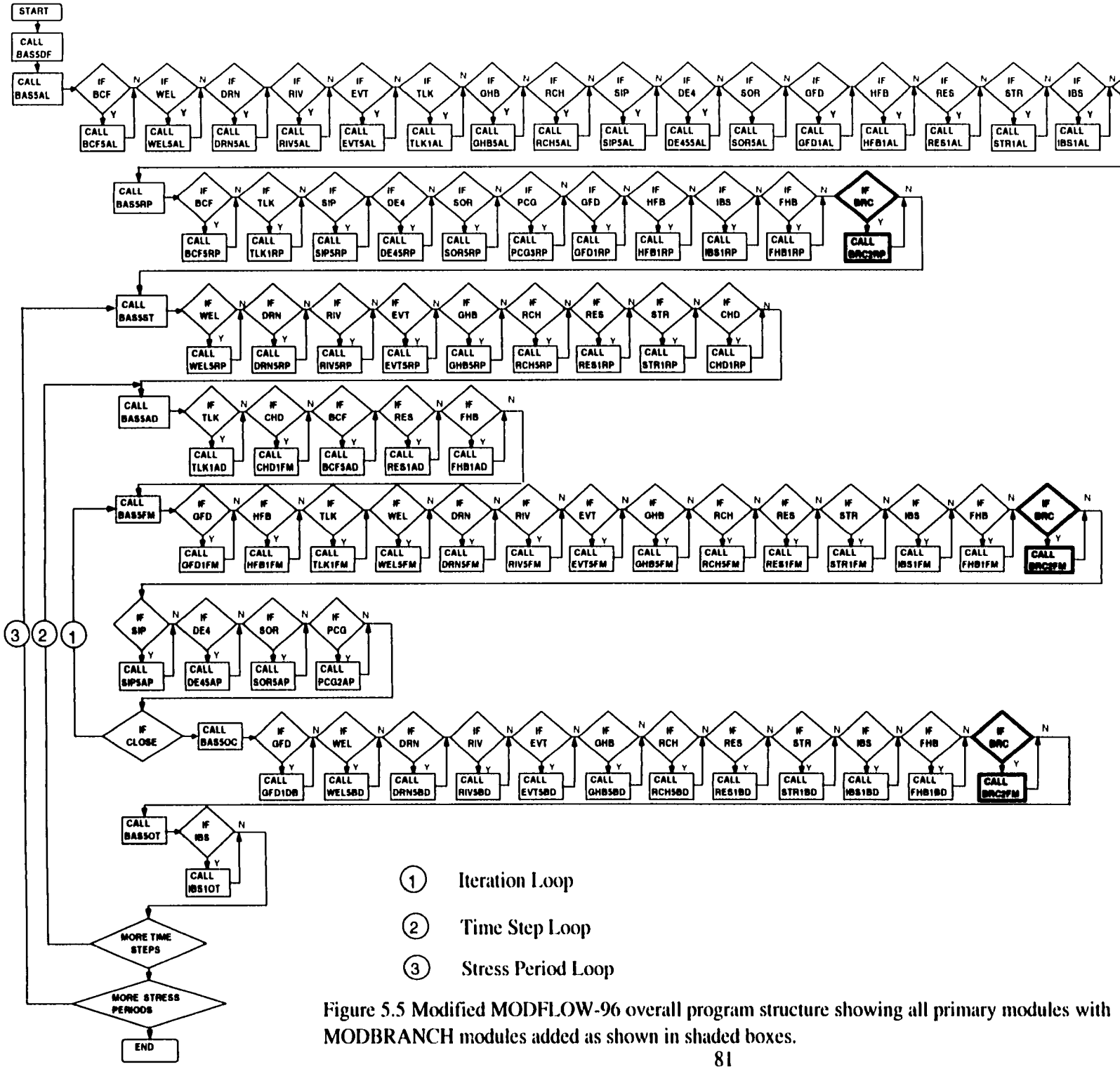


Figure 5.5 Modified MODFLOW-96 overall program structure showing all primary modules with MODBRANCH modules added as shown in shaded boxes.

2. BRC2RP: reads input data for MODBRANCH

3. BRC2FM: calls MODBRANCH and incorporates leakage to the RHS terms in each aquifer model cell containing a river reach.

4. BRC2BD: calls MODBRANCH to calculate rates and accumulates volumes over a MODFLOW time step. MODBRANCH module called by BRC2FM and BRC2BD simulates the unsteady flow in networks of reaches with leakage to the aquifer.

To link MODBRANCH to SSTM, the SSTMLINK Package is written to save the hydraulic solution parameters of the flow field required by SSTM. These parameters include leakage rates between stream and aquifer; discharge; cross sectional area; mean depth; and mean width.

5.4 MT3D Structure

MT3D version 1.11 (Zheng, 1990) will be described here. The MT3D transport model uses a modular structure similar to that implemented in MODFLOW. Like the MODFLOW model, the MT3D model consists of a main program and a number of independent subroutines, called modules, which are grouped into a series of packages. Each of these packages deals with a single aspect of transport simulation. The general procedures in the MT3D model for a typical simulation run are illustrated in Fig. 5.6. These general procedures are implemented for each of the four components in the transport equation. Each component is represented by a package. These packages are: Advection (ADV), Dispersion (DSP), Sink and Source Mixing (SSM), and Chemical Reaction (RCT). In addition to the four transport packages, the MT3D model program includes three additional packages: The Basic Transport Package (BTN), the Flow Model Interface Package (FMI), and the Utility Package (UTL). Figure 5.7 shows primary modules of MT3D organized by

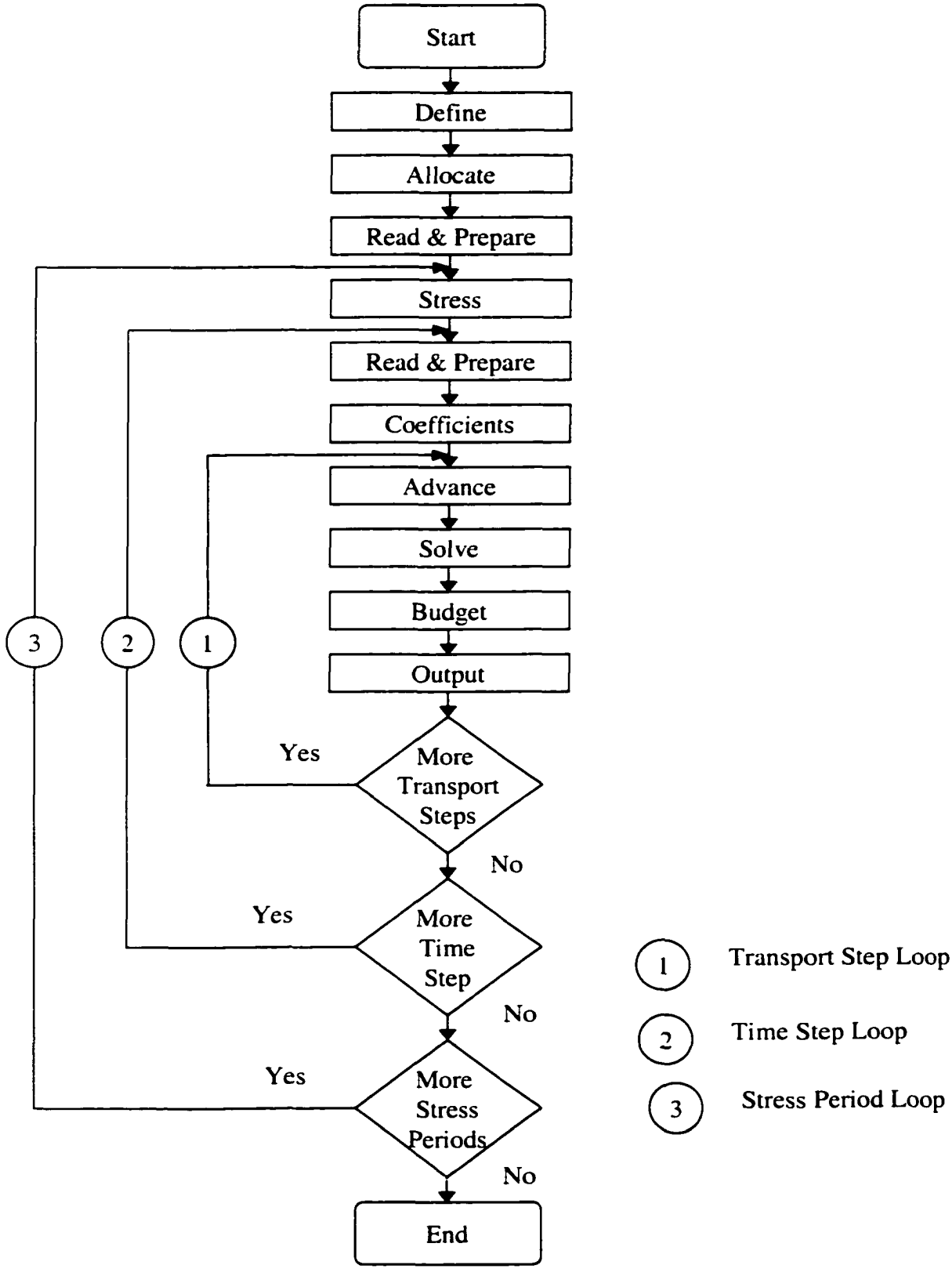


Figure 5.6 MT3D general procedures for a typical transport simulation (Zheng, 1990)

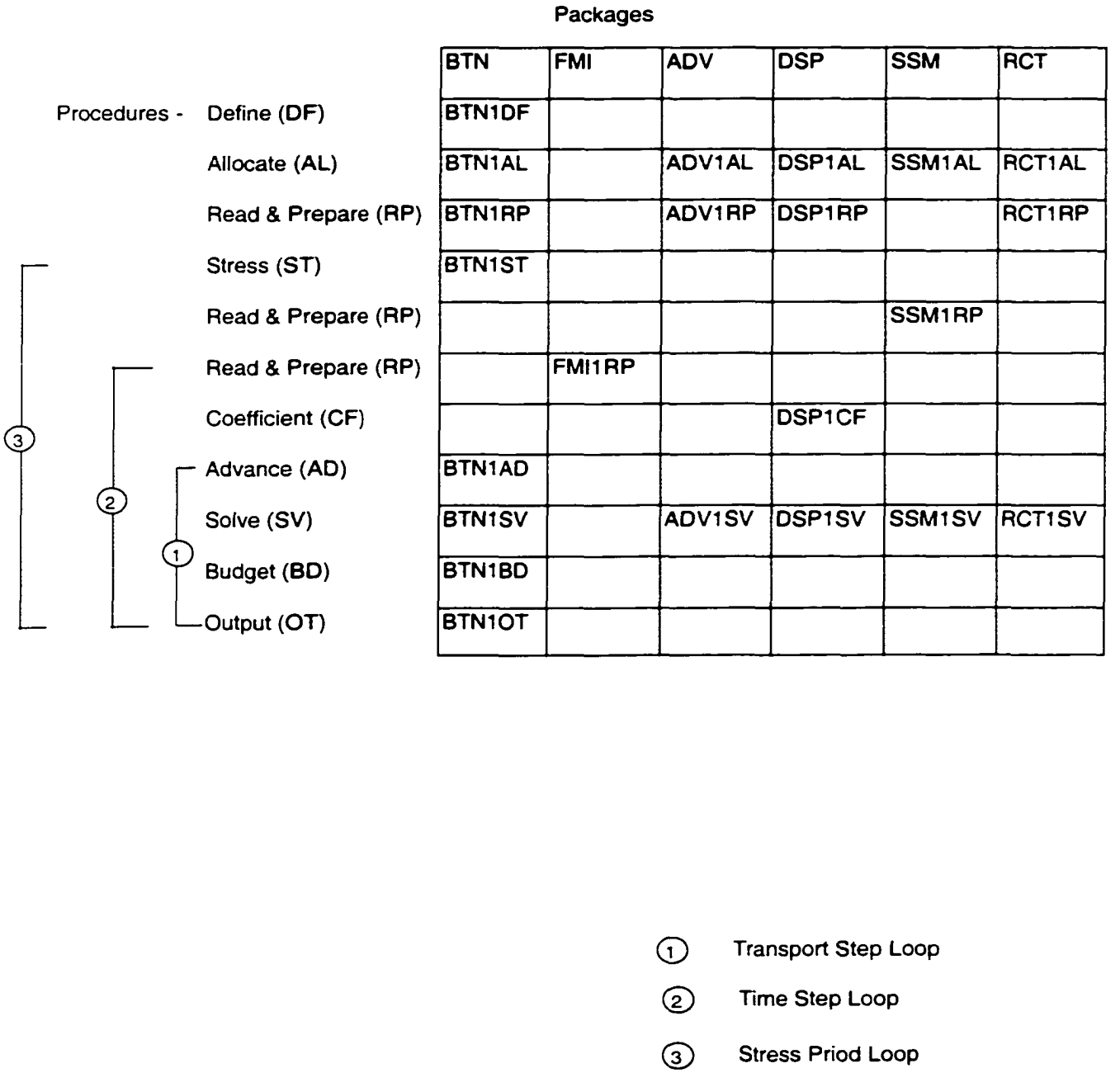


Figure 5.7 Primary modules of MT3D as organized by procedures and packages (Zheng, 1990).

procedures and packages. The main program controls the overall execution of the entire program. A flow chart showing all the primary modules called by the main program is shown in Fig. 5.8. For detailed description of the MT3D structure refer to the MT3D Manual (Zheng, 1990).

To link MT3D with MODFLOW, a package has been written by Zheng (1990) for use with MODFLOW-88 code to save heads and flow terms needed by MT3D. The package is named LKM Package . In MT3D, the Flow Model Interface Package (FMI) consist of secondary modules that read hydraulic heads and fluxes across cell interfaces and read and prepare the locations and flow rates of the various sink/source terms.

5.5 Modification of Main Models

In this study, several modifications are conducted to MODFLOW, MODBRANCH, and MT3D models. These modifications include adding the SSTMLINK Package to the MODFLOW-BRC2-MODBRANCH combination and adding the Stream Solute Transport Package (SSL1) to the MT3D model. These modifications are explained in detail in the following three sections.

5.5.1 Modification of MODFLOW-96 Structure

In this study, a modification is done to the MODFLOW model that is linked to MODBRANCH by the BRC2 Package. The flow chart of this model is explained in detail in Fig. 5.5. Figure 5.9 shows a more clear image of Fig. 5.5 by hiding other subroutines and emphasizing the BRC2 Package subroutines that are called by MODFLOW main program. The processes executed through the BRC2 Package are explained previously in Section 5.3. Before adding subroutines to MODFLOW-BRC2-MODBRANCH combination, the LKM Package that links MODFLOW to MT3D is incorporated in the main program of MODFLOW-96. The LKM Package

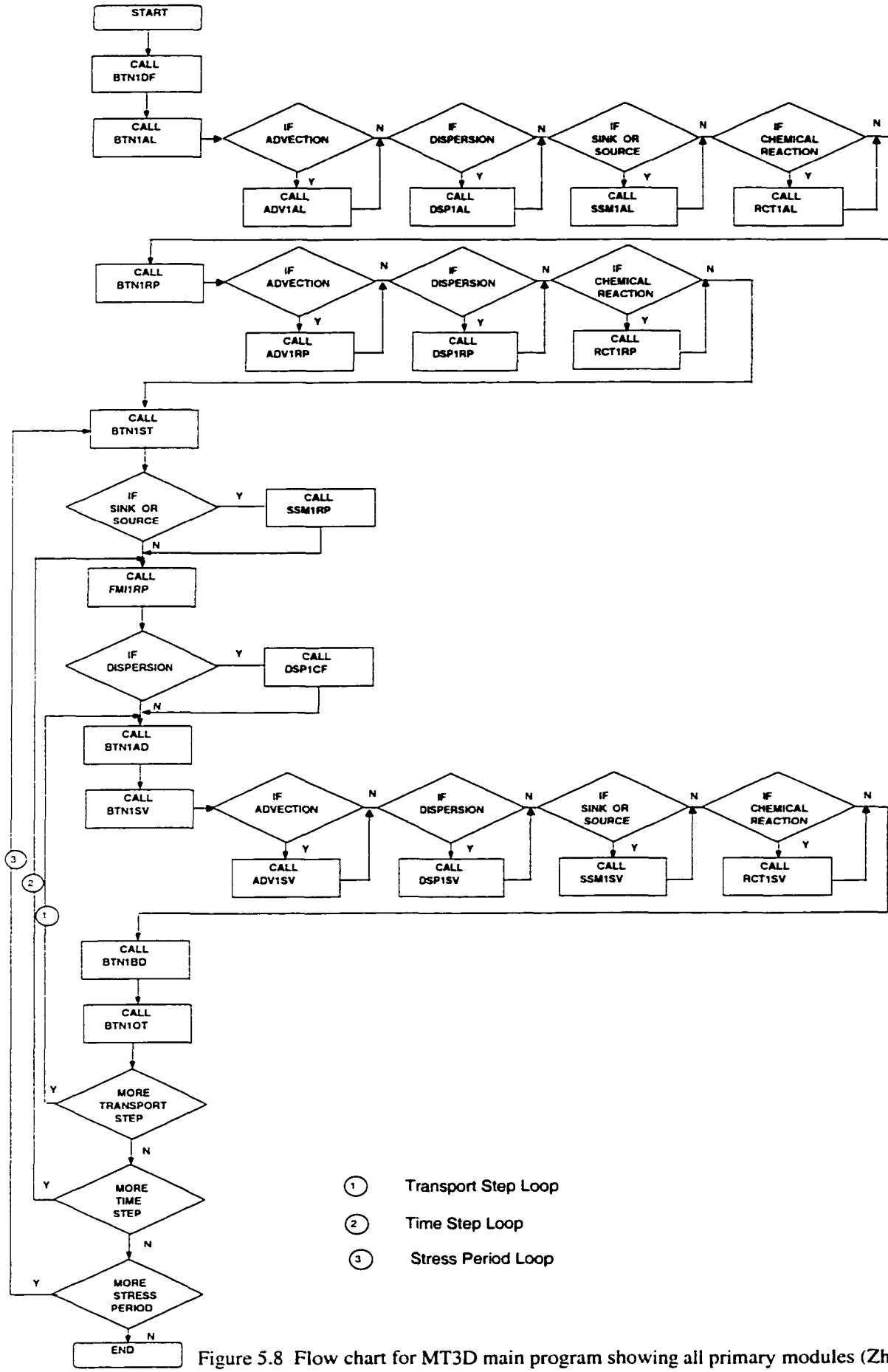


Figure 5.8 Flow chart for MT3D main program showing all primary modules (Zheng , 1990).

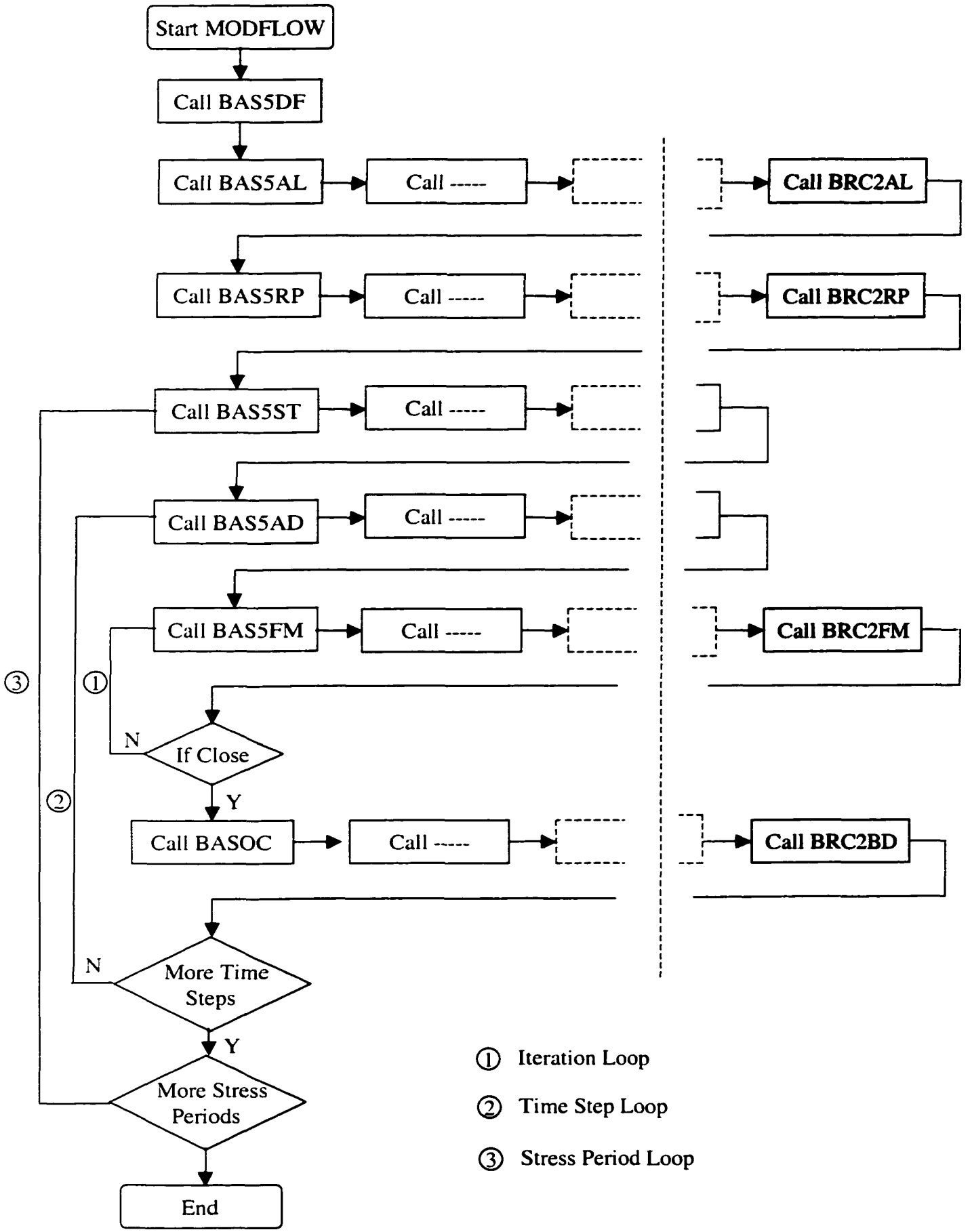


Figure 5.9 Shaded rectangles are BRC2 Package subroutines in MODFLOW96 main program that link to MODBRANCH

was developed by Zheng (1990) and added to MODFLOW-88 model. This package is added to MODFLOW-BRC2-MODBRANCH combination as shown in Fig. 5.10. The LKM subroutines save the following variables to a file that will be used by MT3D:

1. Heads, flow across cell interfaces in 3 dimensions, x, y, and z,
2. Well locations and rates, drain locations and rates, river cell locations and rates if the RIVER Package is used, recharge layer indices and rates, evapotranspiration layer indices and rates, and general head dependant boundaries and rates, and streams locations and leakage rates.

The SSTMLINK Package is developed in this study to link MODFLOW and MODBRANCH to SSTM. The SSTMLINK Package is composed of subroutines that are called by MODFLOW, BRC2 and MODBRANCH modules to save variables needed by SSTM. The subroutines that are called by MODFLOW-96 main program are described here. These subroutines are SSTMINIT and MODFLWTIME, their location in the MODFLOW-96 main program flow chart is shown in Fig. 5.11. As shown, SSTMINIT is called for each time step of the MODFLOW-96 simulation. It writes to a file the number of stress periods in the MODFLOW-96 simulation and the ratio of MODFLOW-96 time step to MODBRANCH time step for each MODFLOW-96 time step count. MODFLWTIME writes the time length of each stress period and the number of its corresponding time steps to a file. The rest of subroutines in the SSTMLINK Package will be illustrated in the next section.

5.5.2 Modification of BRC2 Package Structure

The MODBRANCH model is composed of three main subroutines and other secondary subroutines. The main subroutines are BRINIT, SOLVER, and BREND. The BRINIT Subroutine

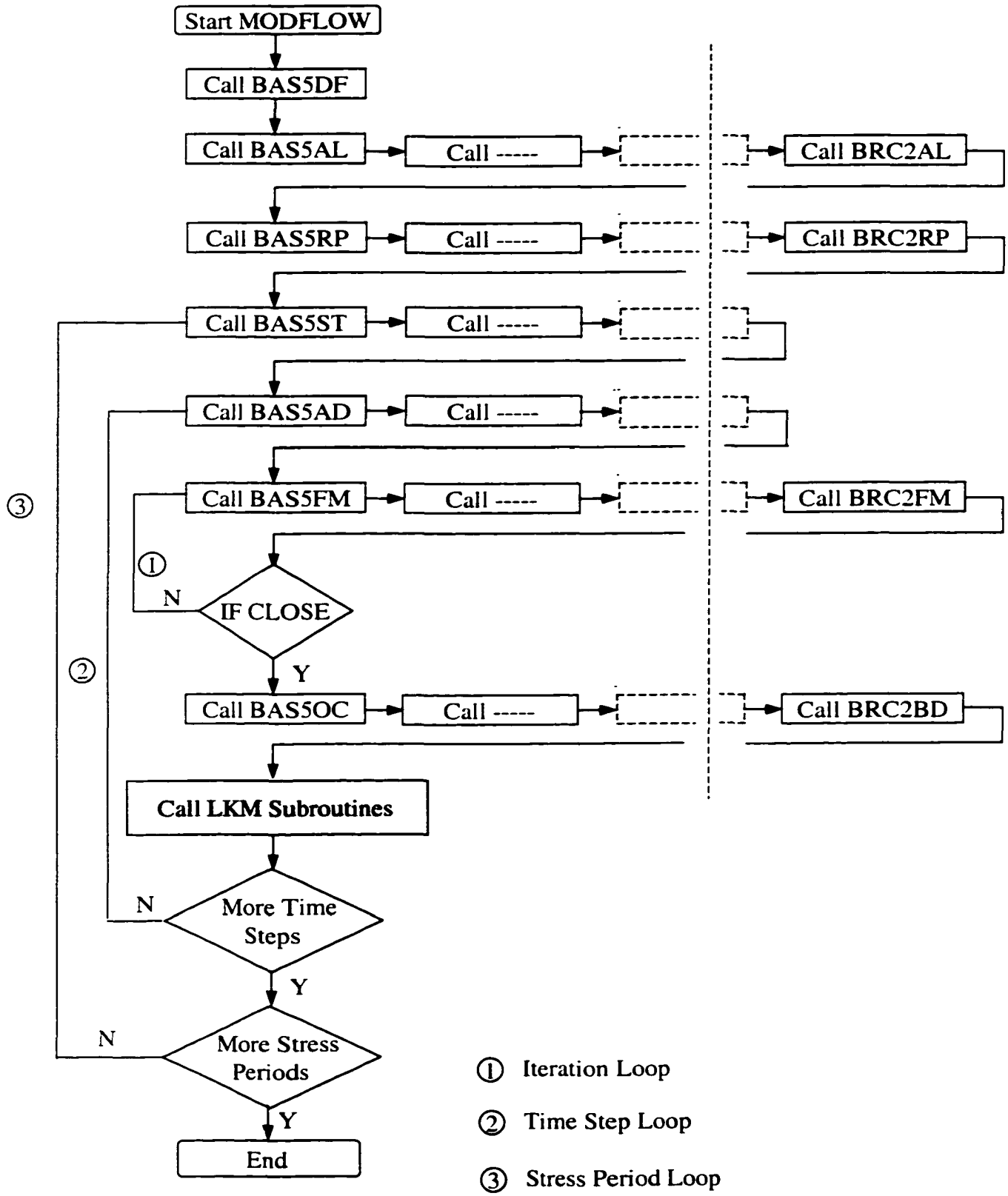


Figure 5.10 Shaded rectangle is where LKM subroutines are called in MODFLOW96 main program that contains the BRC2 Package.

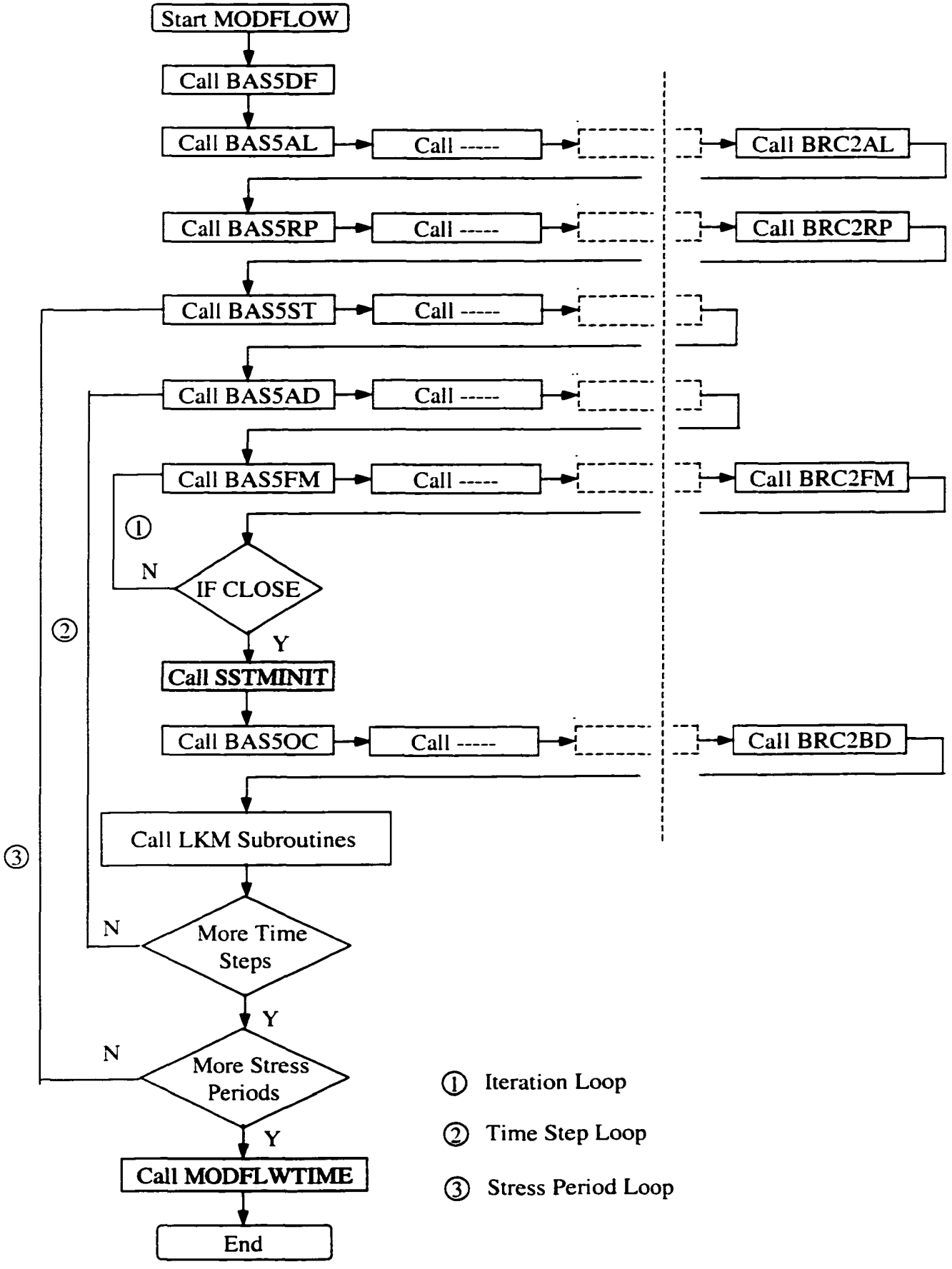


Figure 5.11 Shaded rectangles are subroutines of SSTMLINK Package that added to MODFLOW to link to SSTM.

initializes MODBRANCH computational variables and arrays and reads required data. The SOLVER Subroutine solves the system of equations of a channel network. The BREND Subroutine terminates MODBRANCH execution and calls the final output subroutines. These three major subroutines are called by the BRC2 Package as shown in Fig. 5.12. Subroutine BRC2RP calls BRINIT Subroutine to read and prepare variables needed by BRC2 Package. BRC2FM calls SOLVER Subroutine a number of times equal to the ratio of MODFLOW time steps to MODBRANCH time steps then add leakage from or to the aquifer to MODFLOW system of equations. At the end of simulation BREND is called by BRC2BD to estimate volumetric budget of the streams. The rest of subroutines in the SSTMLINK Package are called from BRC2 subroutines. The BRC2RP Subroutine calls BRNCHCGI Subroutine as shown in Fig. 5.13. This subroutine writes MODBRANCH geometry parameters to MODBRANCH-SSTM Interface File. These parameters include number of branches in the stream network, number of junctions, number of open boundaries, stream segments length, layer, column and row of aquifer model cells that correspond to stream segments. Subroutine SOLVER calls BRANCHFLO to write flow computation results to MODBRANCH-SSTM Interface File for each MODBRANCH time step. These results include channel flow discharge, area, mean width, mean depth, flow velocity, and leakage to or from the aquifer.

5.5.3 Modification of MT3D Model Structure

To link MT3D to the SSTM, a package is added in this study to MT3D version 1.11. The MT3D code is modified to account for variability of stream concentration during the groundwater transport step. The before modification version considers the stream as a point source and sink and deals with that using the Sink/Source Mixing (SSM1) Package. The SSM1 package reads

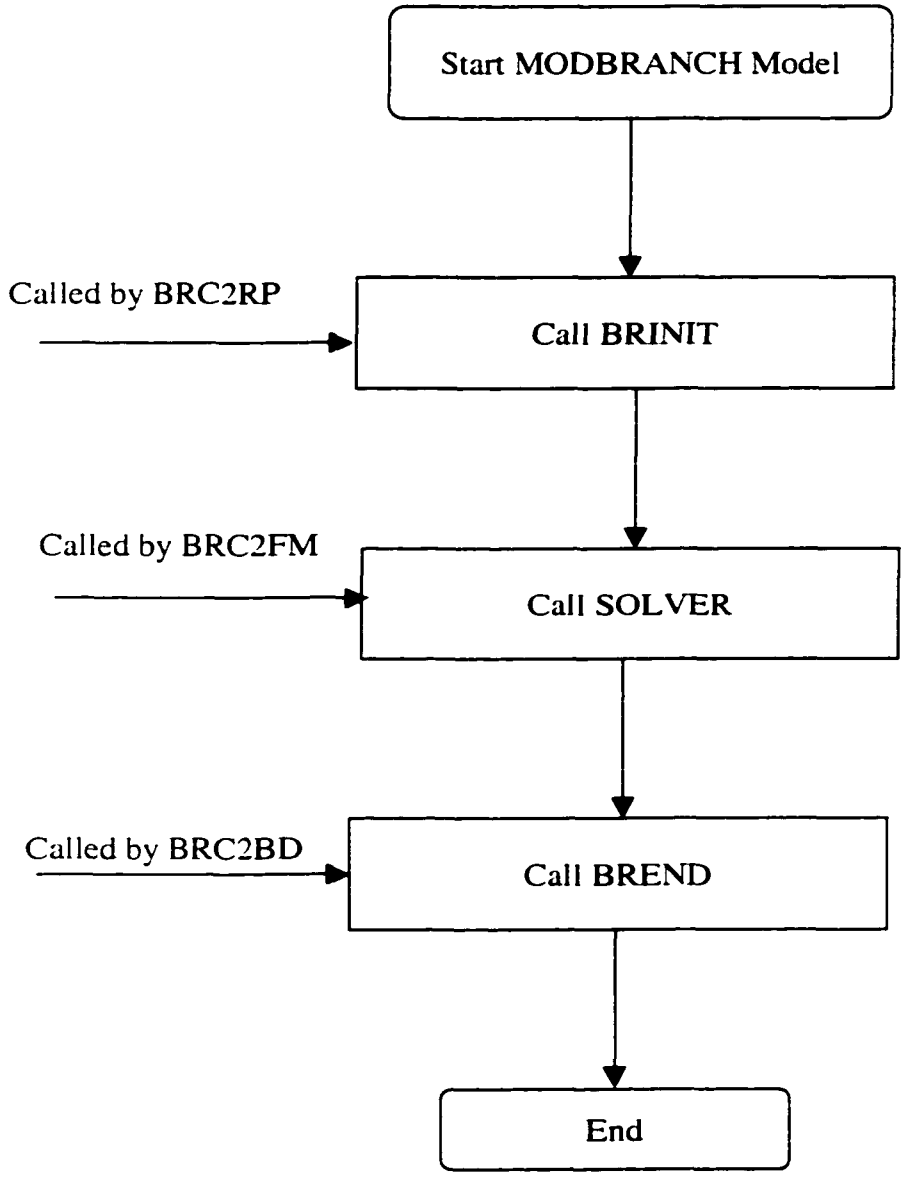


Figure 5.12 Flowchart of MODBRANCH showing main subroutines and where they called by BRC2 Package.

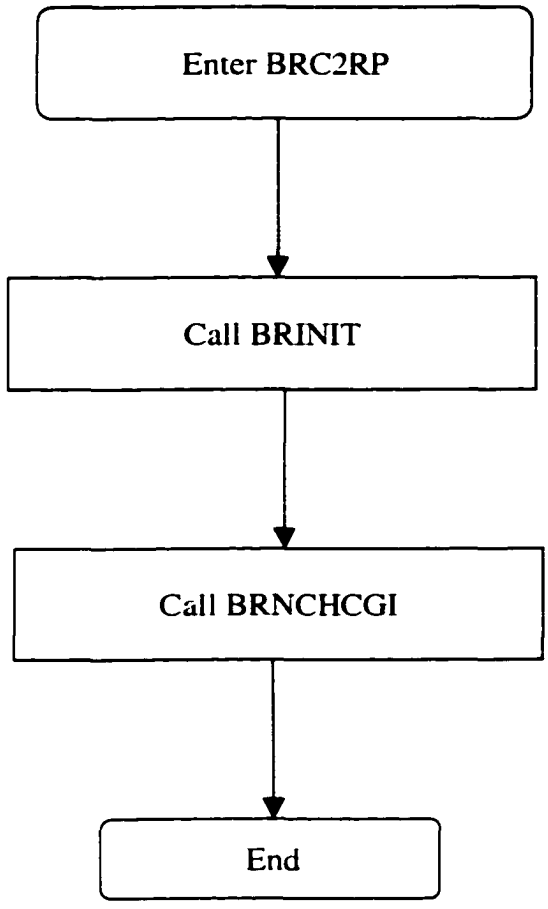


Figure 5.13 Flowchart of BRC2RP after adding BRNCHCGI subroutine

a constant concentration in the stream cells during the stress period. The value of flow leakage for the cells is read from the MODFLOW-MT3D interface file using the Flow Model Interface (FMI1) Package. The MT3D code is modified to account for variability of stream concentration during the groundwater transport step. For this, stream concentration that used to be read as a constant value from an input file will be obtained by calling the SSTM. For this reason, a package is added in this study to MT3D model to link it with the SSTM. This package is referred to as Stream Solute Package and abbreviated as SSL1 Package. The SSL1 Package has a similar structure to other MT3D packages and composed of three modules (subroutines). It is added to MT3D structure as shown in Fig. 5.14. The SSL1AL Subroutine allocates space for data arrays needed by the Stream Solute Package. The SSL1RP Subroutine reads and prepares input data needed for solving the stream solute term. Subroutine SSL1RP calls the SSTM and gets stream network variables like leakage to or from the aquifer, stream hydraulic variables, like discharge, width, depth, mean velocity, stream segments initial concentrations, stream segments bed slope, model cells that corresponds to stream segments. The SSL1SV Subroutine is called in each transport step during MT3D execution. The SSL1SV calls subroutines BSC1AD of the SSTM to advance one time step. The transport step in MT3D is set equal to the time step in SSTM. The SSL1SV calls ADS1SV and DDS1SV of the SSTM and passes the value of aquifer cell concentration to the ADS1SV and DDS1SV. The stream solute transport equation is solved and the value of solute in the stream is passed to MT3D. The stream concentration is included in MT3D transport equation and solved for in the SSL1SV subroutine.

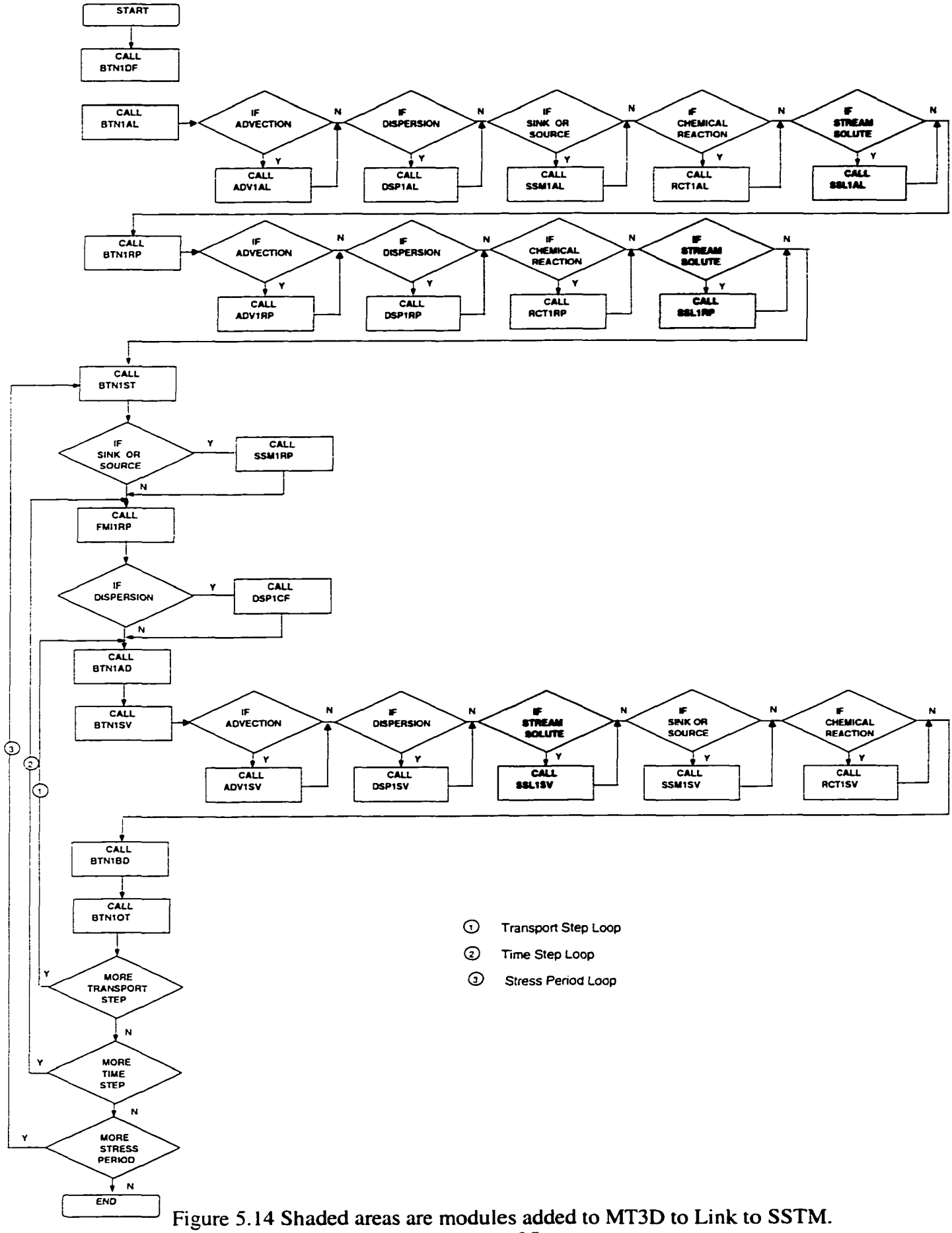


Figure 5.14 Shaded areas are modules added to MT3D to Link to SSTM.

5.4 Development of the Stream Solute Transport Model, SSTM

The SSTM is developed as a primary model of the main model, MSAST. It is coded based on the governing equations explained in Chapter 4 Section 4.3. The model is designed with similar modular structure as the previous models (MT3D, MODFLOW and MODBRANCH). This will facilitate its links to MODBRANCH and MT3D, and allow adding new modules for more stream processes to the main model in the future. The SSTM consists of a main program and a number of independent modules that are grouped into a series of packages. The general procedures performed for a typical simulation run are illustrated in Fig. 5.15. The time step utilized is the same as the MODBRANCH time step and the MT3D transport step. Prior to entering the time step loop, the program executes three procedures. In the Define Procedure, the simulation problem is defined; that is, the size of the model, and the various transport options to be used in the simulation are specified. In the Allocate Procedure, computer memory is allocated for the data arrays whose dimensions depend on the parameters specified in the Define Procedure. In the first Read and Prepare Procedure, stream variables contained in the interface file produced by MODBRANCH are read. In the second Read and Prepare Procedure, input data that are constant throughout the simulation are read and processed. These input data include spatial and temporal discretization information, boundary conditions, initial conditions, and output control options.

The first procedure within the time step loop is the Advance procedure. The Advance procedure advances the simulation one time step. The Solve Procedure solves each transport component using an implicit finite difference technique. The Output Procedure prints or saves simulation results as needed according to the user-specified output control option. Classification of modules by procedure and packages is shown in Fig. 5.16. Figure 5.17 shows the SSTM main program and its modules and links to the SSL1 Package.

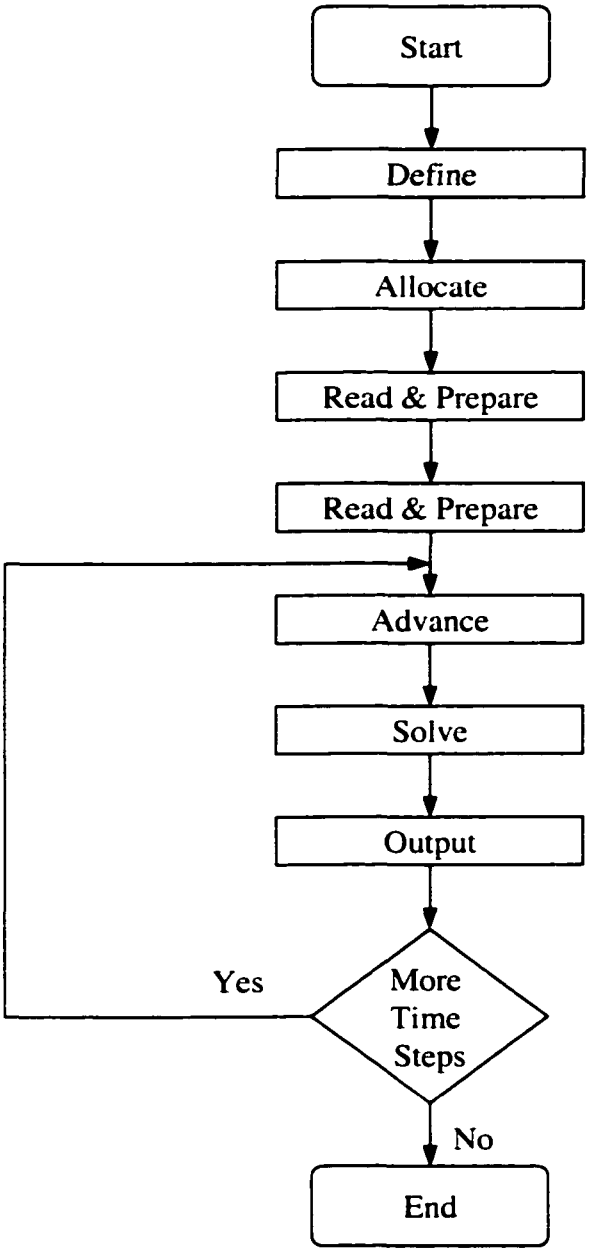


Figure 5.15 SSTM general procedures for a stream solute transport simulation.

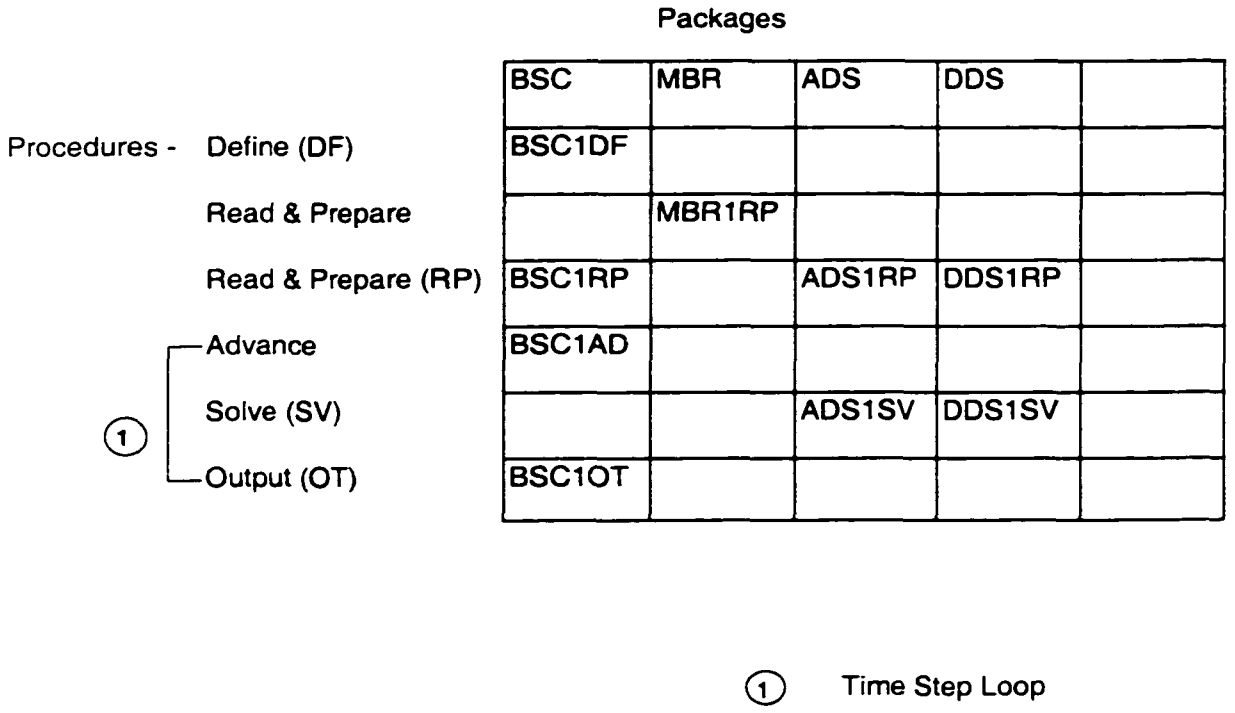


Figure 5.16 Primary modules of SSTM as organized by procedures and packages.

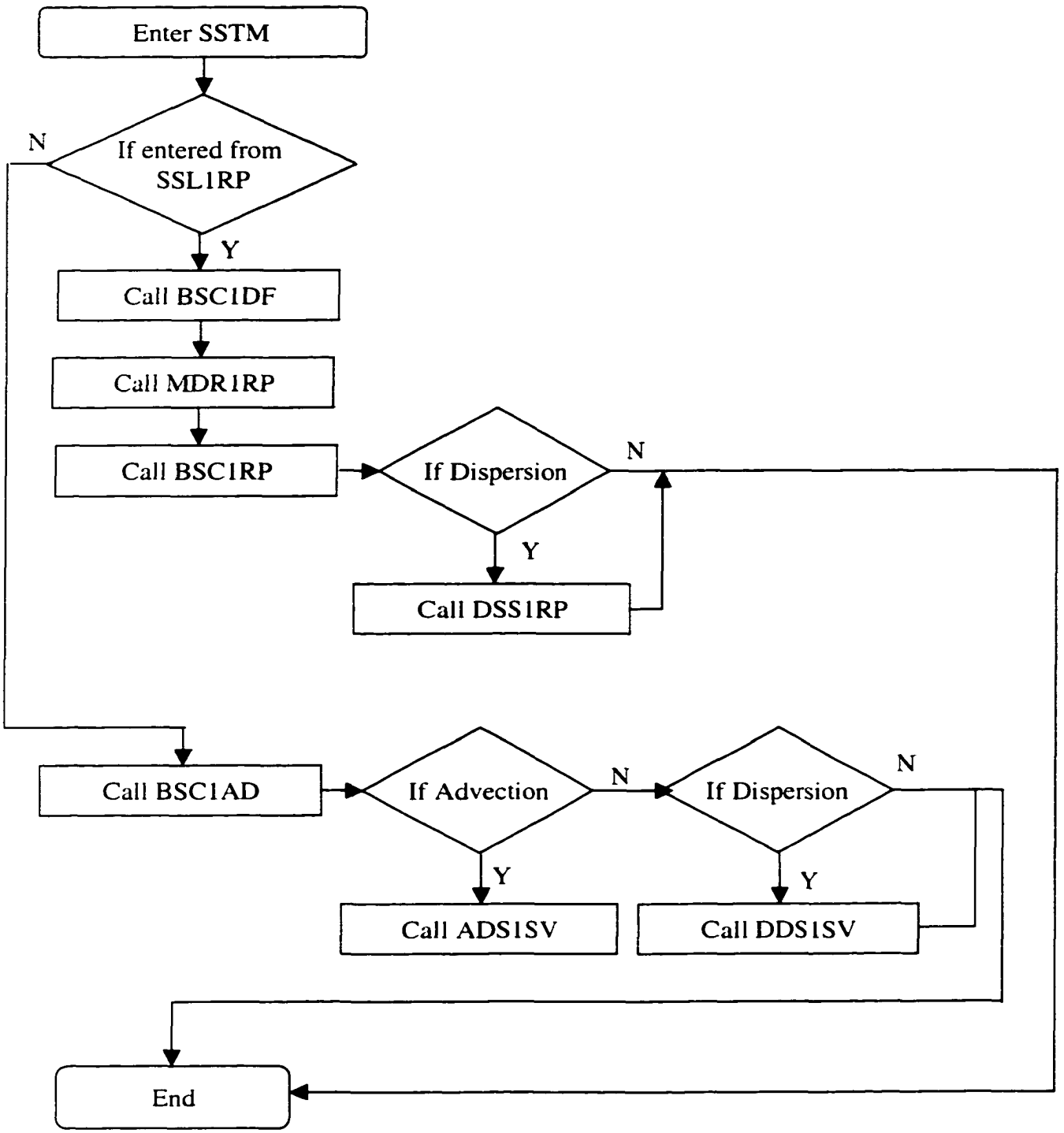


Figure 5.17 Flow chart of SSTM main program showing primary modules and link to SSL1 Package

5.5 Time Discretization

The Model for Stream Aquifer Solute Transport, MSAST simulation time is based on MODFLOW stress period. MODFLOW stress period is the time interval during which all external parameters are constant. Stress period is, in turn, divided into time steps. MODFLOW time step is referred to as (mf) here. Because of the disparity in time scales between groundwater and surface water, there are multiple MODBRANCH time steps in one MODFLOW time step. MODBRANCH time step is referred to as (nf). The same time step is maintained in the SSTM and referred to as (ns). MT3D stress period and time step are set equal to MODFLOW time step and stress period. MT3D transport step is set equal to SSTM time step.

The developed model is used to simulate chloride transport in the stream-aquifer system of the Arkansas River and the Equus Beds aquifer in south-central Kansas. This application is explained in Chapter Six.

Chapter Six

MODEL APPLICATION

6.1 Background

In 1989, the Bureau of Reclamation started modeling the Equus Beds aquifer to investigate management issues regarding water quality degradation of the aquifer. The Equus Beds aquifer provides most of the fresh and usable water in south-central Kansas. Groundwater withdrawals from the Equus Beds aquifer between Hutchinson and Wichita in Kansas have been increasing since the 1940's. The city of Wichita's principal water supply, Wichita Well Field, is located in the Equus Beds aquifer east of Burrton. The study area is located in south-central Kansas as shown in Fig. 6.1. The quality of groundwater in the area is generally good, although salinity indicated by the presence of chloride, has entered the aquifer from several sources.

The modeling examined groundwater and the transport of chloride in the aquifer. The primary objective is to determine how aquifer use affects the distribution of chloride from the main sources of chloride within the aquifer. The Arkansas River and the Little Arkansas River are the major streams in the study area (Fig. 6.1). The USGS set up a flow model for the Arkansas River-Equus Beds aquifer system using MODFLOW. Simulation of groundwater flow for calibration purposes cover the period 1940-1989. The Bureau of Reclamation used the USGS flow model after regriding the finite difference mesh to better define the flow field and applied MT3D for simulation of chloride transport in the aquifer. Simulations were made to characterize the transport of chloride from specific sources during the calibration period (1940-1989) and the projection period (1990-2049). These chloride sources are: the Arkansas River, deep natural saltwater, and saltwater from the Burrton Oil

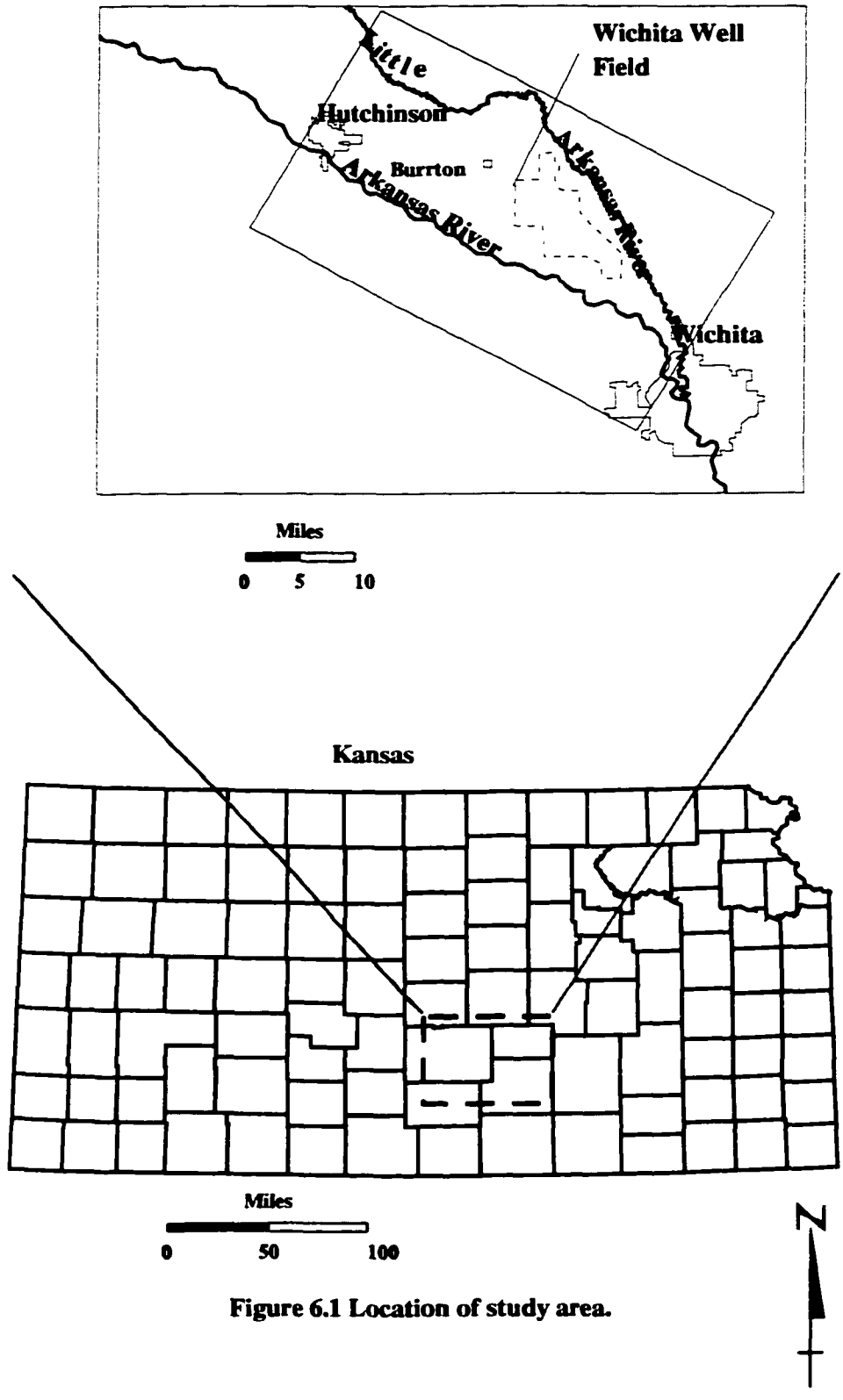


Figure 6.1 Location of study area.

Field. Simulations were also performed to investigate potential management strategies and issues.

6.2 Objective of Model Application

The Bureau of Reclamation MODFLOW-MT3D model (data set) of Equus Beds aquifer are used in the application of the Model for Stream-Aquifer Solute Transport, MSAST. The MSAST is composed of four models: MODFLOW, MT3D, MODBRANCH, and SSTM. The case study is adopted because the data available are the most appropriate to construct the input files for the MSAST modules. Data for two primary models in the MSAST which are MODFLOW and MT3D are available from the USGS and Bureau of Reclamation studies. Other data to drive MODBRANCH and SSTM are collected , when data is not available parameters are assumed. The main objective of the application of MSAST is to check the performance of the model for a period of time within the calibrated MODFLOW-MT3D time period. The MSAST is applied for 3 years from the beginning of the year 1987 till the end of the year 1989. The selection of this period of time is based on the availability of surface water data to drive MODBRANCH. This application is not intended to add to the objectives of the previous studies conducted by USGS and the Bureau of reclamation. It is to test the performance of the MSAST in simulating the transport of chloride between the Equus Beds aquifer and the Arkansas River during a specific simulation time.

6.3 MSAST Application

The MSAST is applied at two stages. First, MODFLOW-MODBRANCH is applied to simulate groundwater flow in the aquifer and surface water flow in the stream and the interaction

between them. The second stage is to utilize the first application and apply MT3D-SSTM to simulate chloride transport in the aquifer and the stream and their interaction.

6.3.1 MODFLOW-MODBRANCH Application

The data set obtained from Bureau of Reclamation for groundwater flow and transport model application represent a calibrated MODFLOW-MT3D application for a period of 40 years (1940-1989). The aquifer is represented by a finite difference mesh grid of 54 rows and 84 columns and 3 layers as shown in Fig. 6.2 . The upper, middle and lower model layers correspond to the upper, middle, and lower units of the Equus Beds aquifer. Boundary conditions for upper, middle, and lower layers are shown in Fig. 6.3, Fig. 6.4, and Fig. 6.5 respectively. The initial heads for the three layers of the model at the beginning of year 1987 are shown in Figs. 6.3, 6.4, 6.5 respectively.

Aquifer properties are horizontal hydraulic conductivity, vertical hydraulic conductivity, specific yield and storage coefficient. The distribution of horizontal hydraulic conductivity in the model layers is shown in Fig. 6.9, Fig. 6.10 and Fig. 6.11. A specific yield of 0.15 was assigned uniformly to the upper model layer. For the middle and lower layers, a specific storage of 0 .0001 ft^{-1} was assumed and multiplied by the layer thickness to get values of storage coefficient for each model cell.

Stresses simulated in the Bureau of Reclamation groundwater flow model include recharge, evapotranspiration, streamflow, stream leakage, and pumpage by wells (Myers et al., 1996). Recharge values for the flow model were adjusted based on average precipitation for each stress period. Evaptranspiration rate was determined through calibration with a maximum rate of 35 inches per year with the water table at land surface and a linear decrease to 0 where the watertable is 10 feet

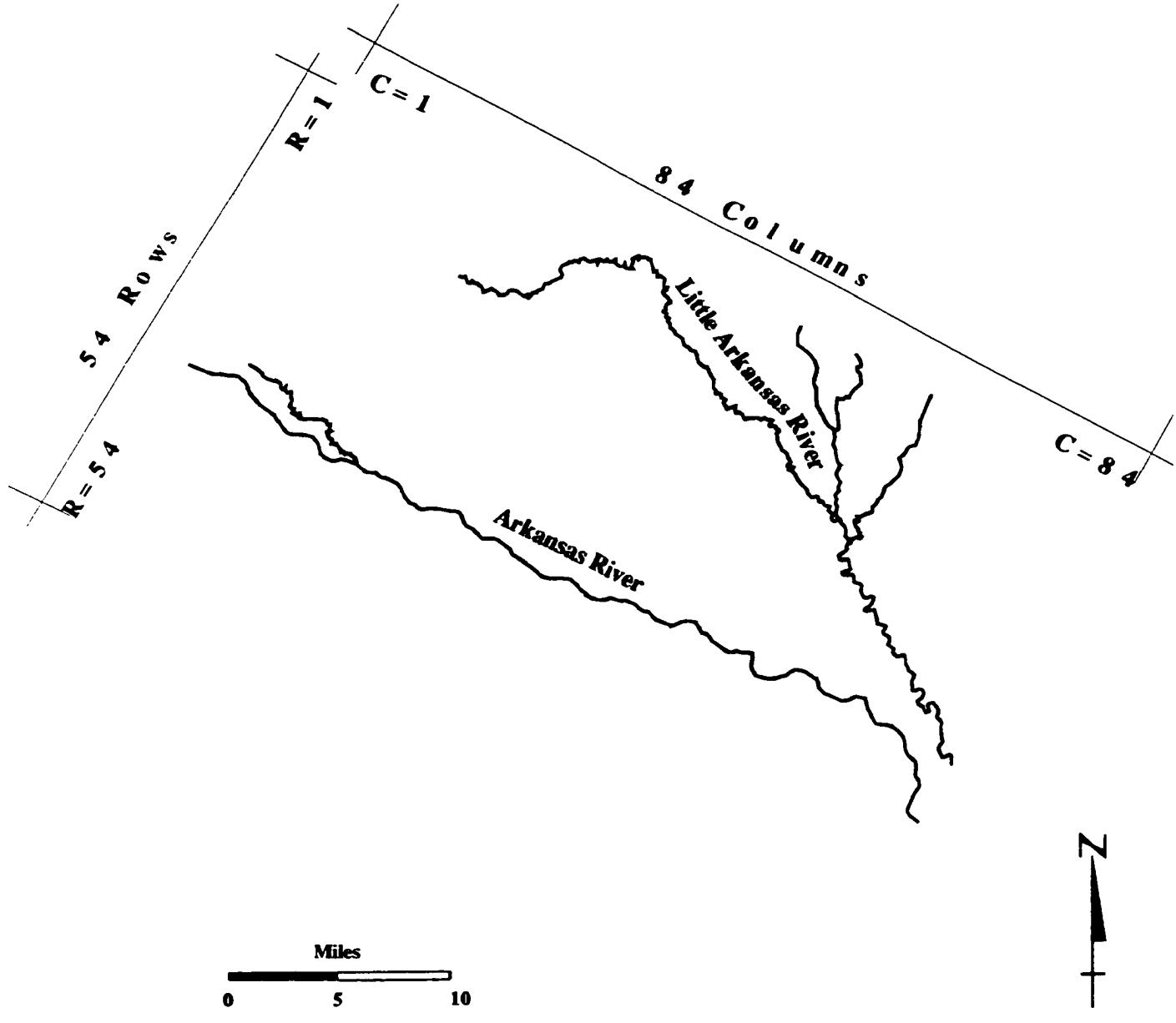


Figure 6.2 Model grid (54 rows X 84 columns X 3 layers).

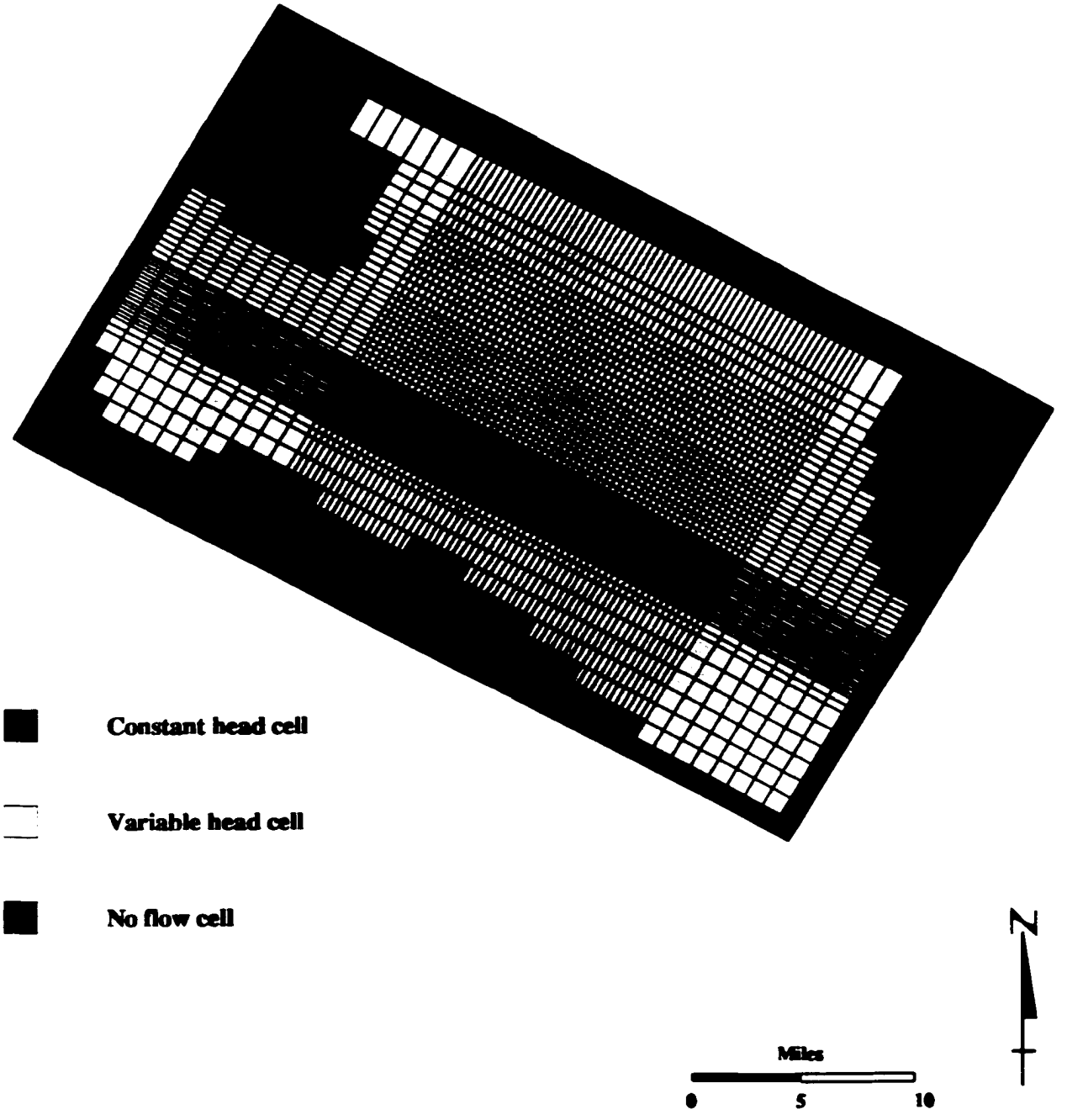


Figure 6.3 Boundary conditions for upper layer of groundwater flow model.

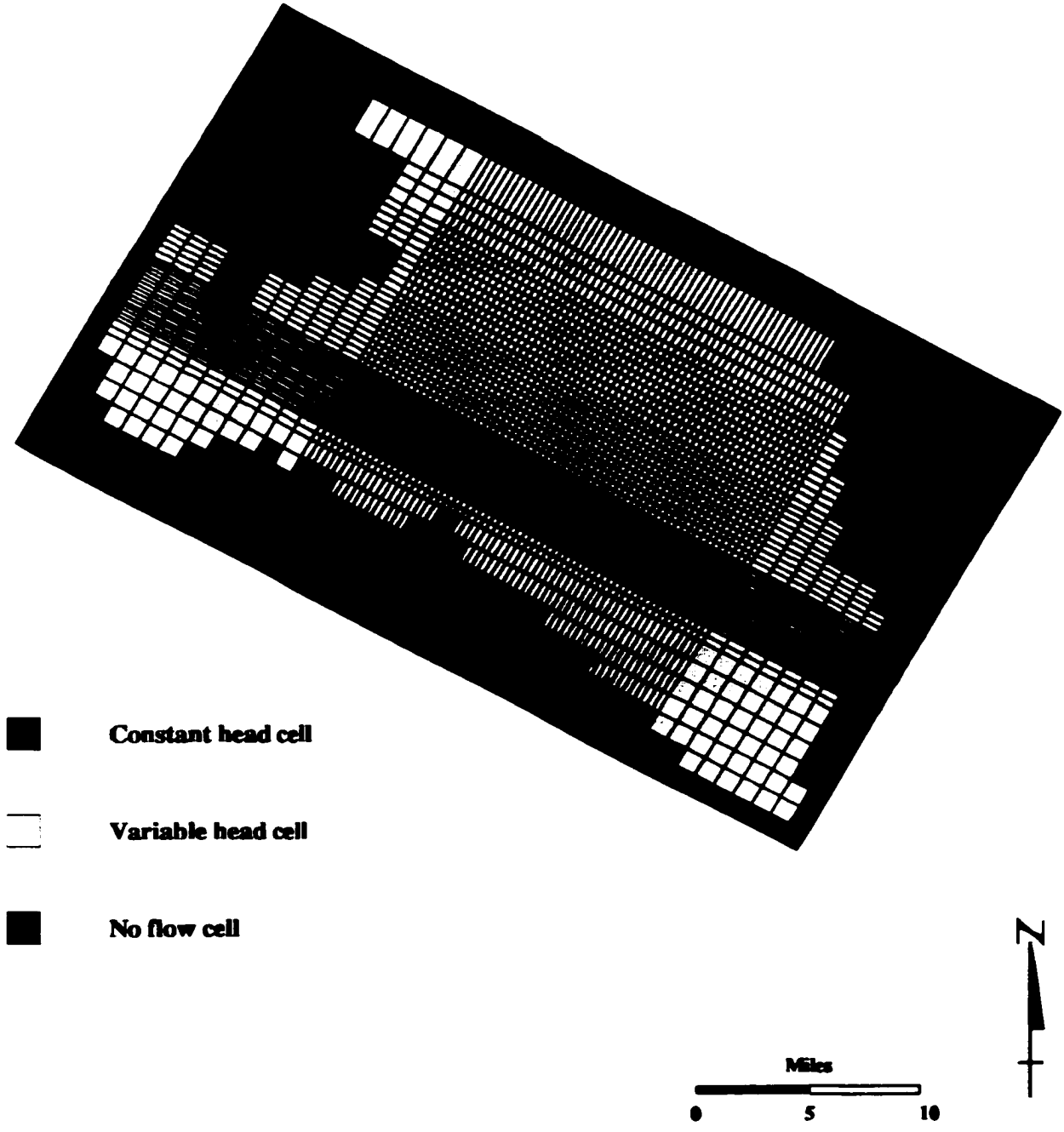


Figure 6.4 Boundary conditions for middle layer of groundwater flow model.

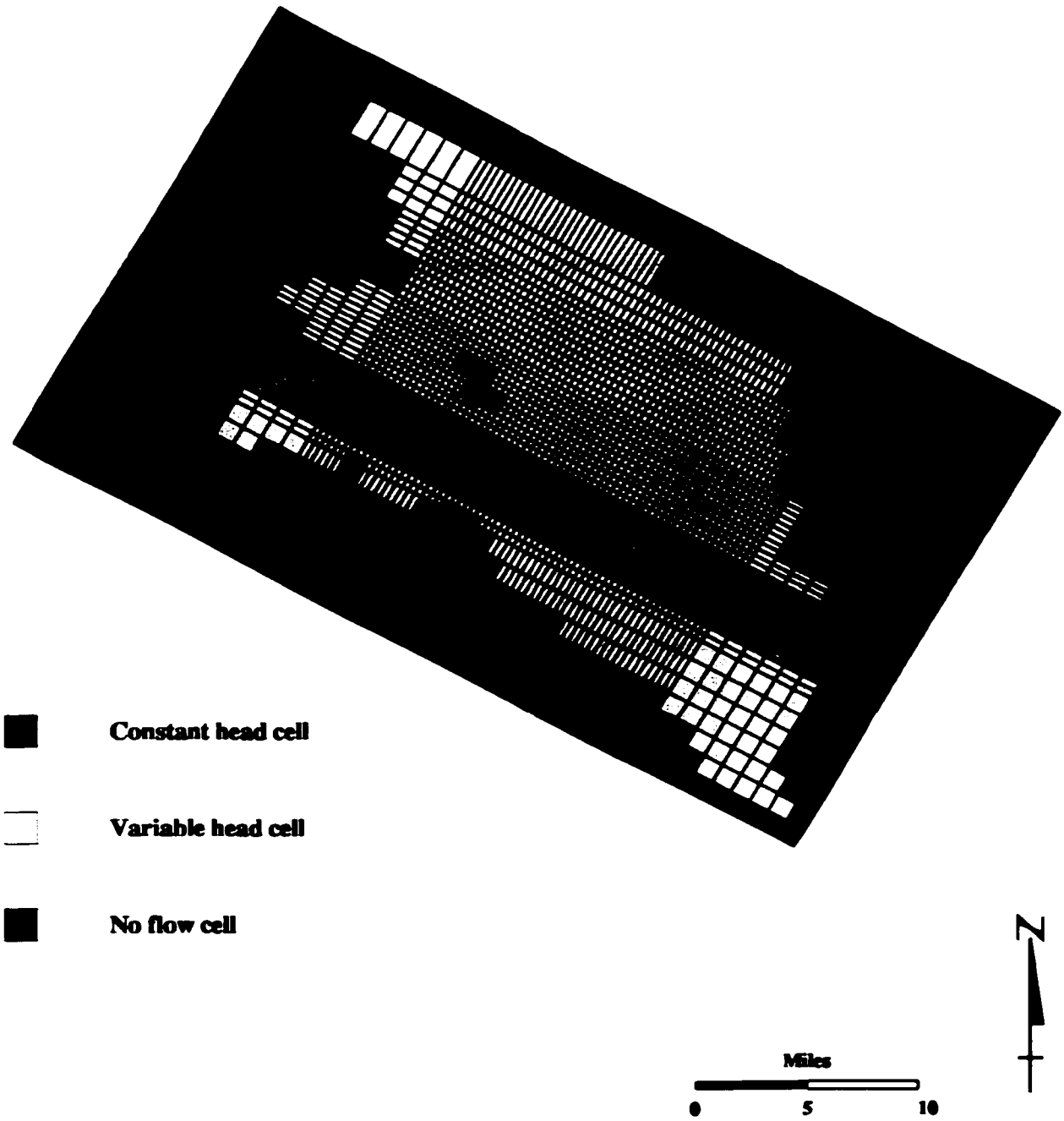


Figure 6.5 Boundary conditions for lower layer of groundwater flow model.

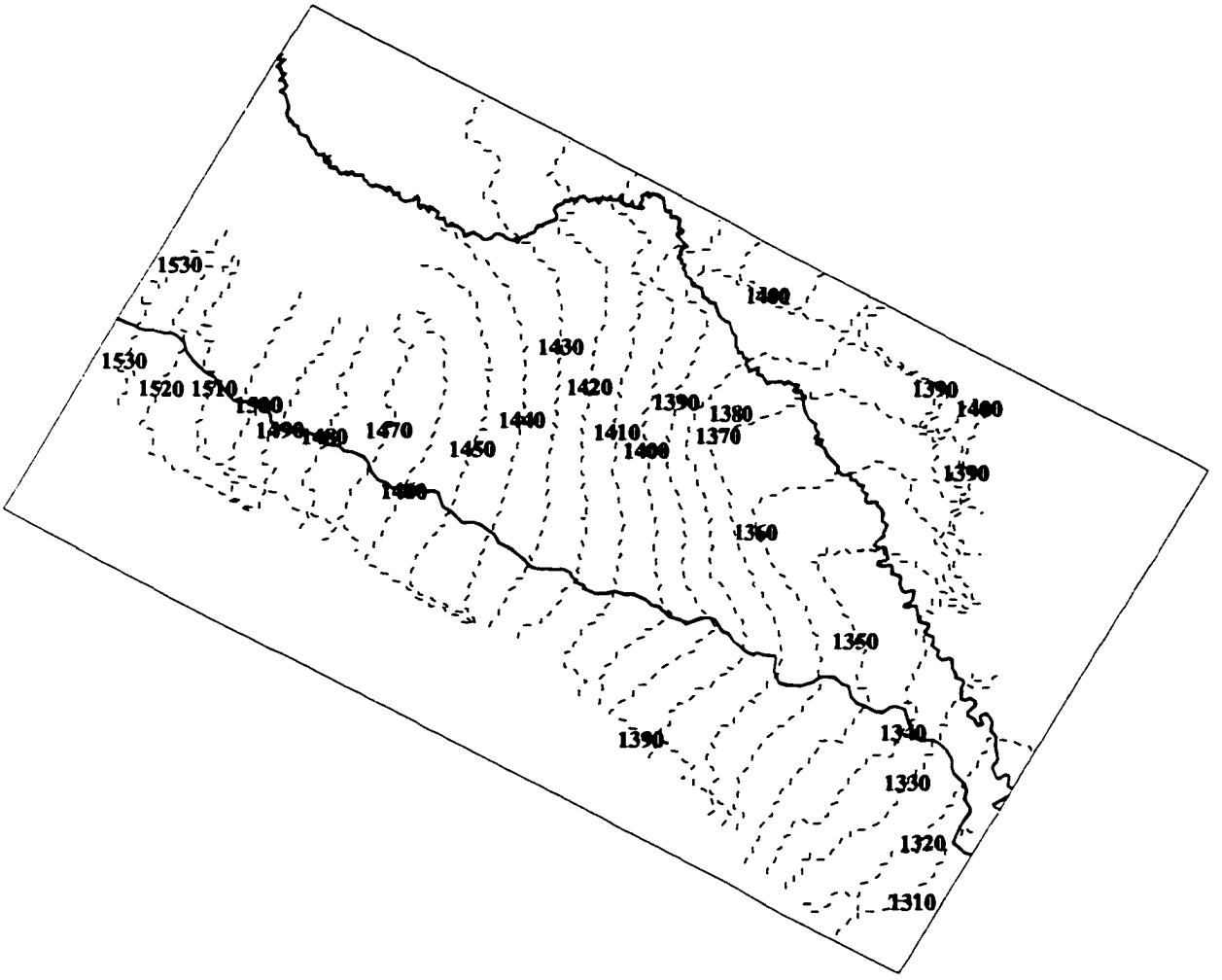


Figure 6.6 Potentiometric contours in upper model layer at the beginning of year 1987.

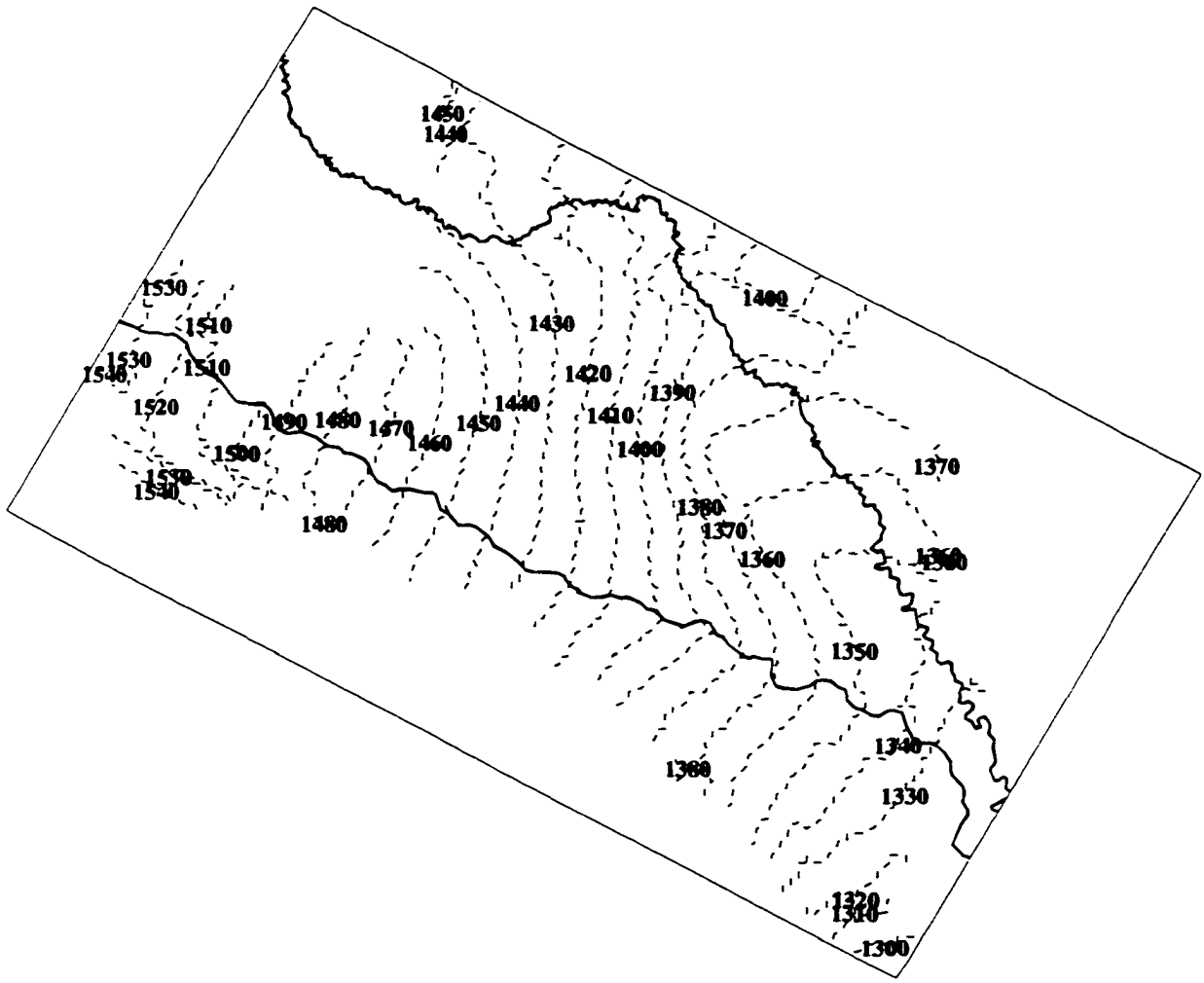


Figure 6.7 Potentiometric contours in middle model layer at the beginning of year 1987.

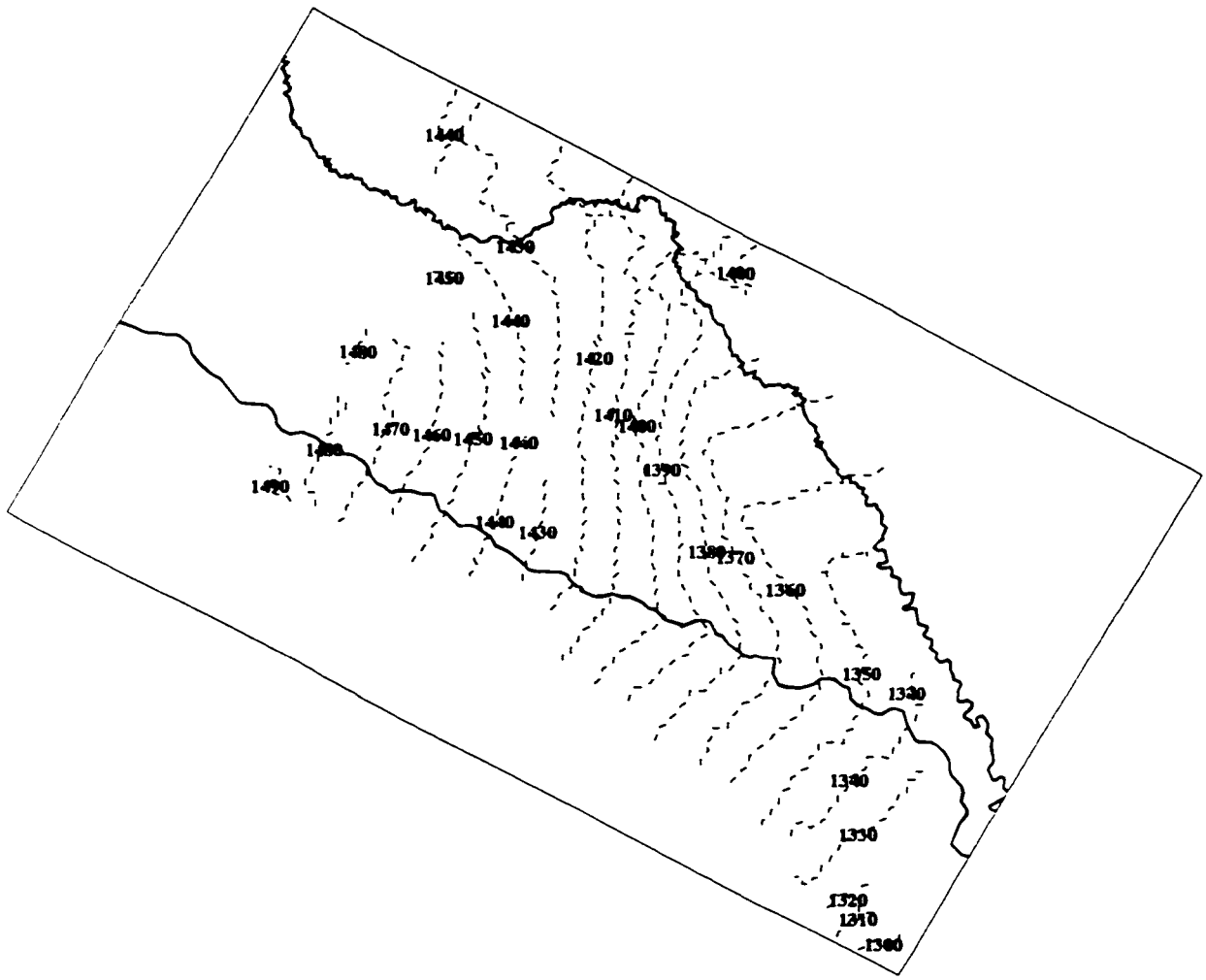


Figure 6.8 Potentiometric contours in lower model layer at the beginning of year 1987.

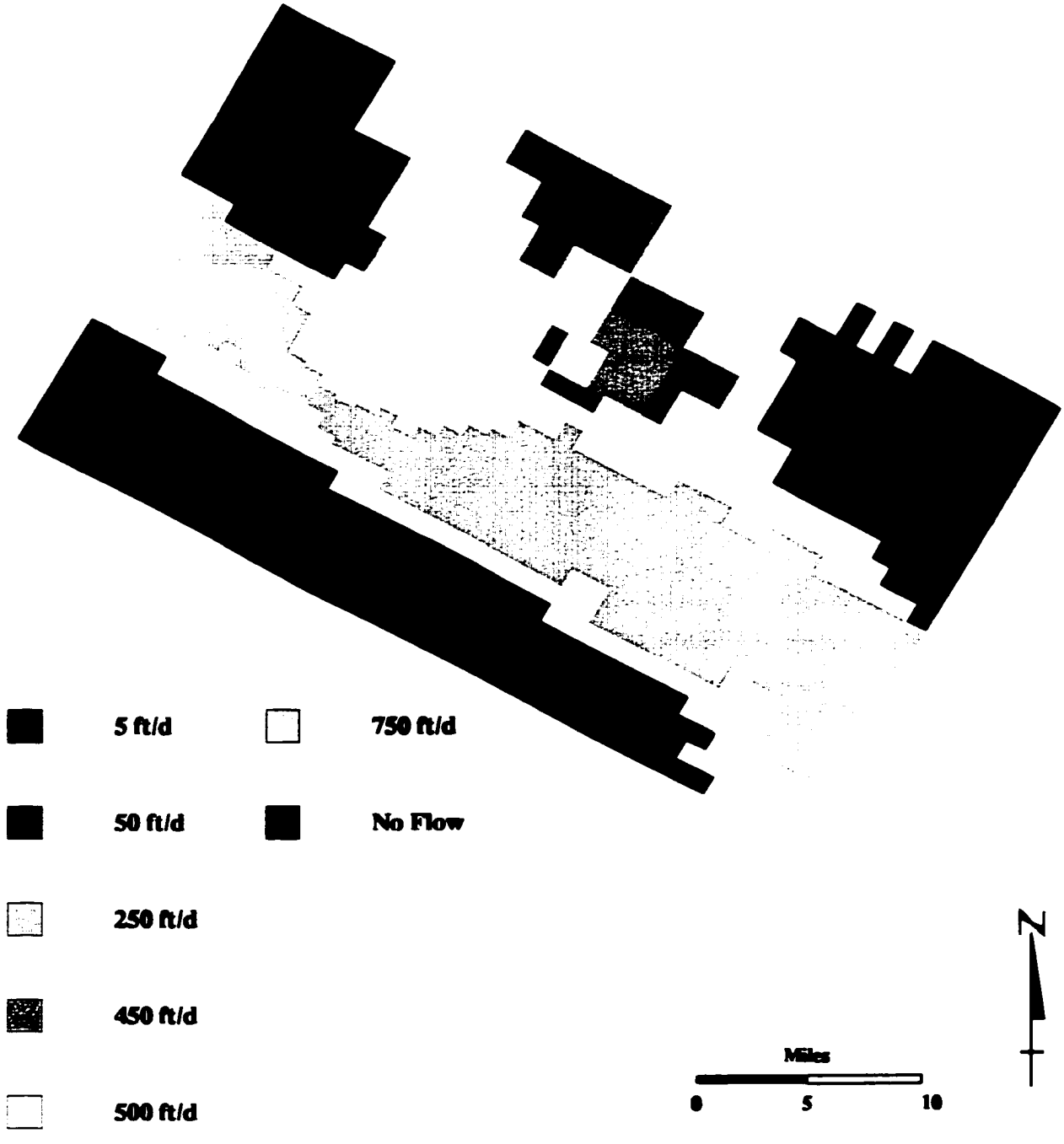


Figure 6.9 Distribution of horizontal hydraulic conductivity in upper model layer.

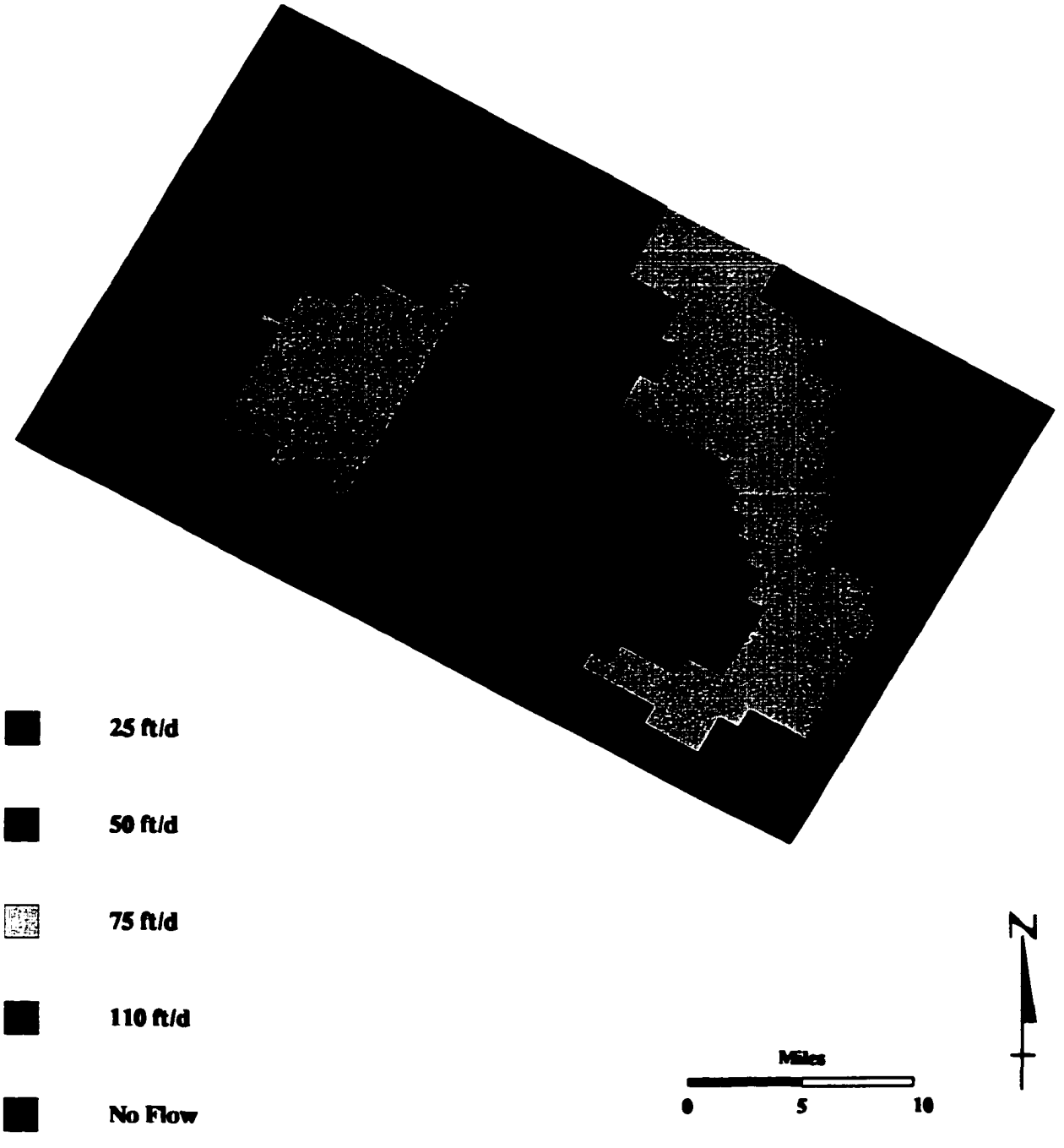


Figure 6.10 Distribution of horizontal hydraulic conductivity in middle model layer.

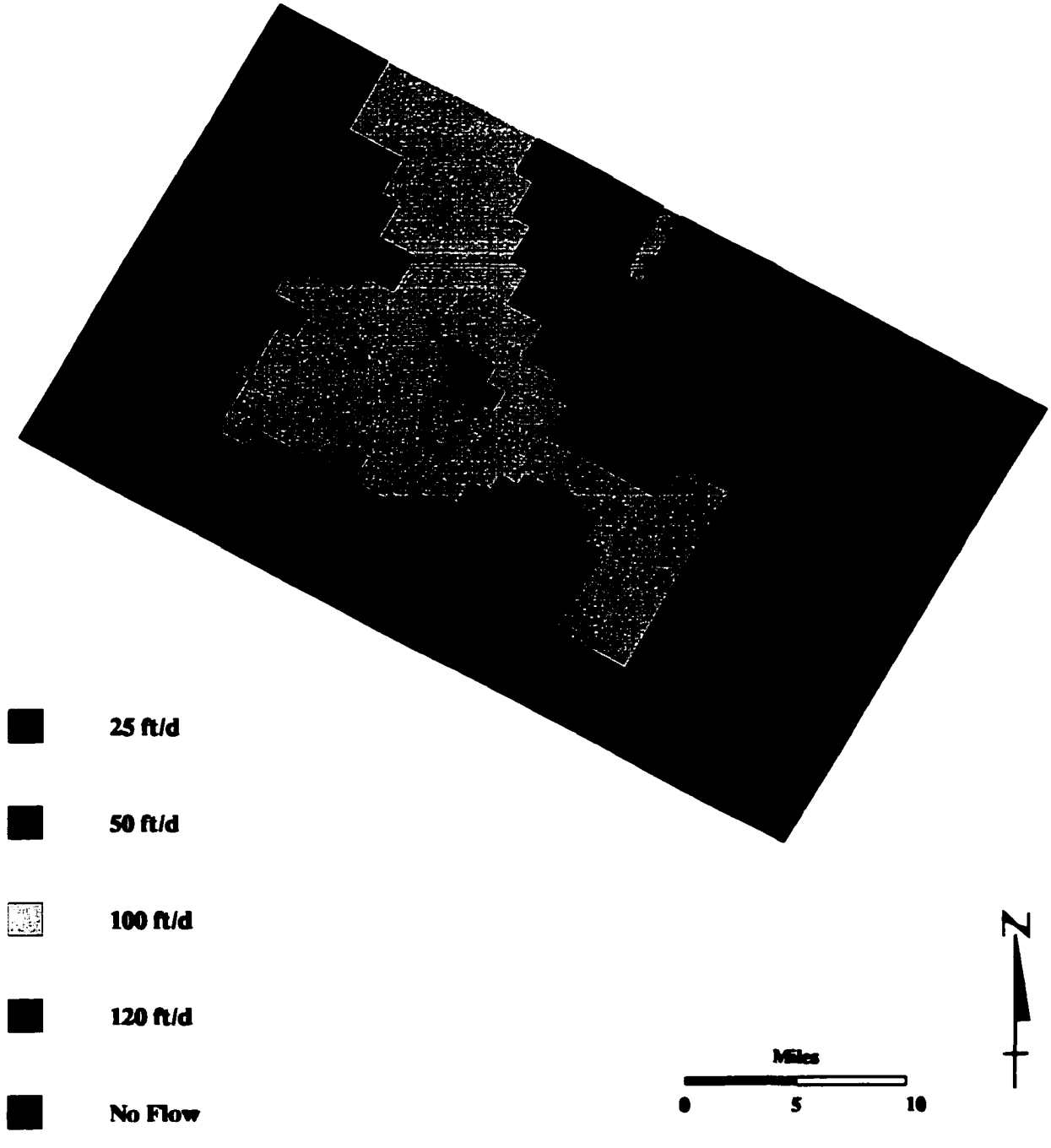


Figure 6.11 Distribution of horizontal hydraulic conductivity in lower model layer.

or more below the land surface (Myers et al., 1996). Myers developed pumpage data for the groundwater flow model.

In the Bureau of Reclamation model, The stream-aquifer interaction was simulated using the STREAM Package in MODFLOW (Prudic, 1989). In the MSAST, the stream-aquifer interaction is represented using the BRC2 Package of MODFLOW and MODBRANCH (Swain et al., 1996). The stream network is composed of 16 branches as shown in Fig. 6.12 and Fig. 6.13. It comprises part of the Arkansas River channel between Hutchinson and Maize. Branches 1-14 are each divided into 5 cross-sections. Branches 15 and 16 are each divided into 3 cross-sections. Table 6.1 lists branch number, number of cross sections in each branch, layer, row, column number of aquifer cell that contains the stream cross-section, the streambed leakage coefficient and streambed bottom elevation. The tabulated parameters are the main parameters used in MODBRANCH to describe the stream-aquifer interaction.

Table 6.1 Parameters describing stream-aquifer interaction for the case study.

Branch No.	Cross Section No.	Accumulated Cross-Section No.	Layer No.	Row No.	Column No.	k/b sec-1	Streambed Bottom Elevation ft
1	1	1	1	40	18	1.142E-05	1453
	2	2	1	40	19	1.142E-05	1453
	3	3	1	39	20	6.208E-06	1453
	4	4	1	38	21	6.208E-06	1453
	5	5	1	39	22	4.064E-06	1449

Table 6.1 continued

Branch No.	Cross Section No.	Accumulated Cross-Section No.	Layer No.	Row No.	Column No.	k/b sec-1	Streambed Bottom Elevation ft
2	1	6	1	41	23	1.2E-05	1449
	2	7	1	41	24	1.2E-05	1449
	3	8	1	41	25	2.069E-06	1443
	4	9	1	42	26	1.628E-05	1443
	5	10	1	41	27	2.069E-06	1443
3	1	11	1	40	28	2.069E-06	1443
	2	12	1	41	29	1.857E-05	1439
	3	13	1	41	30	1.857E-05	1439
	4	14	1	42	31	6.537E-06	1435
	5	15	1	42	32	6.537E-06	1435
4	1	16	1	42	33	6.537E-06	1435
	2	17	1	42	34	6.537E-06	1435
	3	18	1	43	35	9.972E-06	1428
	4	19	1	43	36	9.972E-06	1428
	5	20	1	43	37	1.262E-05	1424
5	1	21	1	42	38	8.114E-06	1424
	2	22	1	41	39	1.077E-05	1420
	3	23	1	41	40	1.077E-05	1420
	4	24	1	41	41	1.077E-05	1420
	5	25	1	41	42	1.077E-05	1420
6	1	26	1	42	43	1.252E-05	1414
	2	27	1	42	44	1.252E-05	1414
	3	28	1	42	45	1.252E-05	1414
	4	29	1	41	46	9.394E-06	1408
	5	30	1	40	47	1.607E-05	1408
7	1	31	1	39	48	1.607E-05	1408
	2	32	1	39	49	2.618E-05	1405
	3	33	1	39	50	2.618E-05	1405
	4	34	1	39	51	2.618E-05	1405
	5	35	1	39	52	4.042E-06	1400
8	1	36	1	39	53	4.042E-06	1400
	2	37	1	39	54	4.042E-06	1400
	3	38	1	39	55	1.422E-05	1395
	4	39	1	39	56	1.422E-05	1395
	5	40	1	38	57	7.449E-06	1389

Table 6.1 continued

Branch No.	Cross Section No.	Accumulated Cross-Section No.	Layer No.	Row No.	Column No.	k/b sec-1	Streambed Bottom Elevation ft
9	1	41	1	36	58	1.765E-05	1389
	2	42	1	35	59	1.765E-05	1389
	3	43	1	36	60	1.765E-05	1389
	4	44	1	37	61	1.881E-05	1384
	5	45	1	37	62	1.881E-05	1384
10	1	46	1	38	63	1.045E-05	1384
	2	47	1	38	64	8.743E-06	1379
	3	48	1	38	65	8.743E-06	1379
	4	49	1	38	66	8.743E-06	1379
	5	50	1	37	67	4.482E-06	1372
11	1	51	1	36	68	4.482E-06	1372
	2	52	1	36	69	4.482E-06	1372
	3	53	1	37	69	4.482E-06	1372
	4	54	1	38	69	6.476E-06	1372
	5	55	1	39	70	4.644E-06	1367
12	1	56	1	40	70	7.372E-06	1367
	2	57	1	40	71	7.372E-06	1367
	3	58	1	40	72	7.372E-06	1367
	4	59	1	39	73	7.362E-06	1360
	5	60	1	38	74	7.814E-06	1360
13	1	61	1	37	74	6.199E-06	1360
	2	62	1	36	75	6.994E-06	1360
	3	63	1	35	75	3.041E-05	1354
	4	64	1	34	76	3.041E-05	1354
	5	65	1	35	77	1.965E-05	1350
14	1	66	1	37	77	5.649E-05	1350
	2	67	1	36	77	6.759E-06	1350
	3	68	1	36	78	4.271E-06	1345
	4	69	1	35	78	1.979E-05	1339
	5	70	1	34	78	4.582E-05	1339
15	1	71	1	34	79	1.527E-05	1339
	2	72	1	35	79	1.932E-05	1339
	3	73	1	36	80	1.222E-05	1335

Table 6.1 continued

Branch No.	Cross Section No.	Accumulated Cross-Section No.	Layer No.	Row No.	Column No.	k/b sec-1	Streambed Bottom Elevation ft
16	1	74	1	37	80	8.093E-06	1335
	2	75	1	37	81	2.007E-05	1328
	3	76	1	38	82	1.863E-05	1324

USGS two gaging stations have available streamflow data for the time of simulation. These stations are gaging station of Arkansas River near Hutchinson, Kansas (No. 0714330), and gaging station of Arkansas River near Maize, Kansas (No. 07143375). The two stations are shown in Fig. 6.12. The observed daily streamflow for these gaging stations are shown in Fig. 6.14. Parameters of Table 6.1 and streamflows values at the two gaging stations are used to construct a MODBRANCH input file. Streamflow of gaging station number 0714330 is considered as the upstream boundary condition and streamflow of gaging station number 07143375 is considered as the downstream boundary condition.

The streamflow records for the gaging stations are available for each day. A 1-day time step is used in MODBRANCH and 30-day time step is used in MODFLOW. This makes the ratio of MODFLOW time step to MODBRANCH time step to be 30. The simulation is run for 1080 MODBRANCH time steps from 1/12/1987 to 12/26/1989. The simulated streamflow at stream cross-section No. 33 located in branch No. 7 is shown in Fig. 6.15.

6.3.2 MT3D-SSTM Application

The MT3D-SSTM is applied using MODFLOW-MODBRANCH flow solution. The

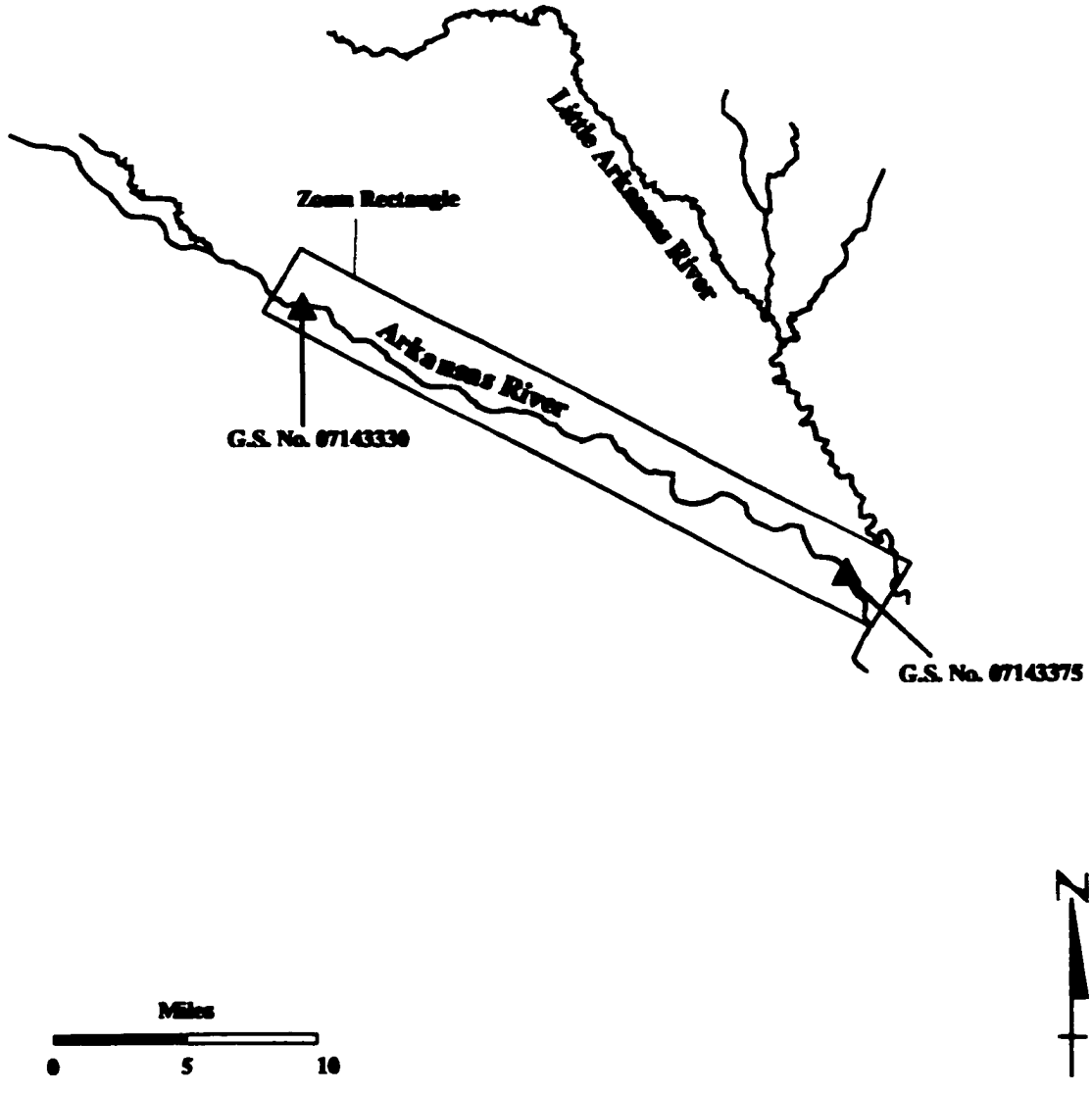


Figure 6.12 The simulated channel located between two USGS gaging stations.

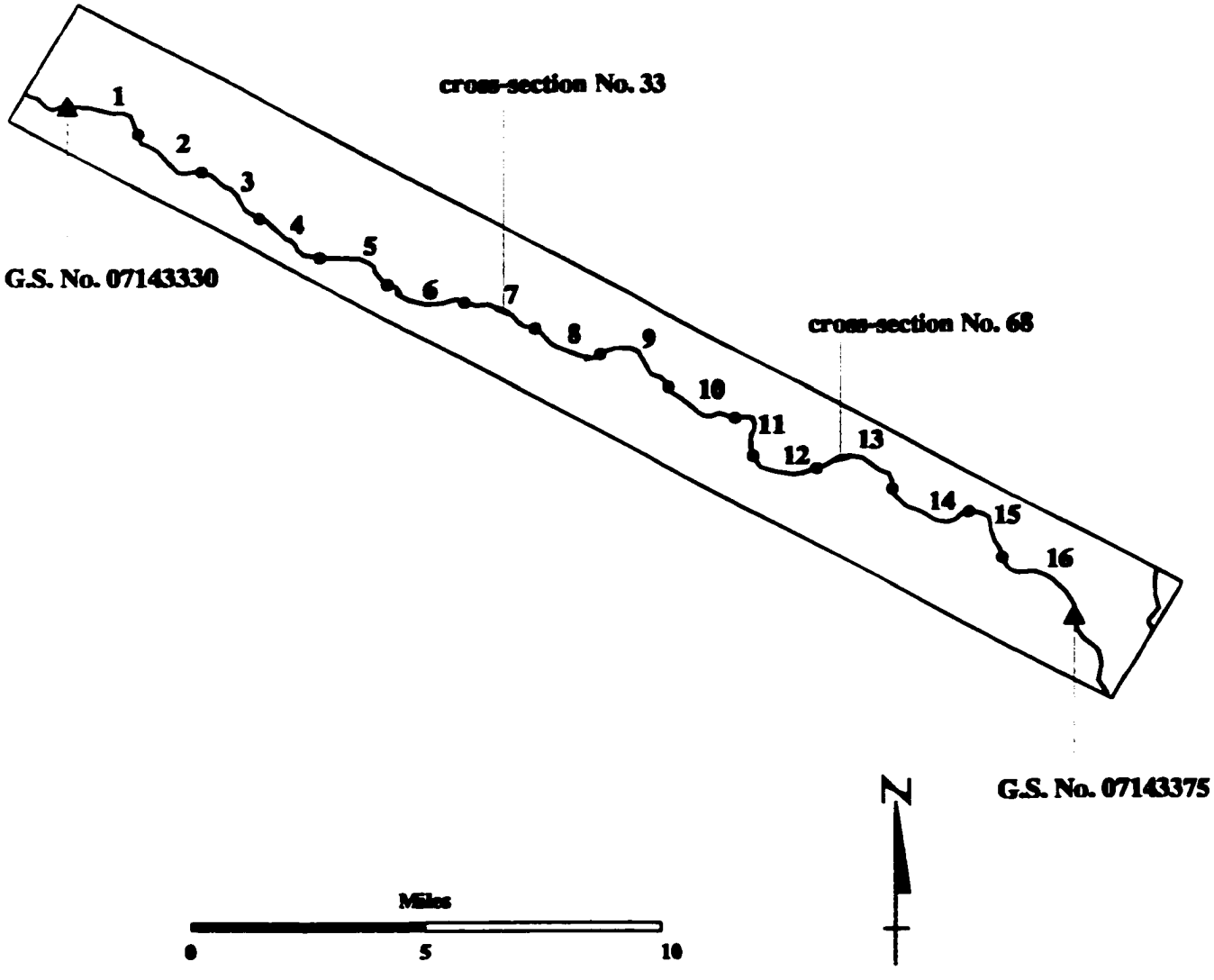


Figure 6.13 Enlarged plot of the zoom rectangle of Figure 6.12 showing the 16 branches.

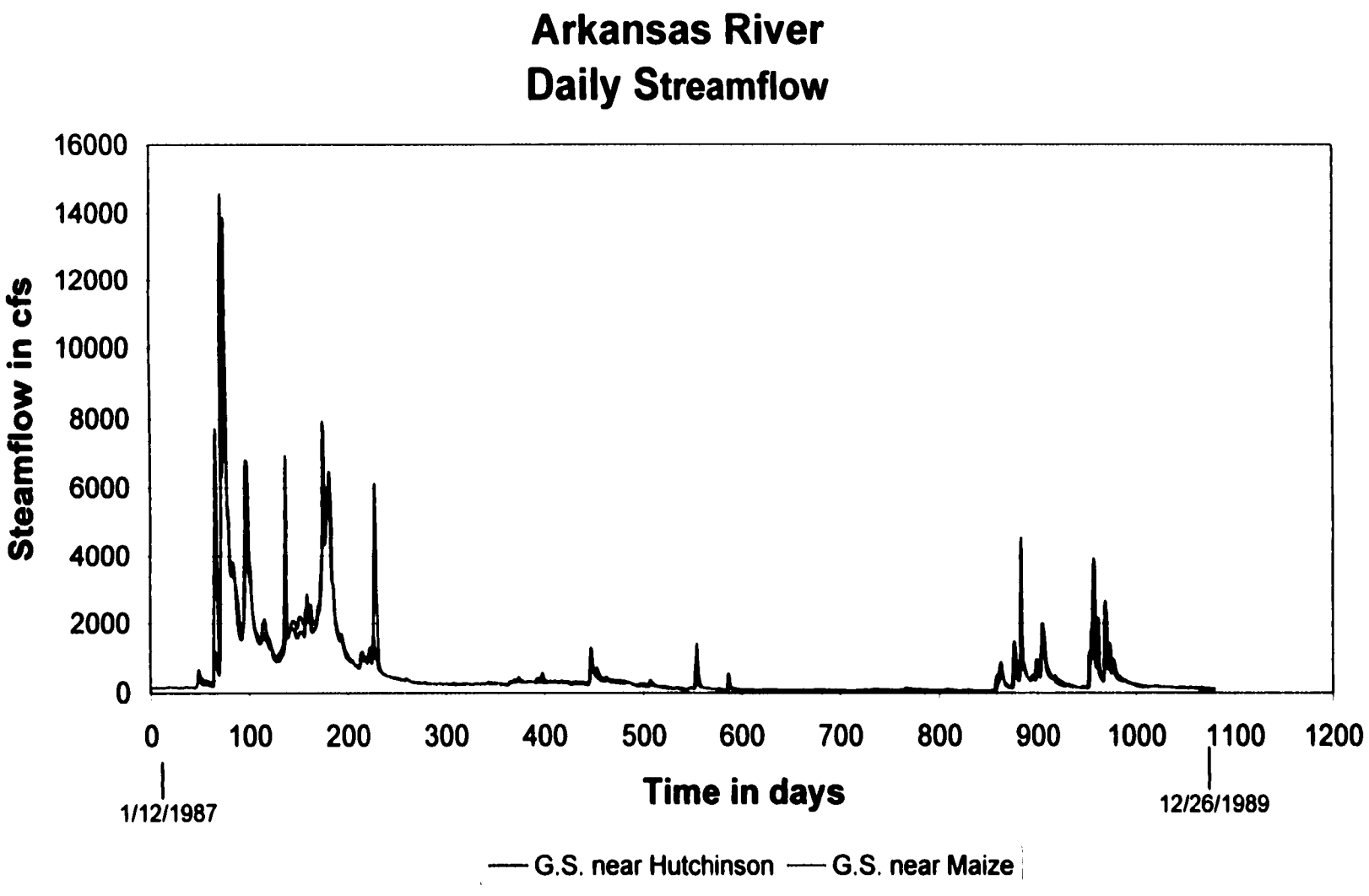


Figure 6.14 Observed daily streamflow from 1/12/1987 to 12/26/1989 at Hutchinson and Maize gaging stations.

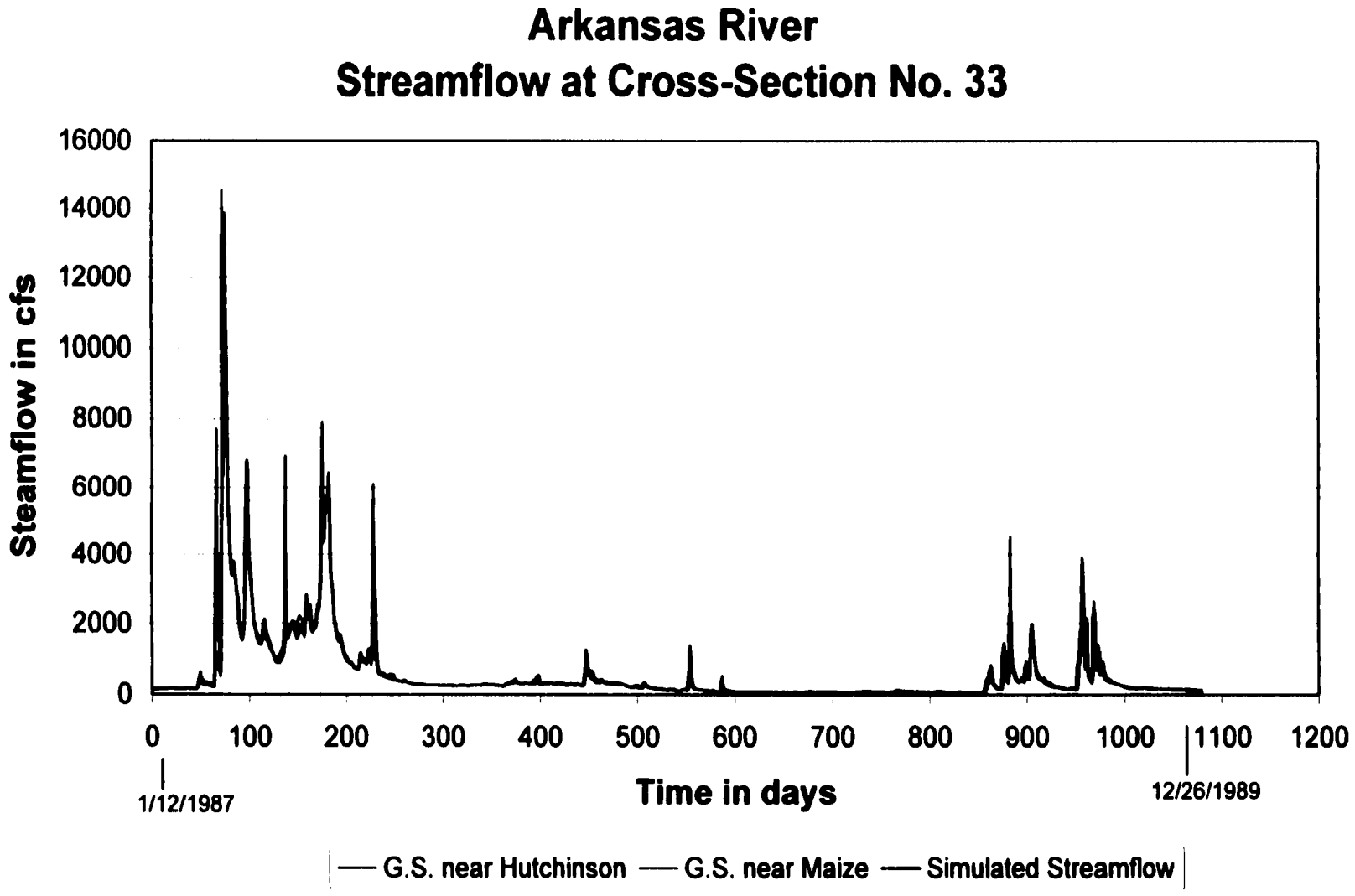


Figure 6.15 Simulated daily streamflow from 1/12/1987 to 12/126/1989 at cross-section No. 33.

boundary conditions regarding transport in the aquifer include active concentration cells, inactive concentration cells, and constant concentration cells. All cells which were active in the groundwater flow model are considered to be active concentration cells. Constant concentration cells were located in the lower layer below the Arkansas River to represent deep natural saltwater indicated by chloride near the bedrock. MT3D concentration boundary conditions for upper, middle and lower layers are shown in Fig. 6.16, Fig. 6.17, and Fig. 6.18 respectively. Bureau of Reclamation MT3D application was used to simulate initial chloride concentration (1/12/1987) in the aquifer for the MT3D-SSTM application. The initial concentration for the three layers in the Bureau of Reclamation MT3D model was for the year 1940. The initial concentrations were concluded by combining data from studies done by Spinazola et al. (1985) and Myers et al. (1996). The sources considered in the model are: oil field brine from Burrton Oil Filed, saltwater from the Arkansas River, and deep natural saltwater. Year 1940 initial concentrations for the upper, middle, and lower layers used in Bureau of Reclamation application are shown in Fig. 6.19, Fig 6.20, and Fig. 6.21 respectively. Simulated initial concentration at the beginning of year 1987 used in the MT3D-SSTM application are shown in Fig. 6.22, Fig. 6.23, and Fig. 6.24.

Values of effective porosity for the upper, middle, and lower model layers were 0.3,0.2 and 0.3 respectively. These values were estimated in the Bureau of Reclamation MT3D model by calibration. Longitudinal and transverse transmissivity values are 100 and 0.3. These values were obtained from the study conducted by Spinazola et al. (1985). In the Bureau of Reclamation MT3D model, the Arkansas River was modeled as a continuous source of chloride using the Sink/Source Mixing (SSM1) Package of MT3D. The chloride concentration was assumed to be equal to 630 mg/l. In the MSAST application, the Package developed in this study and referred to as the Stream

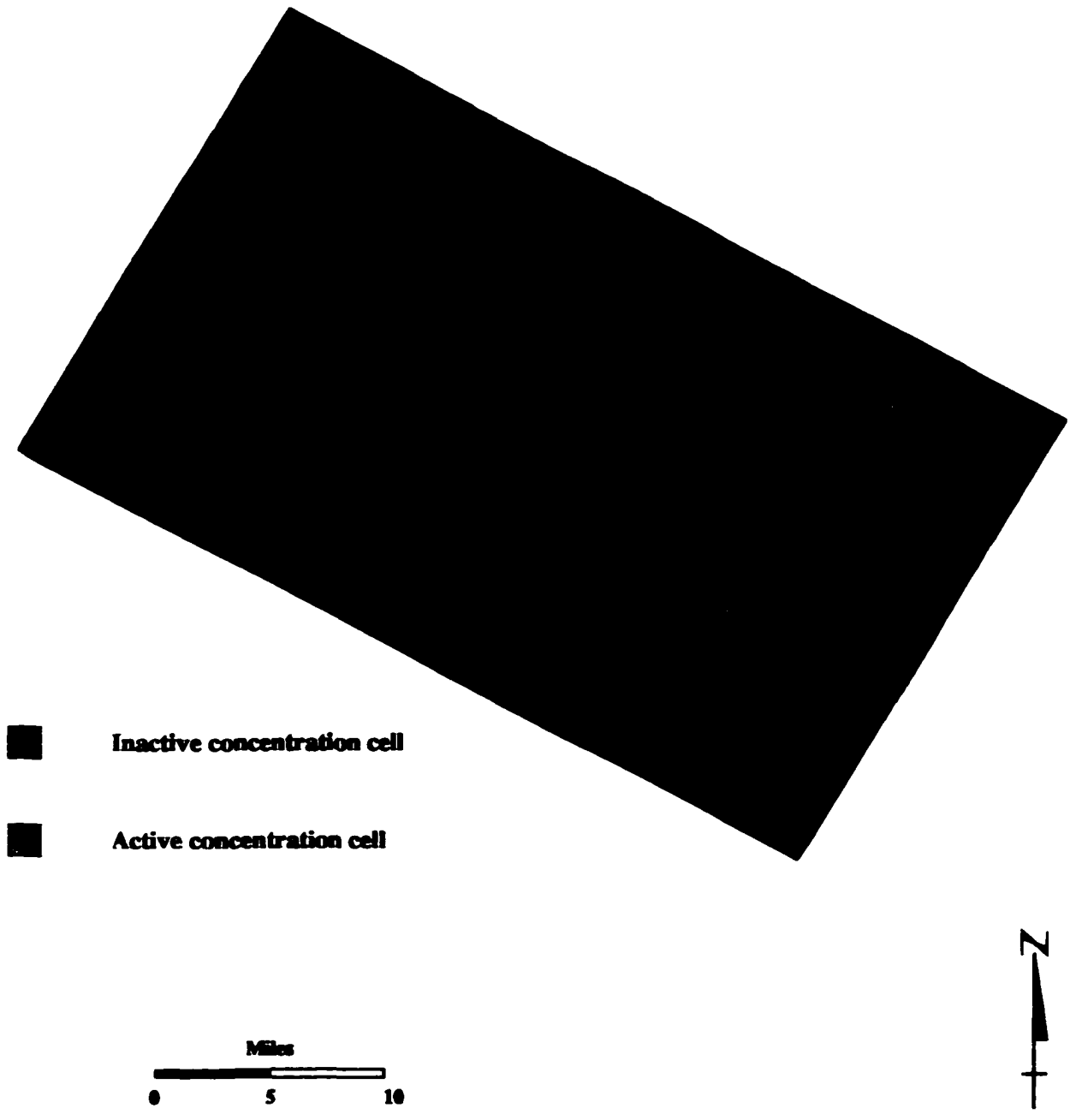


Figure 6.16 Concentration boundaries for upper layer of groundwater transport model.

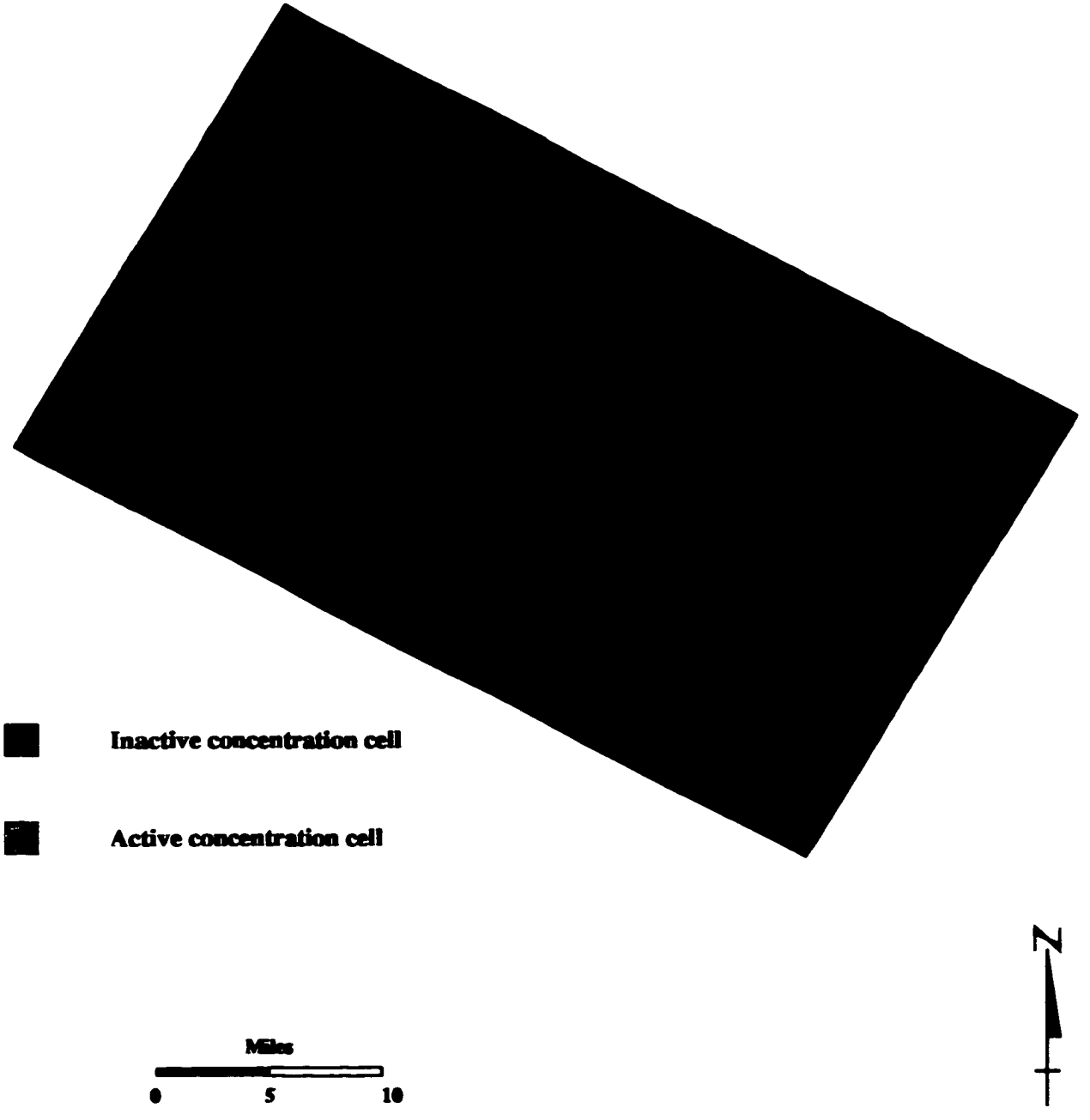


Figure 6.17 Concentration boundaries for middle layer of groundwater transport model.

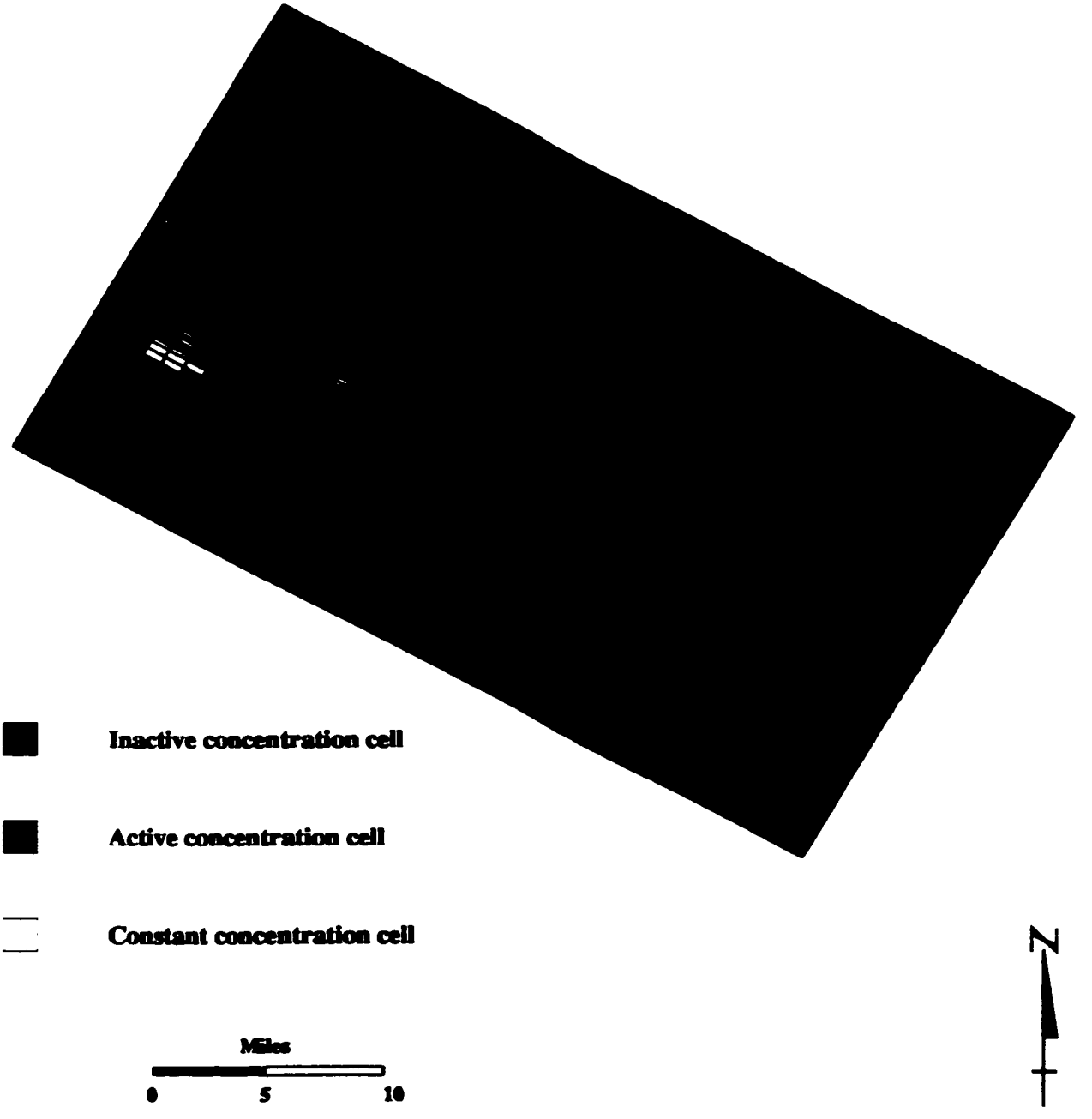


Figure 6.18 Concentration boundaries for lower layer of groundwater transport model.

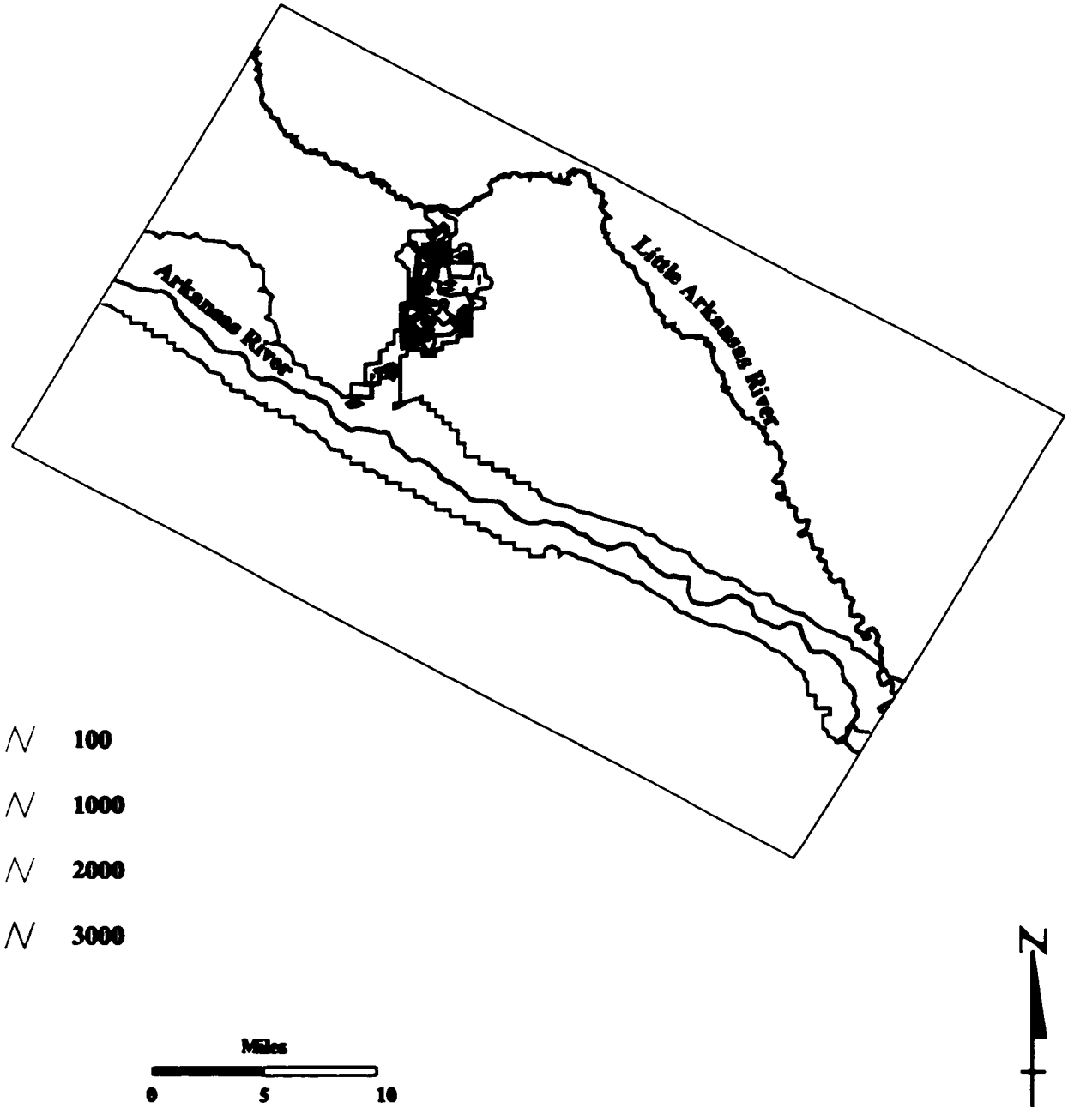


Figure 6.19 Initial concentration of chloride in the upper model layer in 1940, adapted from Bureau of Reclamation, 1993.

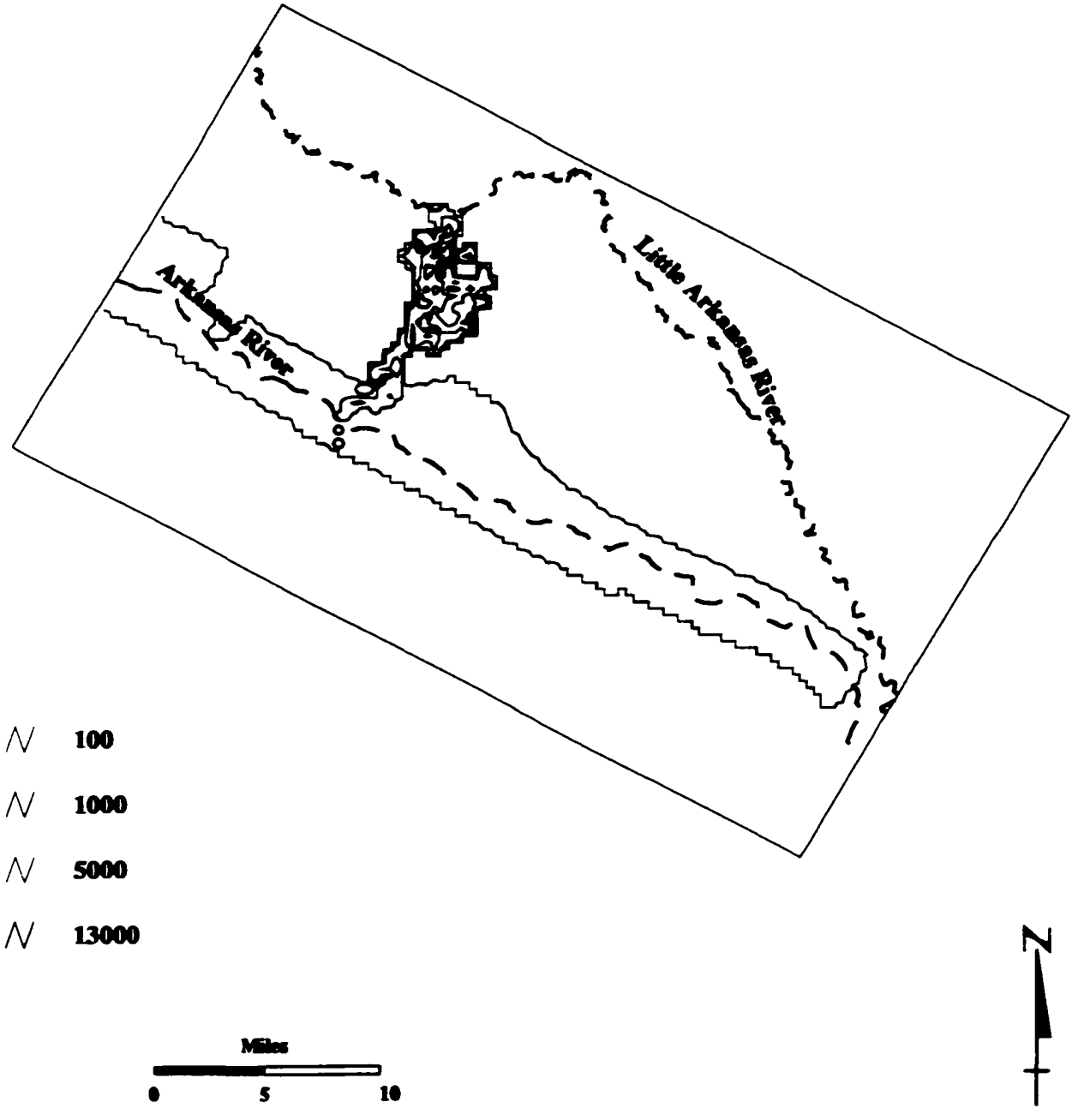


Figure 6.20 Initial concentration of chloride in the middle model layer in 1940, adapted from Bureau of Reclamation, 1993.

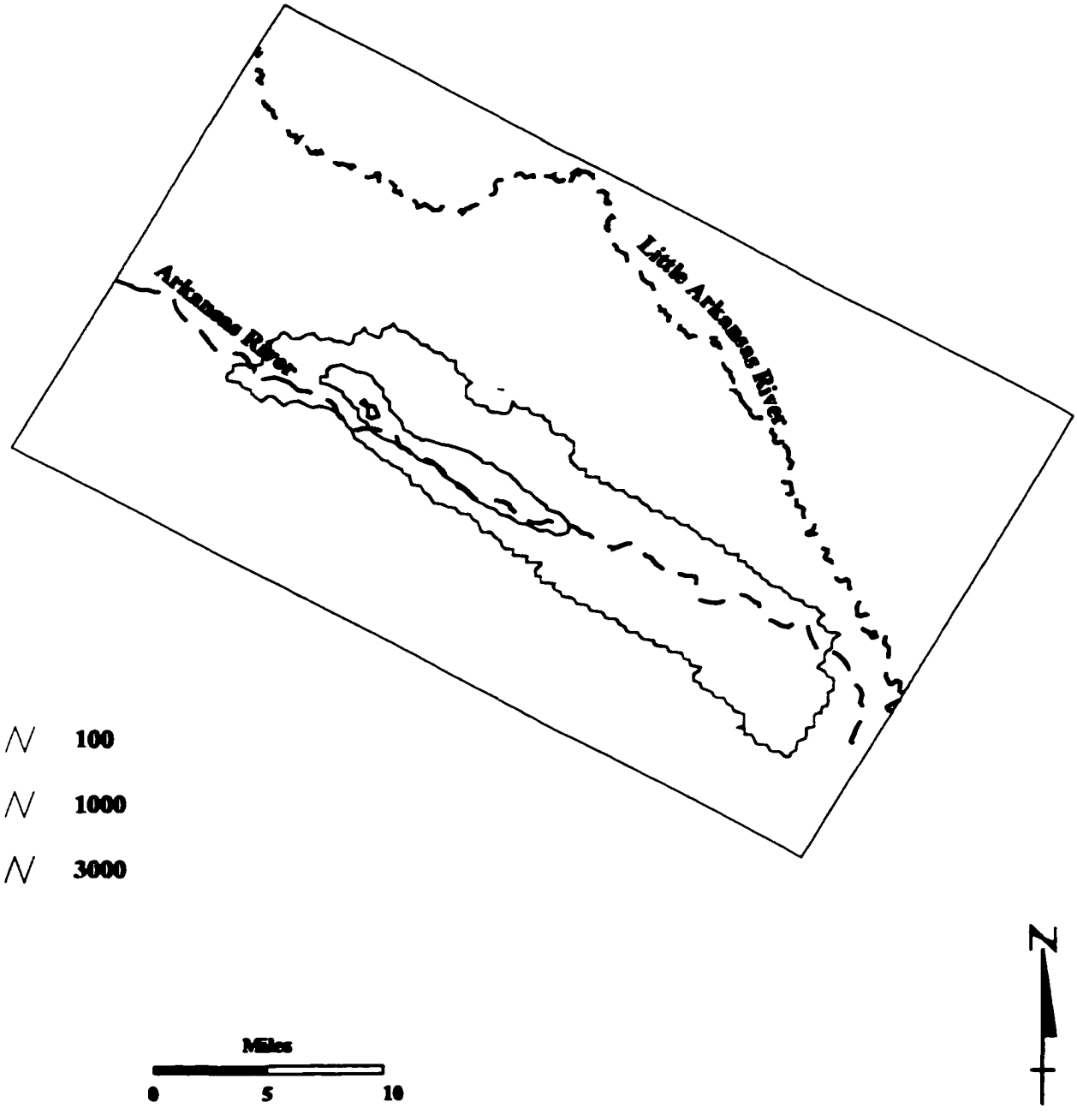


Figure 6.21 Initial concentration of chloride in the lower model layer in 1940, adapted from Bureau of Reclamation, 1993.

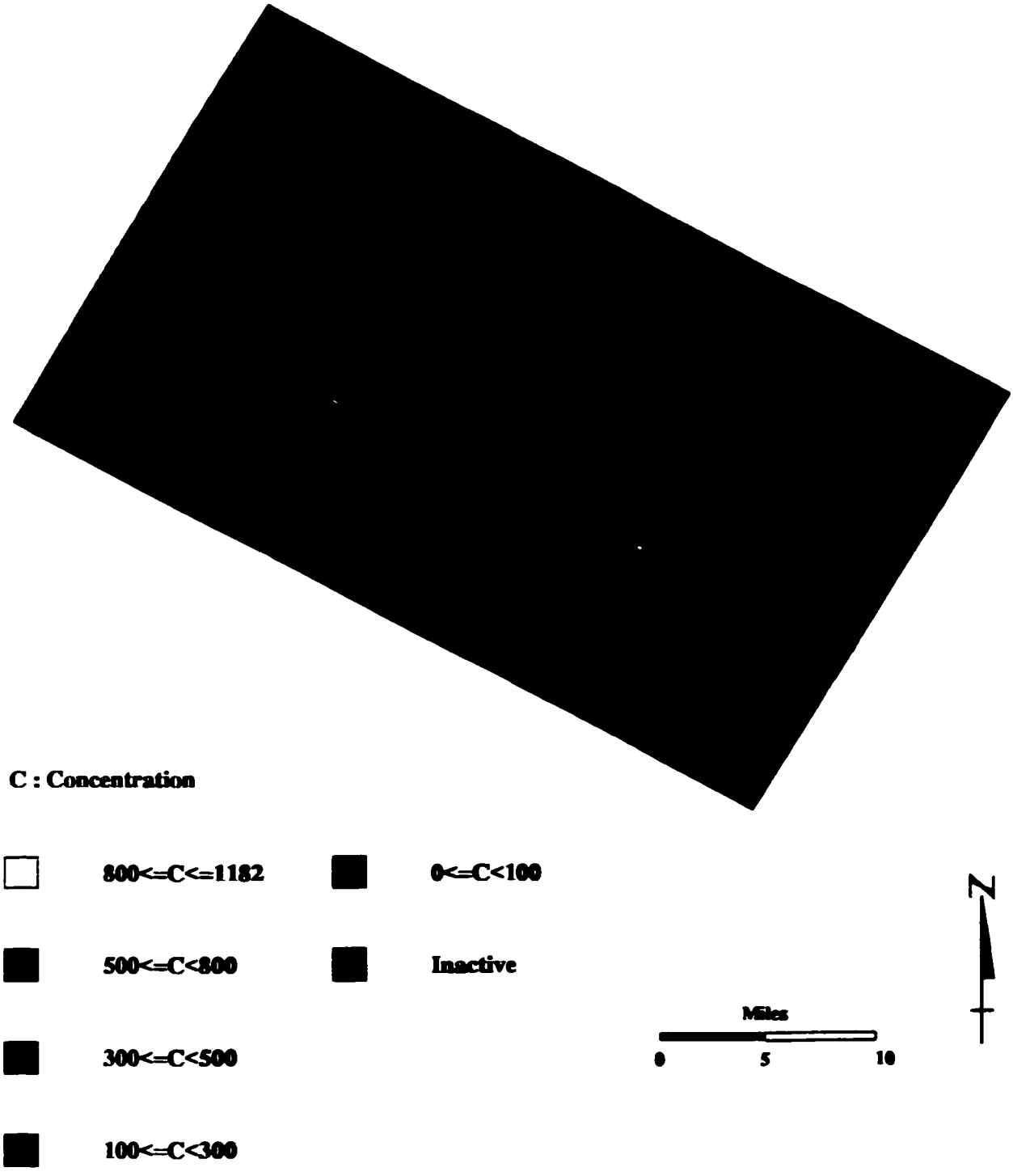


Figure 6.22 Concentration of chloride in the upper model layer at the beginning of year 1987.

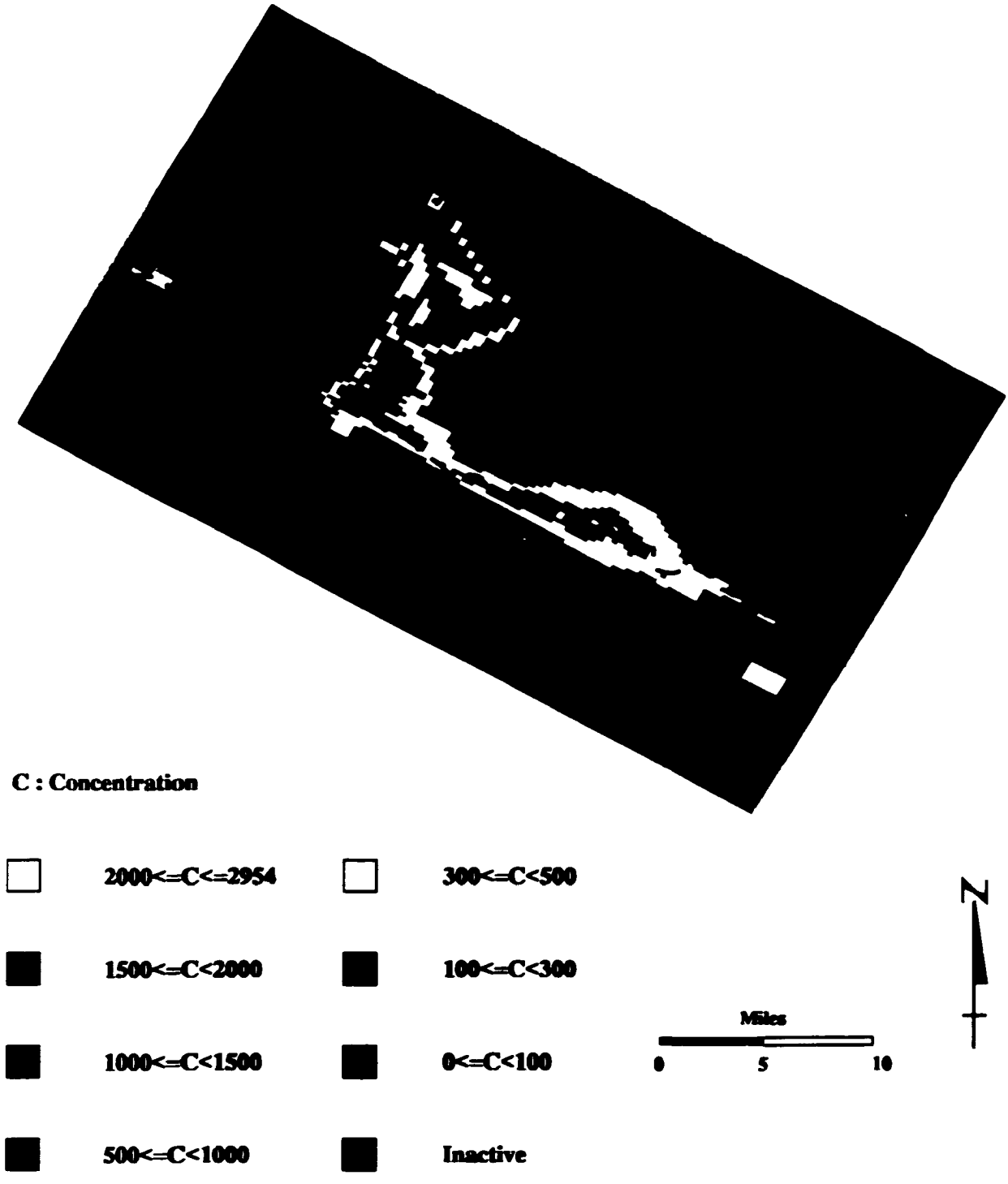


Figure 6.23 Concentration of chloride in the middle model layer at the beginning of year 1987.

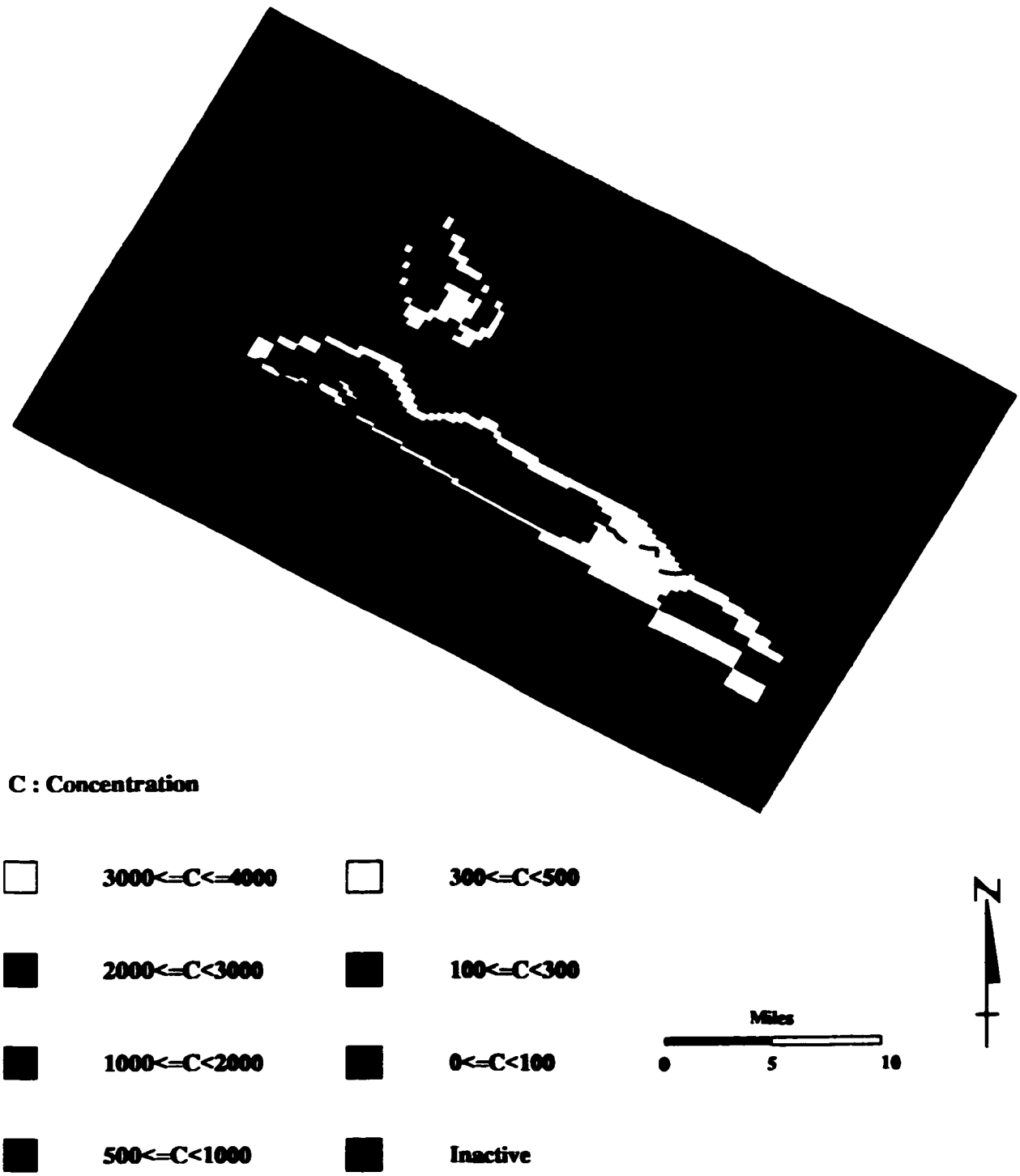


Figure 6.24 Concentration of chloride in the lower model layer at the beginning of year 1987.

Solute Transport (SSL1) Package is used to model the chloride transport between the Arkansas River and the aquifer using the SSTM. Branches 1-16 as shown in Fig. 6.13 are considered in MT3D-SSTM simulation.

In the study conducted by Myers et al. (1996), samples of chloride were collected at sampling sites along the river. The mean chloride concentration was 630 mg/l. This value is used in the Bureau of Reclamation MT3D application. No chloride concentration profile for the Arkansas River is available in space or in time.

The SSTM is executed from the SSL1 Package that is added to MT3D in this study. The transport step of MT3D is set to 1 day. The SSTM time step is set to 1 day to be compatible with MODBRANCH and MT3D. The options or packages considered in MT3D are Advection (ADV1) in the aquifer, Dispersion (DSP1) in the aquifer, and Source/Sink Mixing (SSM1) and the new package added in this study, the Stream Solute Transport (SSL1). The options considered in the SSTM are Advection (ADS1) in the stream and Dispersion in the stream (DDS1).

Since there is no chloride concentration profile for the Arkansas River available in space or in time. The boundary value of chloride concentration is assumed 630 mg/l in the two gaging stations shown in Fig 6.12. This is the mean value of measured values recommended by the Bureau of Reclamation for the concentration of chloride in the Arkansas River for the period 1980-1989. The initial concentration of chloride in the stream cross sections is also assumed 630 mg/l. The time step of MT3D is set equal to 30 days and its transport step is set to equal 1 day. The SSTM time step is set to 1 day to be compatible with MODBRANCH and MT3D. The simulation is run for 1080 SSTM time steps from 1/12/1987 to 12/26/1989.

The simulated chloride concentration at the end of year 1989 in the aquifer upper model layer

is shown in Fig. 6.25. The concentration values in the vicinity of Arkansas river generally decreased. To quantify this decrease, Fig. 6.26 is created by subtracting cell concentration values for the beginning of year 1987 (Fig. 6.22) from those at the end of year 1989 (Fig. 6.25). This simulation is referred to as the Basic Simulation to distinguish it from the sensitivity analysis simulations that will be described later. Figure 6.26 is compared to Fig. 6.27 which represent the difference in chloride concentration between the end of year 1989 and the beginning of year1987using the Bureau of Reclamation model which assumes a constant chloride concentration in the stream segments contained by aquifer cells. It is clear that MT3D-SSTM showed more variability in the vicinity of simulated channel. As shown in Fig. 6.26, the range of concentration decrease in the vicinity of simulated channel was between -589mg/l and -41 mg/l . The number of aquifer cells in which this decrease occurs are 343 cells. Increase in chloride concentration in the vicinity of the river occurred on a much lower scale. An Increase in chloride concentration between 60mg/l and 812 mg/l occurred in 22 aquifer cells. Figure 6.28 shows a detailed distribution of chloride decrease in the vicinity of Arkansas River. Table 6.2 lists the discretized ranges of chloride change occurred in the vicinity of the simulated channel and the number model cells fall in these ranges.

Table 6.2 Distribution of chloride change in the vicinity of simulate channel.

Range	Number of cells
60 <= Concentration difference < 812	22
-100 <= Concentration difference < -41	109
-200 <= Concentration difference < -100	96

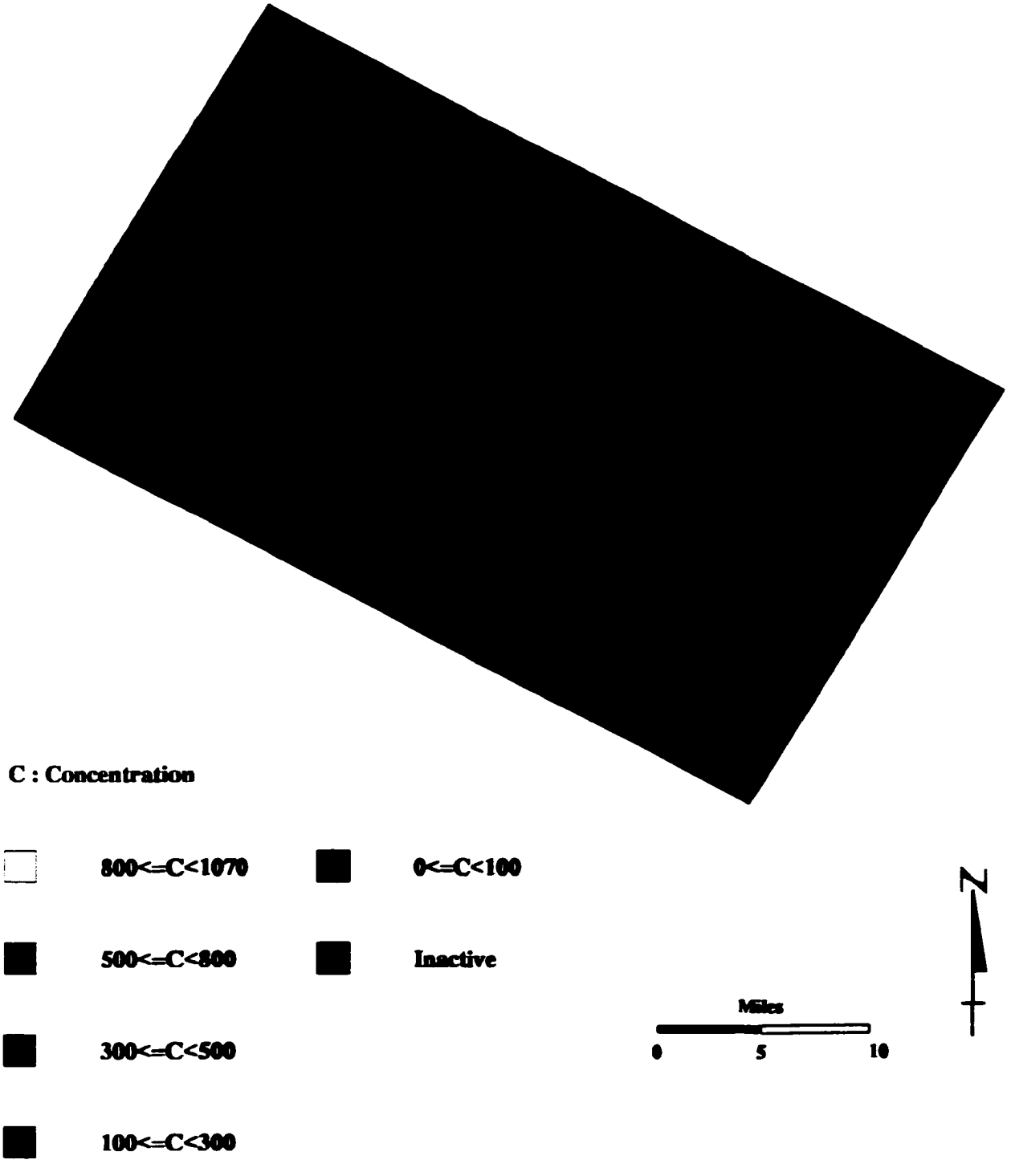


Figure 6.25 Simulated concentration of chloride in the upper model layer at the end of year 1989 using the basic MT3D-SSTM simulation.

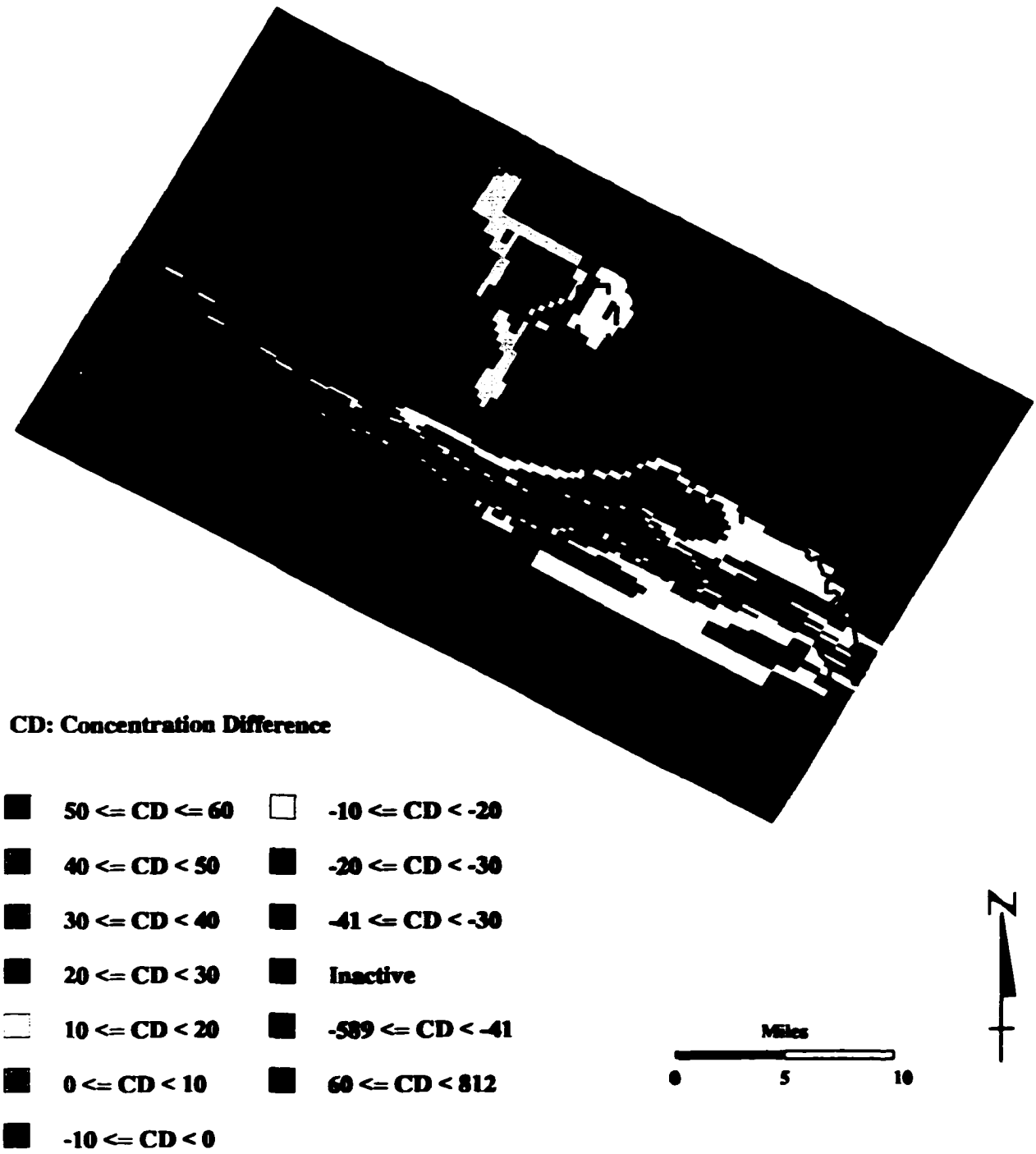
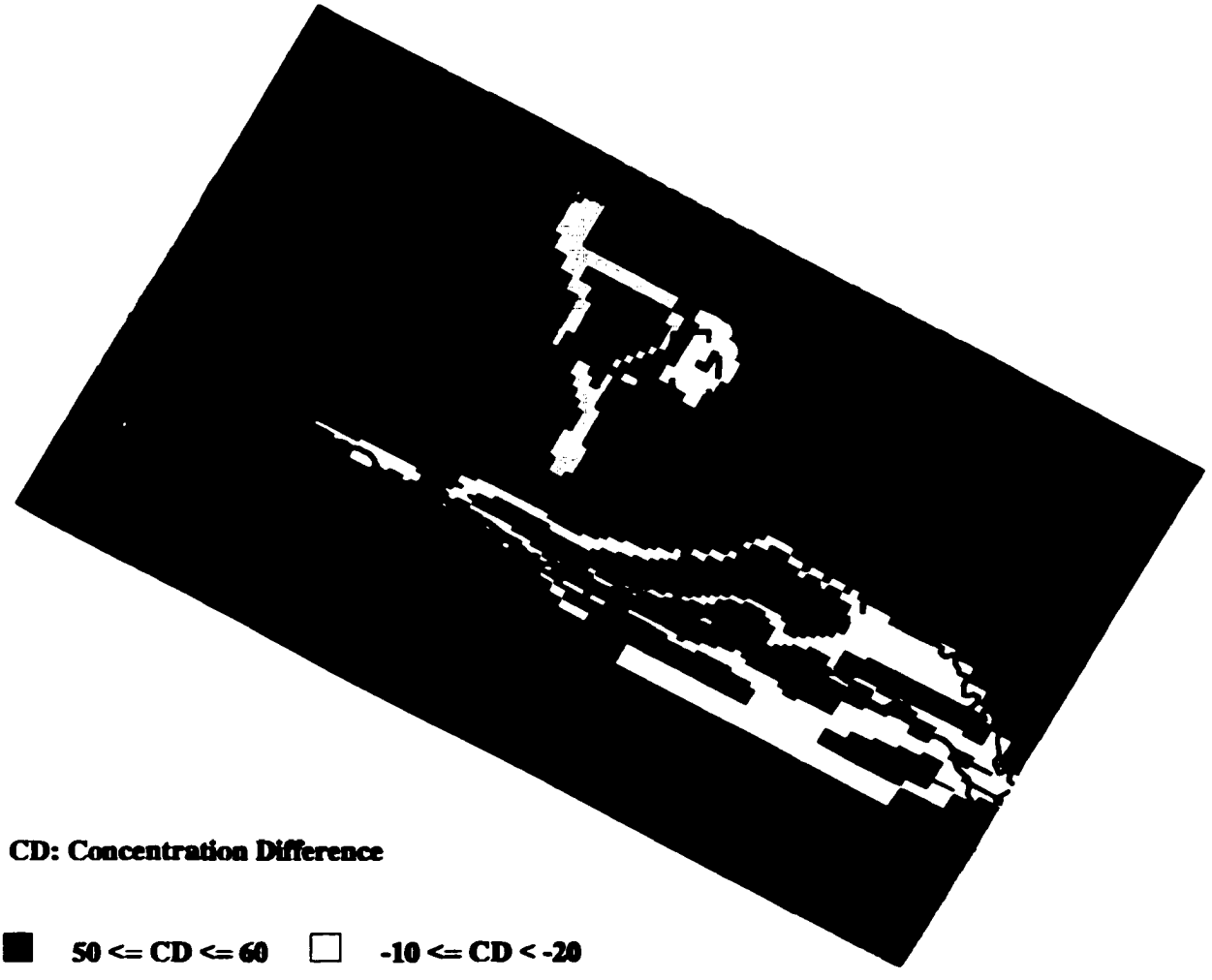


Figure 6.26 Difference in concentration of chloride between the end of year 1989 and the beginning of year 1987 in the upper model layer using MT3D-SSTM basic simulation.



CD: Concentration Difference

- 50 <= CD <= 60
- 40 <= CD < 50
- 30 <= CD < 40
- 20 <= CD < 30
- 10 <= CD < 20
- 0 <= CD < 10
- -10 <= CD < 0
- -10 <= CD < -20
- -20 <= CD < -30
- -41 <= CD < -30
- Inactive

Miles

0 5 10

N

Figure 6.27 Difference in concentration of chloride between the end of year 1989 and the beginning of year 1987 in upper model layer using the Bureau of Reclamation simulation.

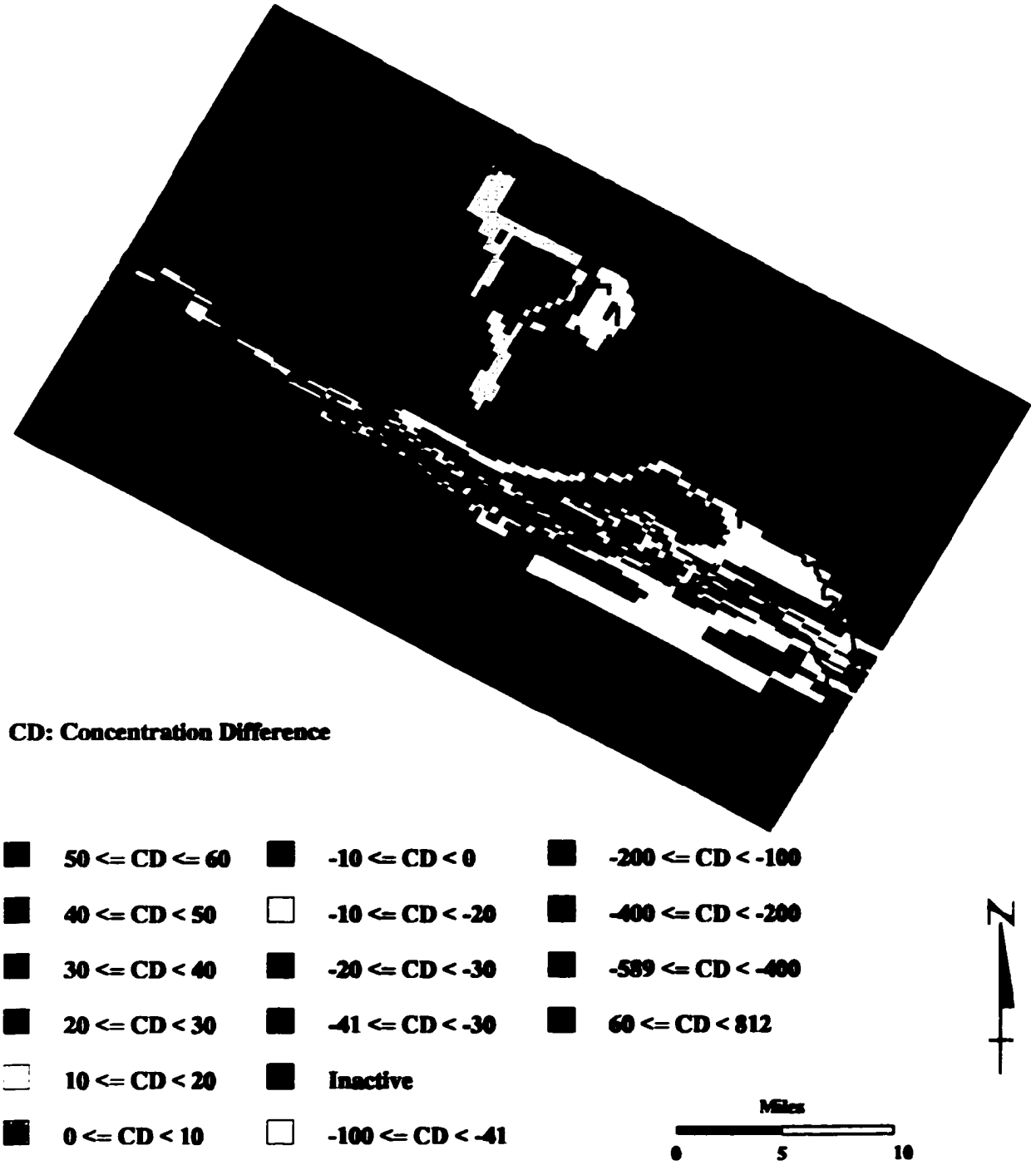


Figure 6.28 Difference in concentration of chloride between the end of year 1989 and the beginning of year 1987 in the upper model layer showing detailed distribution in the vicinity of the Arkansas River.

Table 6.2 continued

Range	Number of cells
400 <= Concentration difference < -200	102
-589 <= Concentration difference < -400	36

Figure 6.29 shows the percentage difference in chloride concentration between the end of year 1989 and the beginning of year 1987. Percentages of change are higher in the vicinity of the simulated channel. The conclusion drawn from the decrease in aquifer concentration is that aquifer leakage to the stream was more than outflow from the stream to the aquifer during the simulation time.

The chloride concentration simulated in the Arkansas River are plotted in space and time over the simulation period. Figures 6.30, 6.31, 6.32, and 6.33 show chloride concentration for several stream cross-sections along the simulated channel. Chloride concentration values are plotted versus time for accumulated stream cross-sections numbers: 4, 10, 33, and 68. Stream cross-sections No. 4 and No. 10 are close to the Hutchinson upstream boundary. Values of chloride concentration in cross-section No. 4 show less variability during low streamflow periods with a value close to the observed mean. The maximum and minimum simulated values of chloride occurred following an abrupt change in river streamflow. The simulated mean of chloride in cross-section No. 4 over the 1080 days is 627.3 mg/l. The simulated mean of chloride concentration in cross-section No. 10 is 631 mg/l. Chloride concentration increases as streamflow in the river decreases. The simulated mean of chloride concentration in cross-section No. 33 is 638.5 mg/l. The simulated mean of chloride in cross-section No. 68 is 655 mg/l. The simulated mean increases downstream. This is because streamflow

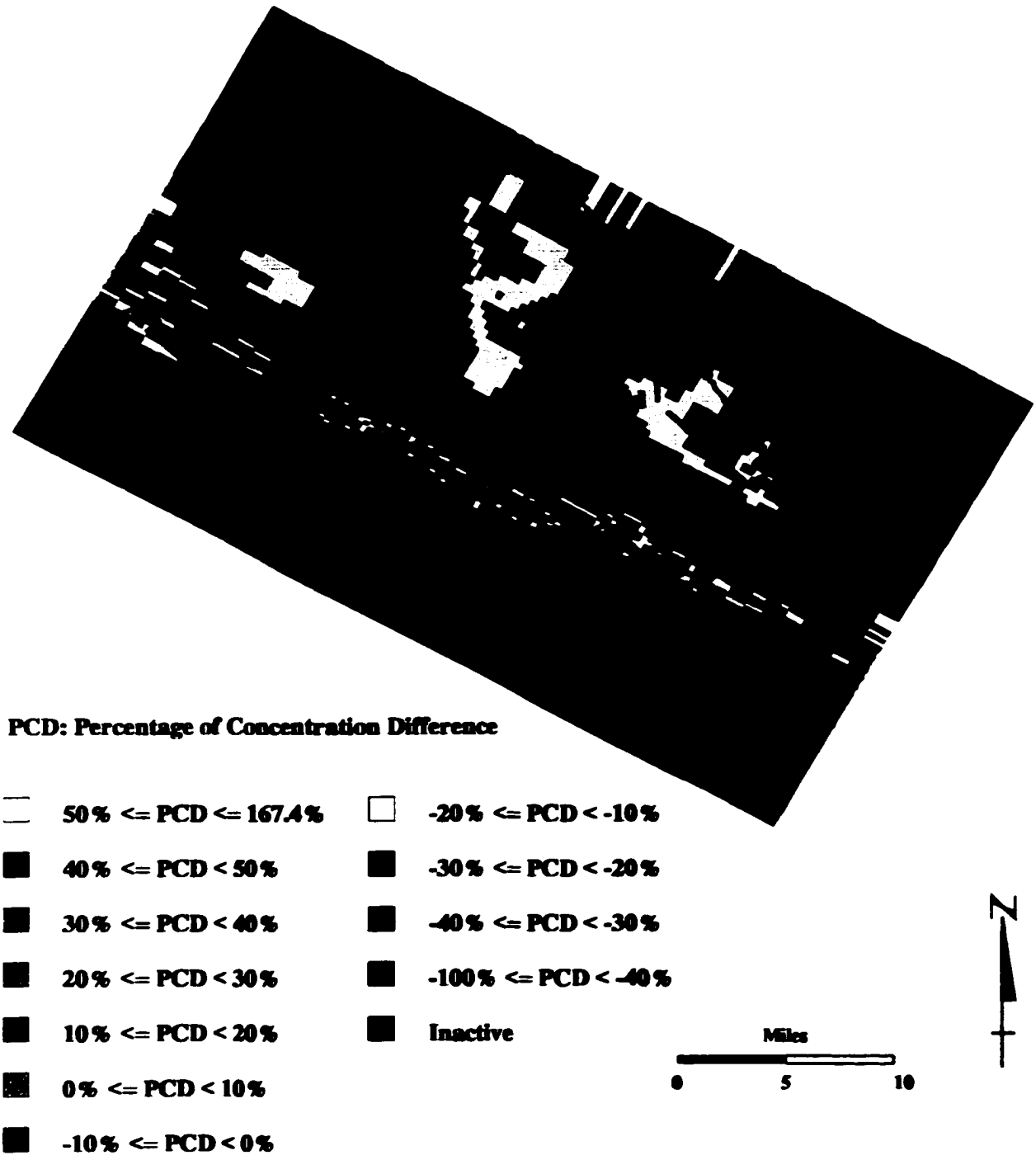


Figure 6.29 Percentage difference in concentration of chloride between the end of year 1989 and the beginning of year 1987 in the upper model layer.

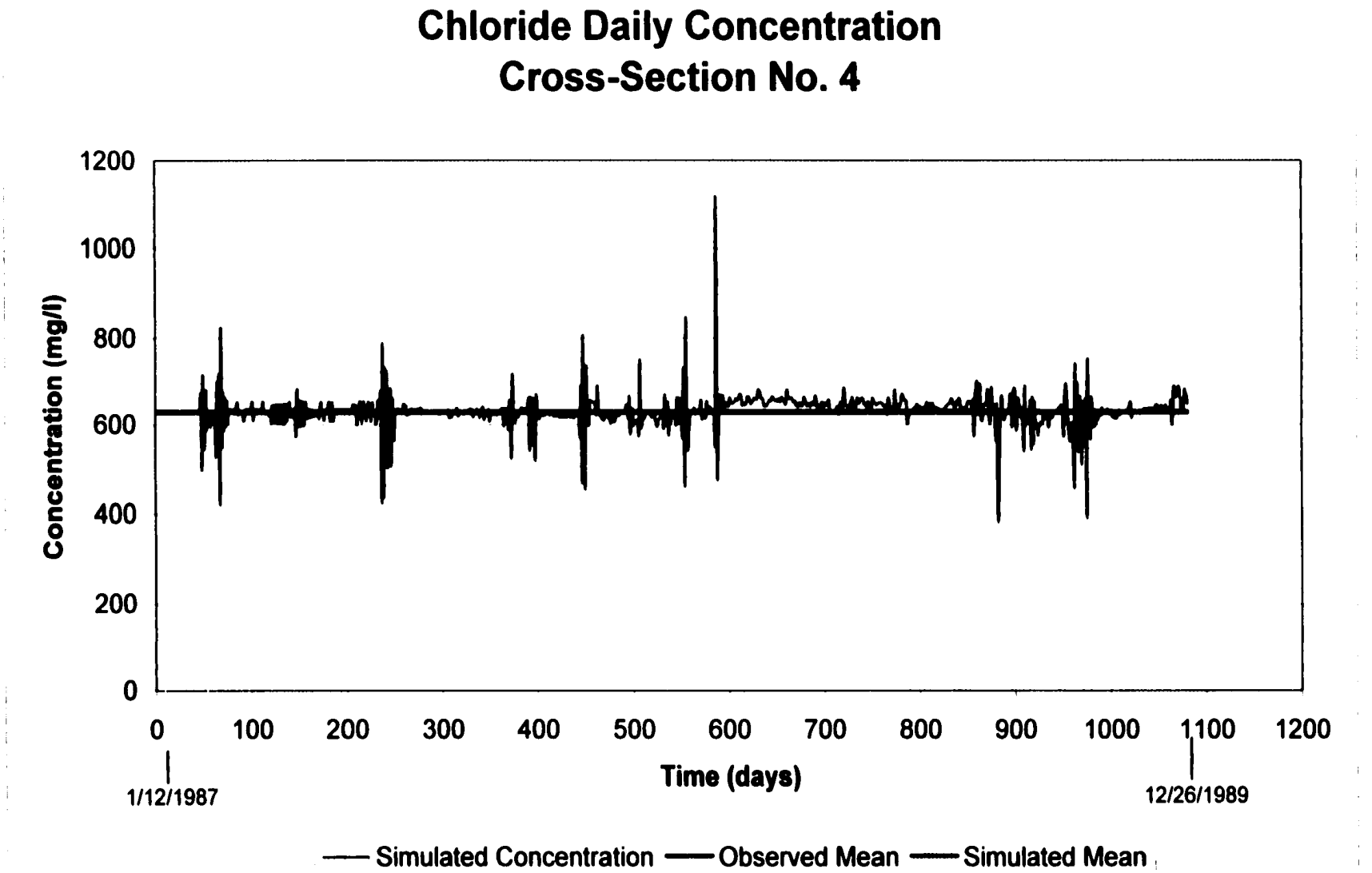


Figure 6.30 Chloride concentration in stream cross-section No. 4 versus time.

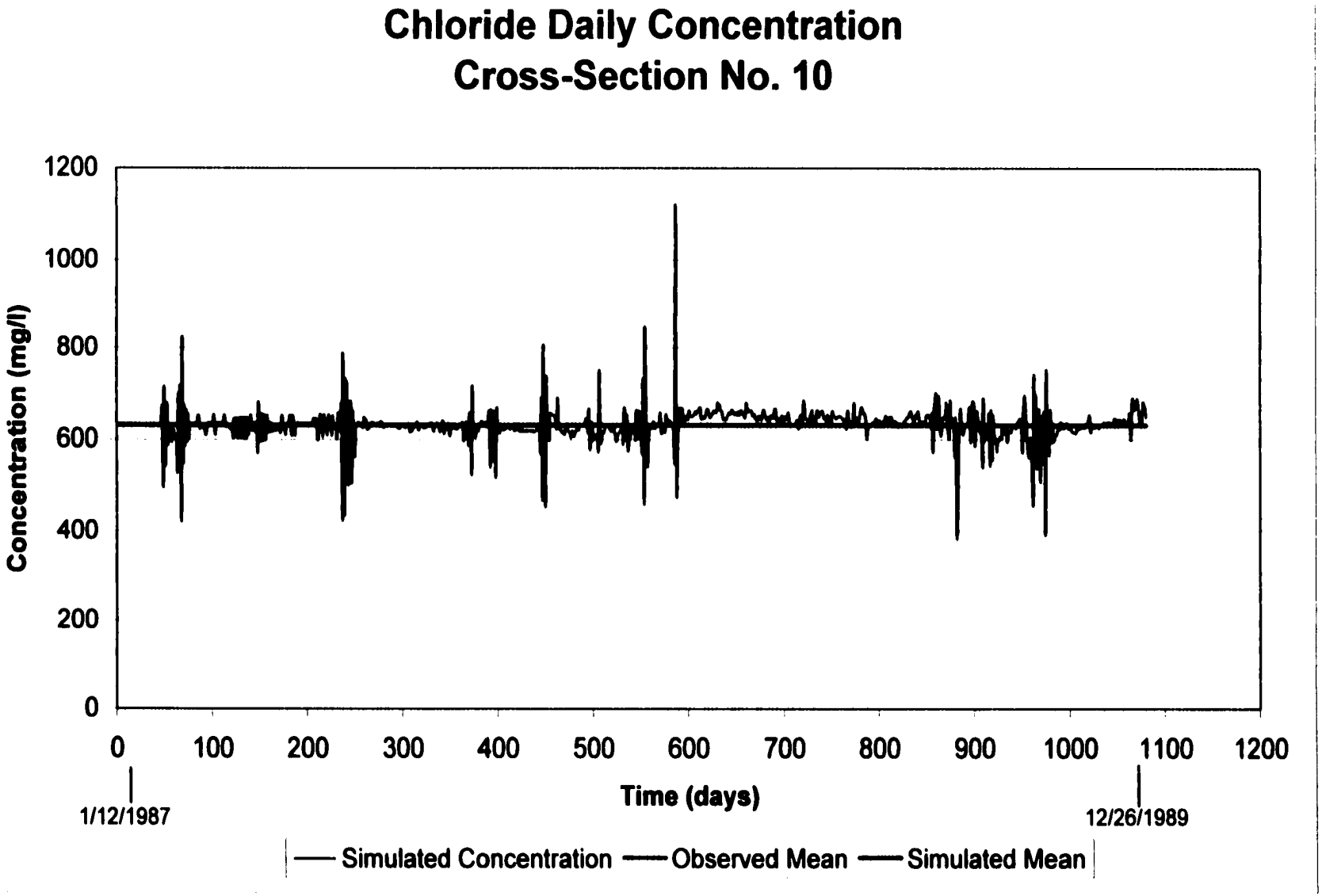


Figure 6.31 Chloride concentration in stream cross-section No. 10 versus time.

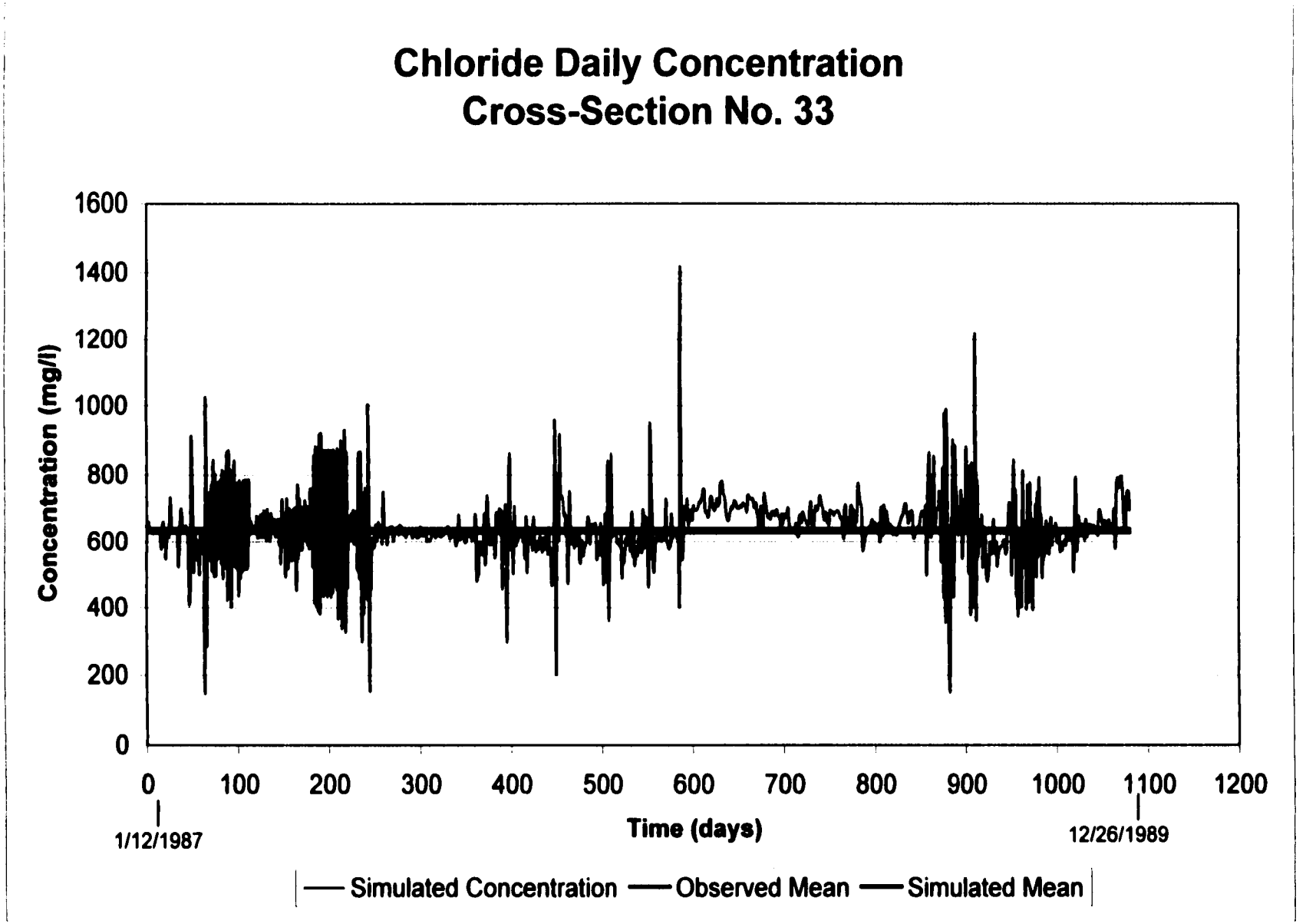


Figure 6.32 Chloride concentration in stream cross-section No. 33 versus time.

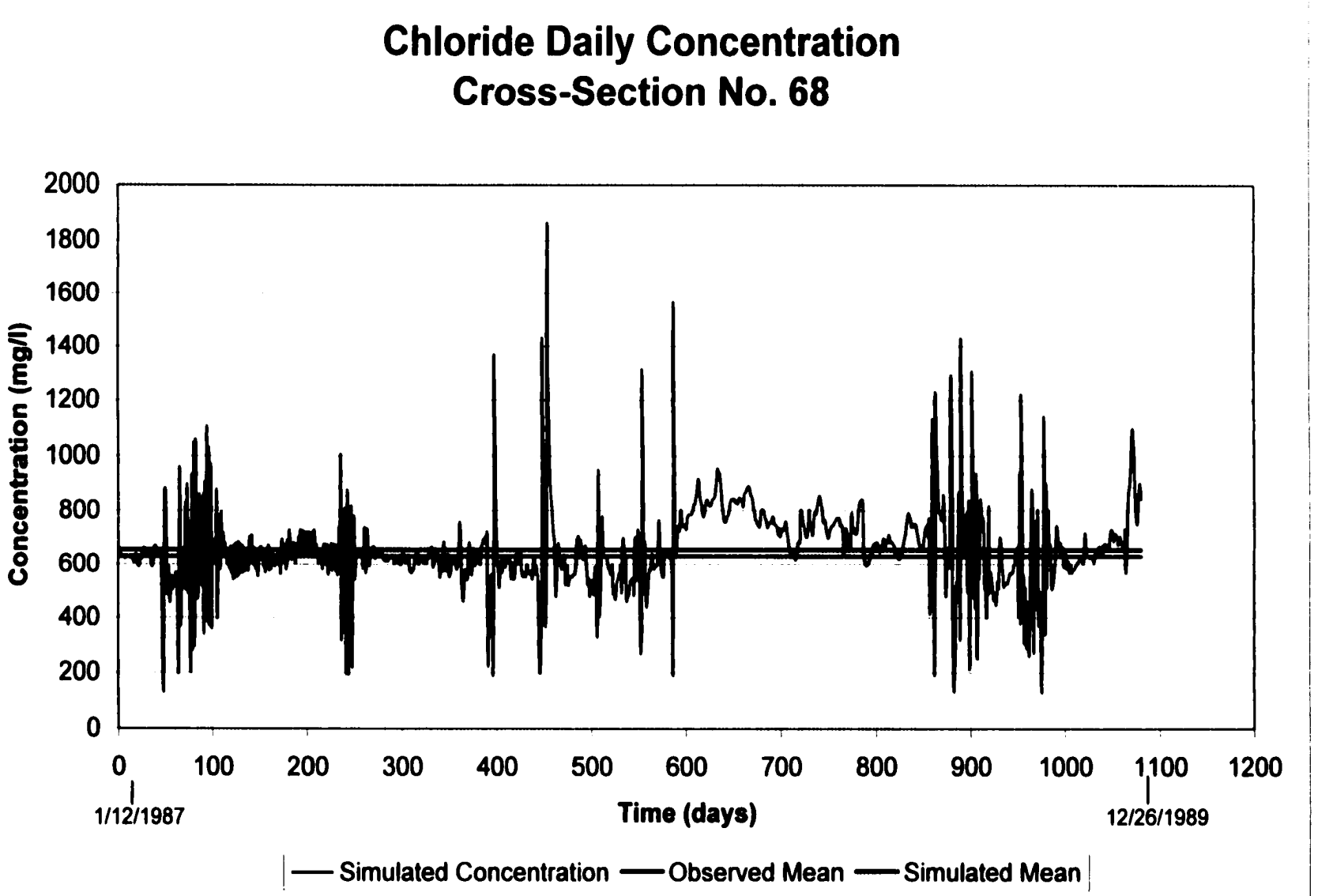


Figure 6.33 Chloride concentration in stream cross-section No. 68 versus time.

values in downstream boundary were less than streamflow values of upstream boundary for most of simulation time. Tables 6.3 and 6.4 shows the available chloride measurements at Hutchinson and Maize gaging stations during 1989 and simulated chloride concentrations at several stream cross-sections close to these stations.

The source of errors in chloride concentration values are mainly due to the non-availability of chloride concentration values at the boundaries with a short time step like every day. The lack of sufficient boundaries could be another source of error. The assumption of average concentration at the boundaries for the whole simulation period might overestimate values of concentration.

Table 6.3 Observed and simulated chloride concentration in Arkansas River near Hutchinson

Date	Time step	Observed Concentration mg/l	Simulated Concentration Cross Section No. 10 mg/l	Simulated Concentration Cross Section No. 4 mg/l
02/24/89	55	650	640	622
03/24/89	83	663	634	622
05/17/89	137	550	600	571
07/31/89	212	518	593	615
08/30/89	242	480	463	580
09/26/89	269	663	626	621
11/01/89	305	643	627	625
11/21/89	325	630	635	629

Table 6.4 Observed and simulated chloride concentration in Arkansas River near Maize.

Date	Time step	Concentration mg/l	Concentration Cross Section No. 68 mg/l	Concentration Cross Section No. 74 mg/l
02/13/89	44	650	710	744
03/23/89	82	650	670	690
05/09/89	129	680	644	683
08/24/89	236	300	322	302
09/25/89	268	590	595	603

6.4 Sensitivity Analysis

The sensitivity analysis is performed to characterize the dynamics of solute interchange between the Arkansas River and the Equus Beds Aquifer during the selected simulation time. Tow simulations are performed. The first simulation referred to as Simulation No.1, is performed to check the change of chloride concentration in the simulated channel resulted from increasing the initial chloride concentration in the aquifer upper model layer 5 times. The second simulation referred to as Simulation No. 2, is performed to check the chloride change in the aquifer resulted from increasing the chloride concentration in the stream 5 times.

6.4.1 Sensitivity Analysis Simulation No. 1

The values of chloride initial concentration in the aquifer upper model layer at the beginning of 1987 are increased 5 times as shown in Fig. 6.34. The model is executed with this increase for a

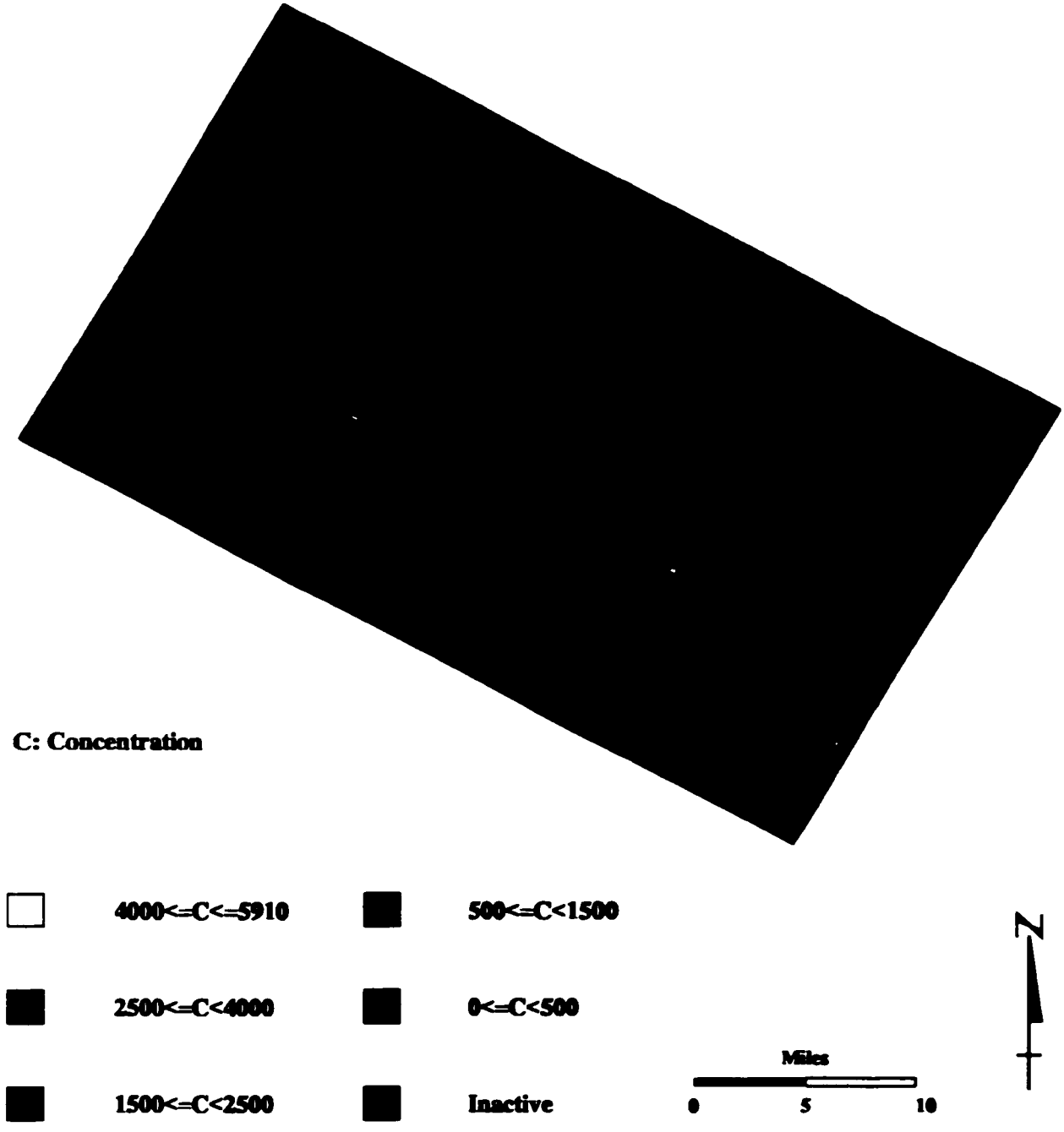


Figure 6.34 Concentration of chloride in the upper model layer at the beginning of year 1987 using Simulation No. 1.

simulation time of 1080 days from 1/12/1987 to 12/26/1989. The increase in chloride in the Arkansas River is tested by checking the increase in stream cross-section No. 33 located in branch No. 7 and stream cross-section No. 68 located in branch No. 13. Locations of both cross-sections are shown in Fig 6.13. The increase in chloride concentration in stream cross-sections No. 33 and stream cross-section No. 68 is shown in Fig. 6.35 and Fig. 6.36 respectively. The percentage increase in chloride concentration for cross-sections No. 33 and No. 68 is shown in Fig. 6.37 and Fig. 6.38 respectively. The secondary y-axis of Fig. 6.37 and Fig. 6.38 shows the simulated chloride concentration in the river versus time. Table 6.5 lists cross-section No. and several statistical parameters of the percentage of chloride increase corresponding to that cross-section.

Table 6.5 Statistical parameters for percentage of chloride increase in the cross-sections No. 33 and No. 68.

Cross section No.	Mean	Standard Deviation	Maximum	Minimum
33	1.46%	2.72%	24.64%	0.003%
68	3.2%	4.32%	40.75%	0.04%

6.4.2 Sensitivity Analysis Simulation No. 2

The values of chloride concentration in the simulated reach of the river are increased 5 times. This is implemented by setting values of chloride concentration at the upstream and downstream boundaries of the simulated channel to 3150 mg/l. The model is executed with this increase for a simulation time of 1080 days from 1/12/1987 to 12/26/1989. The increase in chloride in the aquifer is tested by checking the increase in chloride final concentration in the aquifer upper model layer.

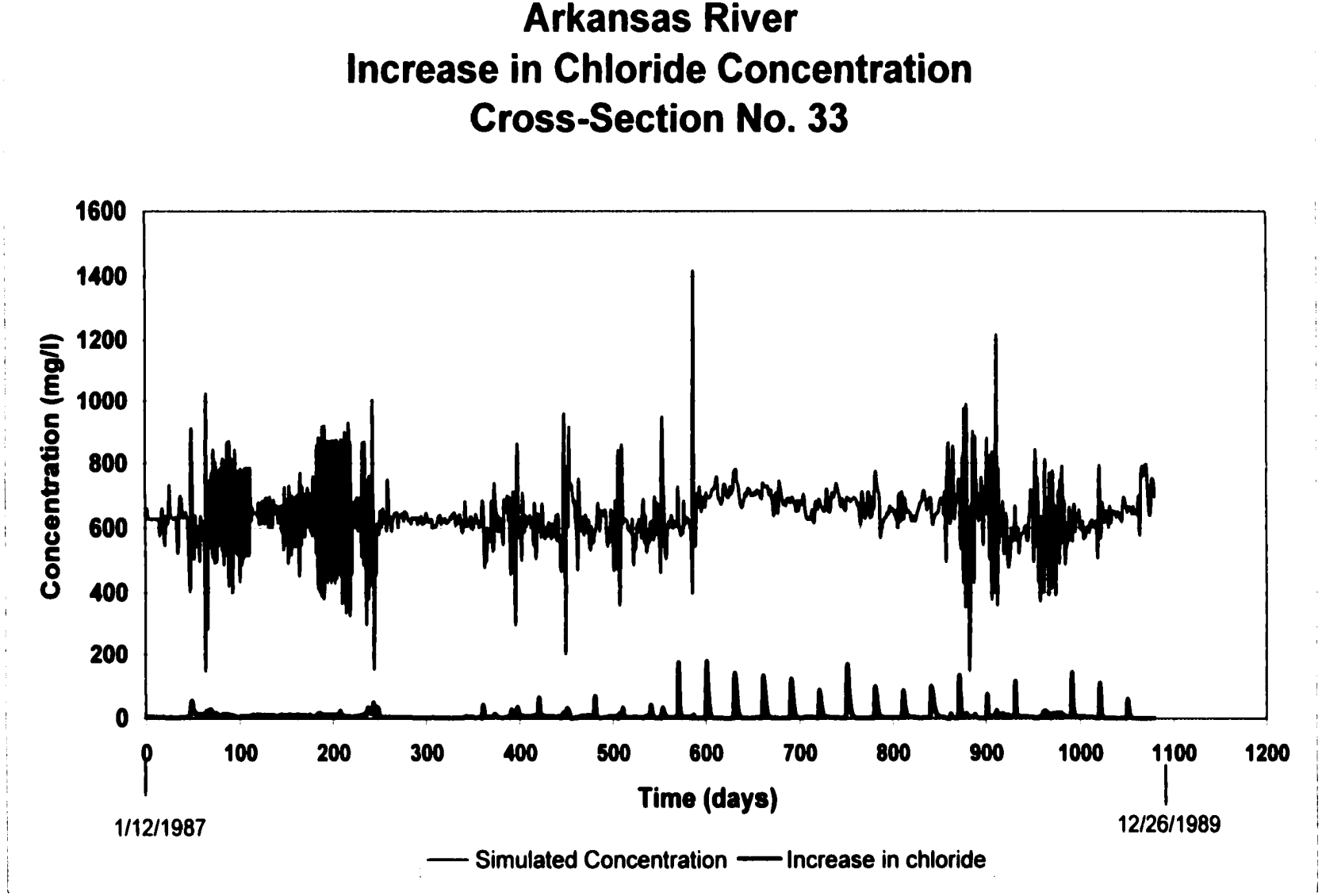


Figure 6.35 Increase in chloride concentration in stream cross-section No. 33 for Simulation No. 1.

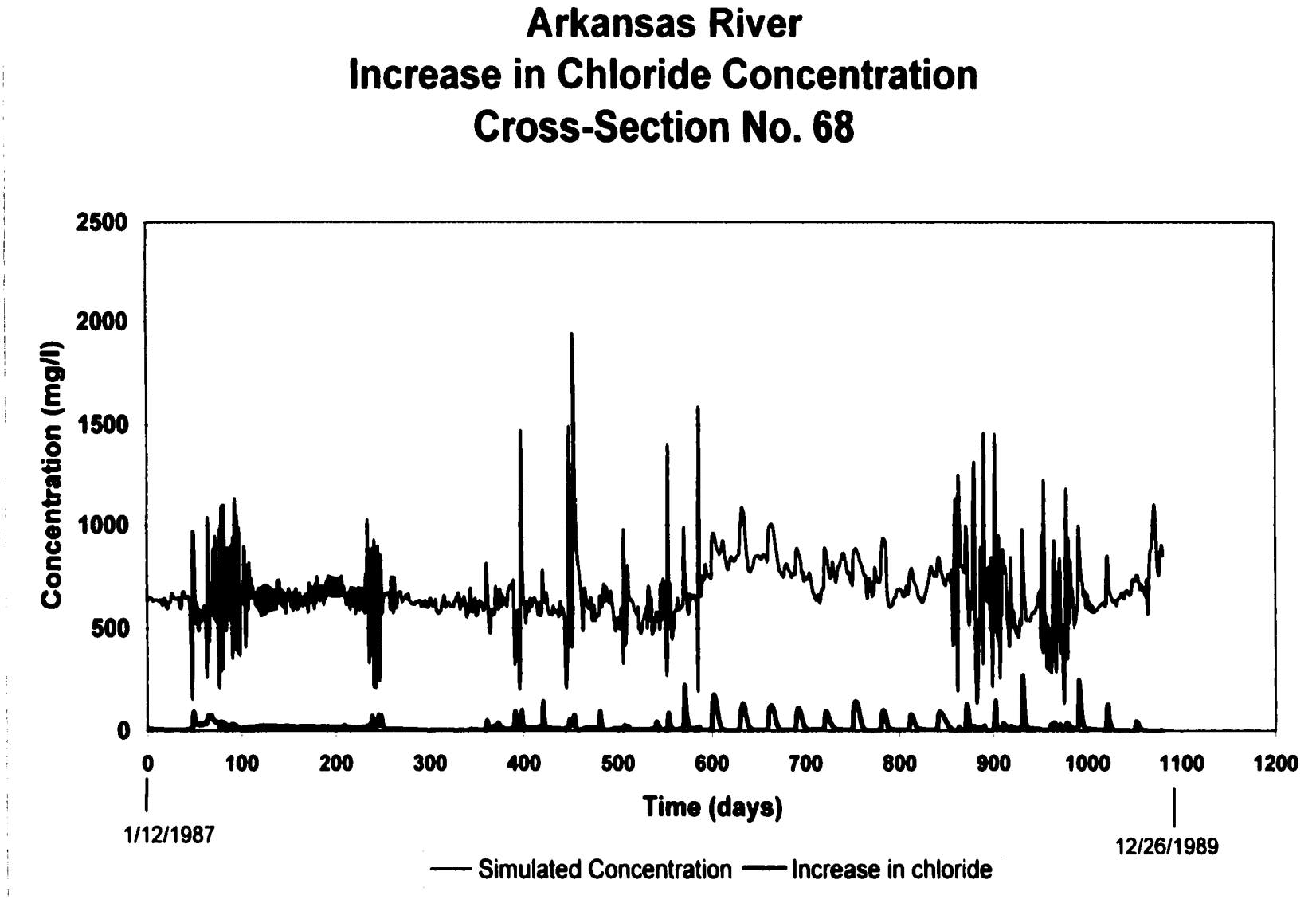


Figure 6.36 Increase in chloride concentration in stream cross-section No. 68 for Simulation No. 1.

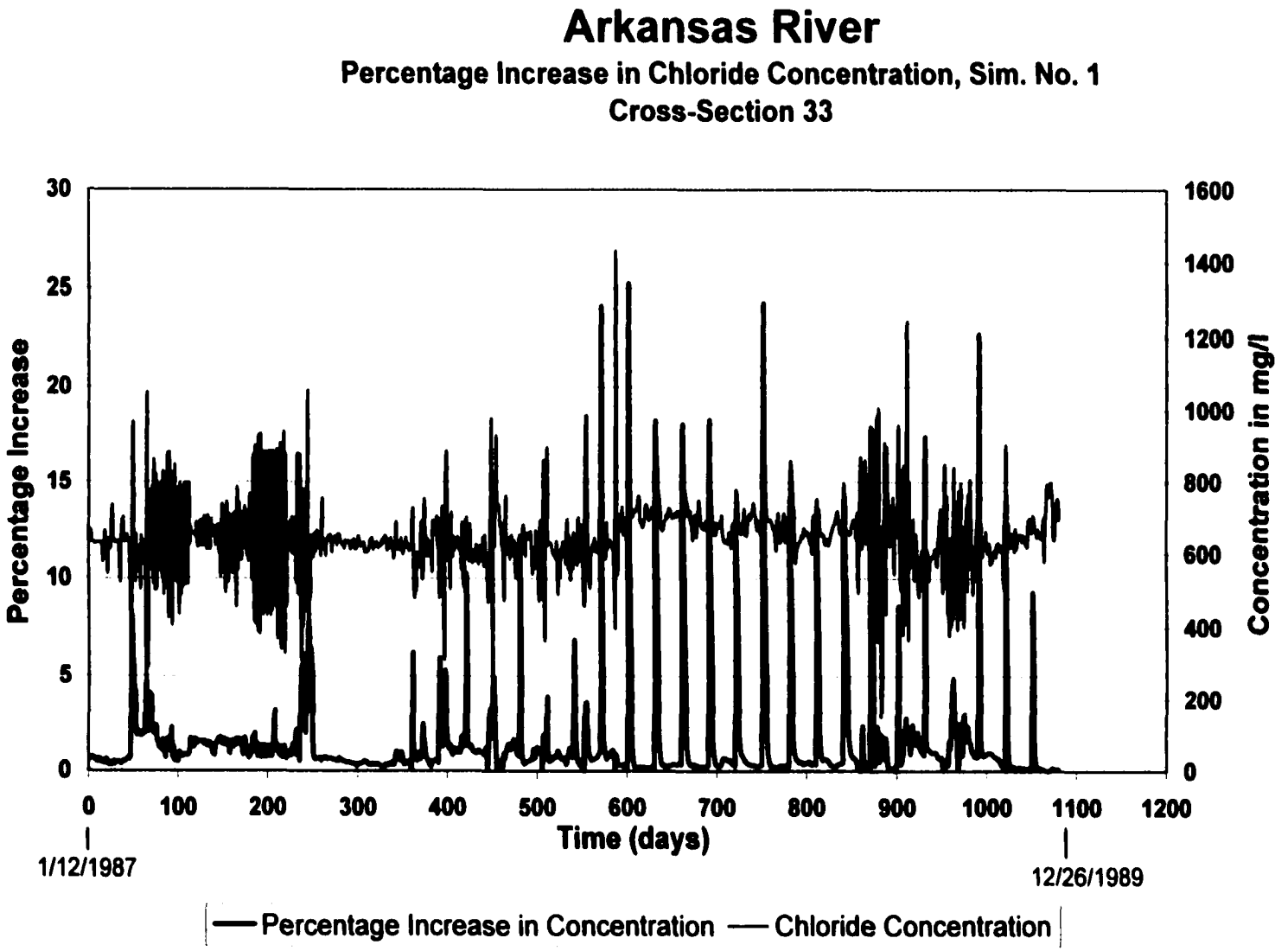


Figure 6.37 Percentage increase in chloride concentration in stream cross-section No. 33 for Simulation No. 1.

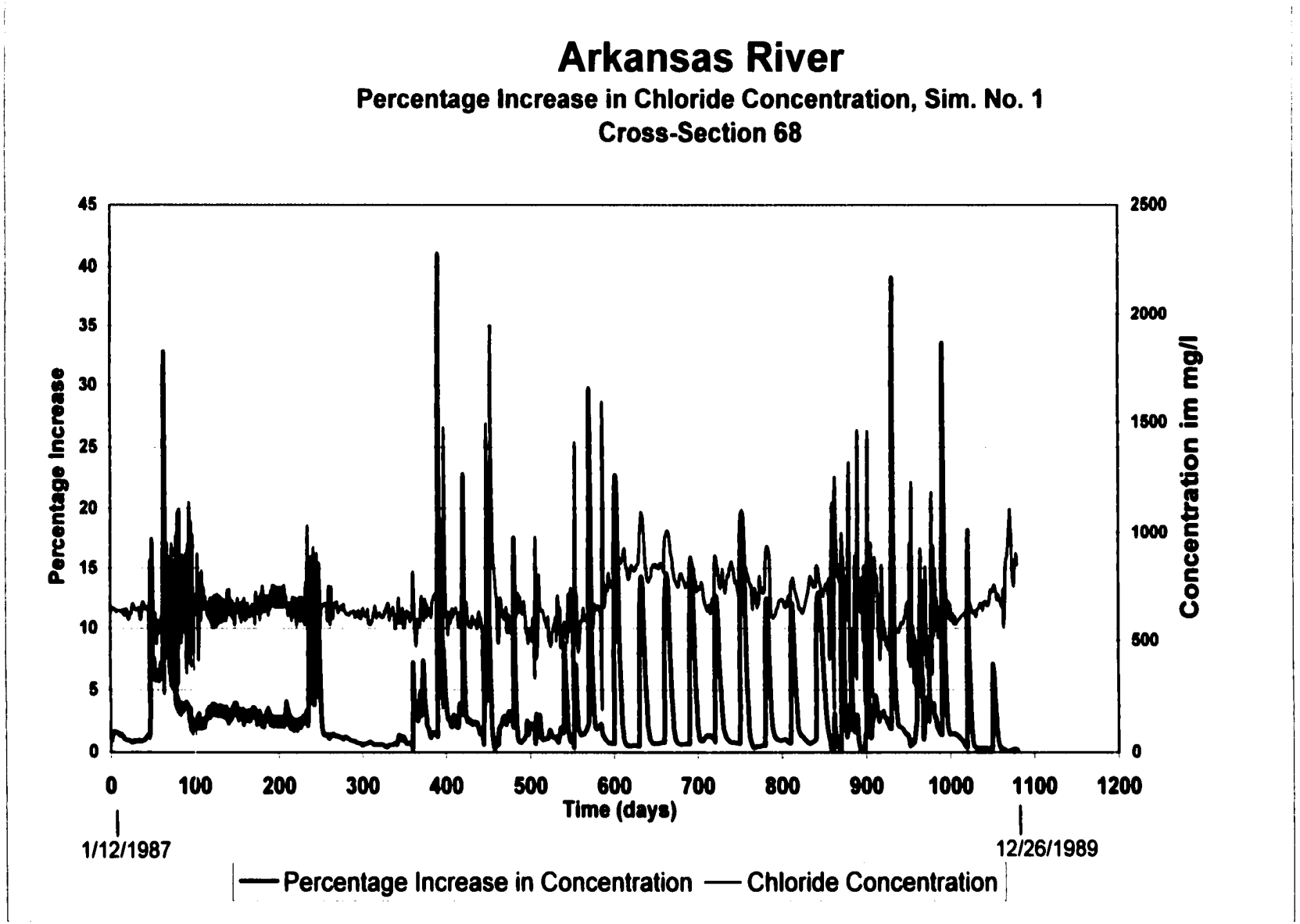


Figure 6.38 Percentage increase in chloride concentration in stream cross-section No. 68 for Simulation No. 1.

Figure 6.39 represents the percentage difference between final chloride concentration in the upper model layer produced by Simulation No. 2 and the chloride concentration produced using the Basic Simulation (Fig. 6.25). Table 6.6 lists the number of cells for each category defined in Fig. 6.39.

Table 6.6 Number of cells for each category defined in Figure 6.39.

Category	Number of grid cells
Inactive concentration cells	559
PCD= 0%	3212
150%≤ PCD ≤249.5%	8
100%≤ PCD <150%	24
50%≤ PCD <100%	50
40%≤ PCD <50%	24
30%≤ PCD <40%	24
20%≤ PCD <30%	46
10%≤ PCD <20%	77
5%≤ PCD <10%	80
0%< PCD <5%	432

Total number of cells that show a percentage increase greater than zero and less than or equal to 249.5% are 765 cells. These cells are located in the vicinity of the simulated channel. The mean percentage of the increase is 15.33% and its standard deviation is 31.75%. From comparing the results of Simulation No. 2 with those of Simulation No. 1, the mean percentage of chloride increase

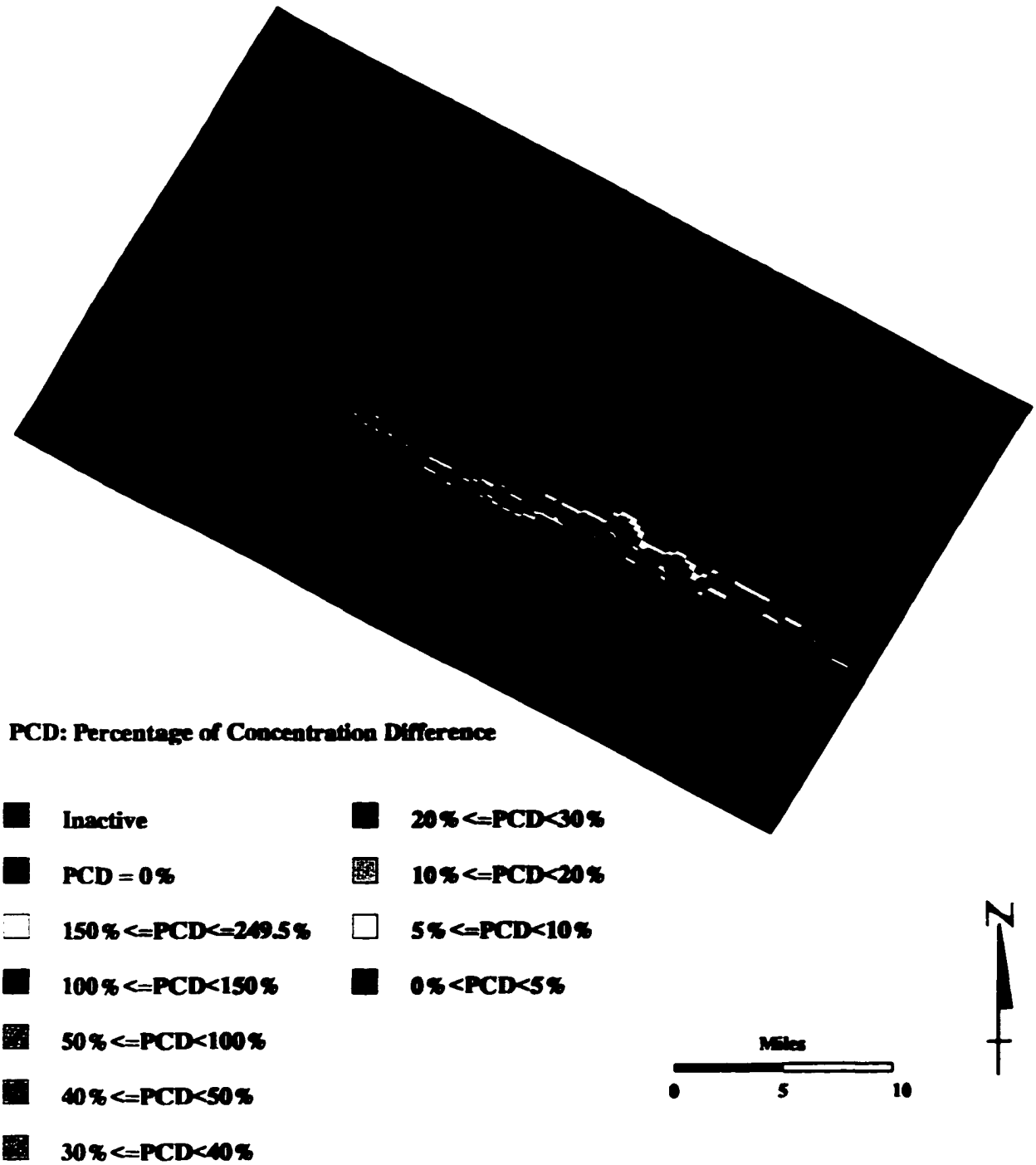


Figure 6.39 Percentage increase in chloride concentration in the upper model layer at the end of year 1989 for Simulation No. 2.

in the aquifer is 15.33% while the mean percentage of chloride increase in the rive is 1.46% for cross-section No. 33 and 3.2% for cross-section No. 68. It is obvious that increasing concentration in the stream channel has more significant effect on the concentration in the aquifer than the effect of increasing concentration in the aquifer has on the concentration in the stream.

Chapter Seven

CONCLUSIONS

7.1 Conclusions

The conclusion that are drawn from this study are :

1. A model for simulating solute transport in a stream-aquifer system is developed. The model is referred to as : Model for Stream-Aquifer Solute Transport or MSAST. The MSAST is developed by coupling four primary models: The groundwater flow model, MODFLOW-96, the coupled groundwater surface water model, MODBRANCH 3.7, the aquifer solute transport model, MT3D 1.11, and a fourth model developed in this study referred to as Stream Solute Transport Model or SSTM 1.0.

2. The Stream Solute Transport Model or the SSTM is developed in this study as a secondary model of the primary model, the MSAST. It is used for the simulation of solute transport in the stream. It is coded based on the one-dimensional solute transport equation in the stream. This equation accounts for solute concentration variation in the stream due to advection, dispersion, and interchange of solute with the aquifer. This equation is solved using finite difference method. The Stream Solute Transport Model is coded having modular structure similar to MODFLOW and MT3D. The modular structure usually consists of a main program for basic tasks and secondary programs for simulating specific processes.

3. Link or interface packages are added to integrate MODFLOW, MT3D, MODBRANCH and SSTM to form the MSAST. Two interface packages are developed in this study. The first package

is the SSTMLINK which is added to MODBRANCH. This package creates an interface file that saves the hydraulic solution of MODBRANCH . This interface file is used by the Stream Solute Transport Model, SSTM. The other package is the Stream Solute Package (SSL1). This package is added to MT3D model. The SSL1 Package calls the SSTM for each transport step in MT3D to get the concentration of solute in the stream segments contained in aquifer cells considered in simulation.

4. The model developed in this study (MSAST) is used to simulate chloride transport in the stream-aquifer system of the Arkansas River and the Equus Beds Aquifer in south-central Kansas. Previous modeling of the aquifer was conducted by the Bureau of Reclamation. MODFLOW and MT3D models were applied to examine groundwater flow and chloride transport in the aquifer. The stream-aquifer flow interaction was simulated using the STREAM Package (Prudic, 1989). The transport of chloride between the Arkansas River and the Equus Beds Aquifer was simulate using MT3D and its secondary package, the Sink/Source Mixing Package (SSM1). The concentration of chloride in the Arkansas River was assumed constant over MT3D stress period. The value of chloride concentration in the Arkansas River was estimated from several disperse measurements in the river.

The MSAST is applied using part of the data set of MODFLOW and MT3D used in the Bureau of Reclamation application. Instead, the stream aquifer interaction is simulated using the BRC2 of Package of MODFLOW and MODBRANCH. An output of this application is an interface file produced by SSTMLINK Package that is used by the SSTM. The interaction of chloride between the Arkansas River and the Equus Beds Aquifer is simulated using the SSL1 Package and the SSTM. The SSL1 Package is developed in this study as a package of MT3D that simulates variable

concentration in a stream connected to an aquifer. The SSTM simulated the transport of chloride in the Arkansas River. The SSTM interfaced with MODBRANCH and used the file created by SSTMLINK Package. The SSTM application requires initial and boundary value of concentration. These values are not available for short time intervals in the study area. The boundary and initial concentration values are approximated to be equal to the value used in the Bureau of Reclamation application.

The simulation is conducted for 1080 days. The results showed that the concentration values of the aquifer cells located in the vicinity of the simulated channel are generally decreased. The chloride concentration in several stream cross-sections is plotted versus time. The simulated means of chloride concentration in the river are close to the observed mean. Sensitivity analysis showed that increasing concentration in the stream channel has more significant effect on the concentration in the aquifer than the effect of increasing concentration in the aquifer has on the concentration in the stream.

Chapter Eight

RECOMMENDATIONS

8.1 Recommendations

1. Efforts should be made to obtain more comprehensive data for future application of this model. The application of the model requires data sets for MODLOW, MT3D, MODBRANCH and SSTM. Having measurements of solute concentrations in the river for several locations and for every short time step intervals (a day or less) will be a good situation to apply the model.

2- Several packages have been added to MODFLOW to simulate specific hydrologic processes. As experienced in this study, the BRC2 Package and MODBRANCH were incorporated in MODFLOW to simulate dynamic connected stream-aquifer system. This development is used in this study to develop a comprehensive model that simulate solute transport in a stream-aquifer system. Recently a Reservoir Package was introduced to MODFLOW-96 (Fenske et al., 1997). A similar study could be undertaken to simulate solute transport in a reservoir-aquifer system.

3- MT3D can simulate reactive transport (non-conservative) using its Chemical Reaction Package (RCT1). The chloride is considered a conservative solute in the MSAST application in this study. The SSTM deals with conservative solute transport in the stream. In a situation of reactive solute transport in a stream-aquifer system, a new package needs to be added to the SSTM to deal with sorption of solute with streambed sediments.

7.3 Recommended Uses of the Model

In general, the model can be used as a water quality analysis tool in a stream-aquifer system. Water quality models for groundwater considers contaminants distribution in the aquifer. Water quality models for surface water deals with the pollution of water in rivers and streams. Contaminated aquifers that discharge to stream can result in contamination of surface water. Conversely, streams can be a major source of contamination to aquifers. The MSAST is a model that can be used to simulate and analyze water quality in a stream-aquifer system. In the application presented in this study, chloride concentration is simulated in the stream-aquifer system of Arkansas River and Equus Beds Aquifer. The distribution of chloride in the stream temporally and spatially were simulated and analyzed. Another use of the model could be in a situation where a contaminated aquifer is connected to a stream. If surface water of the stream is used for irrigation downstream and it is required to estimate downstream level of solute like chloride to make sure that it is not too high to affect irrigation activities.

Environmental tracers are dissolved constituents that are used to track movement of water in a stream-aquifer system. In situation of complex system with several stresses like pumping wells and recharge, it is possible to test the role of these tracers using the MSAST model.

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Appendix A

Description and Listing of Model Code

Modification to MODFLOW Code:

The MODFLOW code utilized is MODFLOW-96. The source code for MODFLOW-96 could be downloaded from the Internet site address: *http://water.usgs.gov/software/modflow-96.html*. Several modification of the modflow code are done to link to Stream Solute Transport Model, SSTM, these modifications are:

1. At the beginning of main modflow code file "modflw96.f", The following variables are declared through line 37-41:

```
REAL PERSS(10)
INTEGER NSTPP1(10)
INTEGER KRAT, NTSAQ1
INTEGER NRATTMM(40)
COMMON /INITIAL/NPER,PERSS, NSTPP1,NRATTMM,KRAT
```

2. The length of stress period array, PERSS , and the number of time steps in each stress period NSTPP1, are stored at line 233 of "modflw96.f", for this, the following lines are added:

```
PERSS(KPER) = PERLEN
NSTPP1(KPER) = NSTP
WRITE (*,*) 'PERLEN =',PERSS(KPER)
WRITE (*,*) ' NSTP  =',  NSTPP1(KPER)
```

3. The of ratio of MODFLOW time steps to MODBRANCH time step is set in variable array NRATTMM(KRAT), for this in line 354 of "modflw96.f", the following lines are added:

```
NRATTMM(KRAT) = NTSAQ1
WRITE (*,*) 'NTSAQ1 =' ,NRATTMM(KRAT)
```

4. In line 357 of file "modflw96.f" subroutine SSTMINIT is called:

```
CALL SSTMINIT
```

5. In line 452 of file "modflw96.f" subroutine MODFLWTIME is called:

```
CALL MODFLWTIME
```

6. The LKM package is the code developed by Zheng (1990) to interface MT3D with

MODFLOW-88. This package is added to MODFLOW-96 main file "modflw96.f". To do that, the following modification are introduced:

A. In line 38 declare the following integer variables

```
      INTEGER IMT3D, IUSTR
```

B. Starting line 46 declare

```
      DATA CUNIT/'BCF ','WEL ','DRN ','RIV ','EVT ','TLK ','GHB ',
     1     'RCH ','SIP ','DE4 ','SOR ','OC  ','PCG ','GFD ',
     2     '    ','HFB ','RES ','STR ','IBS ','CHD ','FHB ',
     3     '    ','    ','    ','    ','    ','    ','    ',
     4     '    ','LKM ','    ','    ','    ','    ','    ',
     5     '    ','    ','    ','    ','    '/
```

C. Starting line 417 add the following code:

```
      IMT3D=IUNIT(30)
      IUSTR=IUNIT(18)
      IF(IMT3D.EQ.0) GO TO 9999
      CALL BAS1MT(X(LCHNEW),X(LCIBOU),
     2NCOL,NROW,NLAY,KKSTP,KKPER,X(LCBUFF),IMT3D)
      IF(IUNIT(1).GT.0) CALL BCF1MT(X(LCHNEW),X(LCIBOU),X(LCCR),
     1X(LCCC),X(LCCV),X(LCTOP),NCOL,NROW,NLAY,KKSTP,KKPER,
     3X(LCBUFF),IMT3D)
      IF(IUNIT(2).GT.0) CALL WEL1MT(NWELLS,MXWELL,
     1X(LCWELL),X(LCIBOU),NCOL,NROW,NLAY,KKSTP,KKPER,IMT3D)
      IF(IUNIT(3).GT.0) CALL DRN1MT(NDRAIN,MXDRN,
     1X(LCDRAI),X(LCHNEW),NCOL,NROW,NLAY,X(LCIBOU),KKSTP,
     2KKPER,IMT3D)
      IF(IUNIT(8).GT.0) CALL RCH1MT(NRCHOP,X(LCIRCH),X(LCRECH),
     1X(LCIBOU),NROW,NCOL,NLAY,KKSTP,KKPER,X(LCBUFF),IMT3D)
      IF(IUNIT(5).GT.0) CALL EVT1MT(NEVTOP,X(LCIEVT),X(LCEVTR),
     1X(LCEXDP),X(LCSURF),X(LCIBOU),X(LCHNEW),NCOL,NROW,NLAY,
     2KKSTP,KKPER,X(LCBUFF),IMT3D)
      IF(IUNIT(4).GT.0)CALLRIV1MT(NRIVER,MXRIVR,X(LCRIVR),
     1X(LCIBOU), X(LCHNEW),NCOL,NROW,NLAY,KKSTP,KKPER,IMT3D)
      IF(IUNIT(7).GT.0) CALL GHB1MT(NBOUND,MXBND,
      IF(IUNIT(4).EQ.0.AND.IUSTR.GT.0)CALLSTR1MT(NSTREM,X(LCSTRM),
     &X(ICSTRM),X(LCIBOU),MXSTRM,NCOL,NROW,NLAY,KKSTP,KKPER,IMT3D)
      IF(IUNIT(4).GT.0.AND.IUSTR.GT.0) THEN
      WRITE(IOUT,9997)
      STOP
      ENDIF
9997  FORMAT(/1X,'STOP.  RIV1 AND STR1 PACKAGES CANNOT BE USED',
     &' CONCURRENTLY IN MT3D SIMULATION')
```

7. In MODFLOW-96 secondary file "bas5.f" under SBAS5O subroutine the following lines are added, starting line 1470:

```
ELSE IF(LINE(ITYP1:ITYP2).EQ.'LKM') THEN
FMTARG='UNFORMATTED'
IUNIT(30)= IU
```

Modification to MODBRANCH Code

The MODBRANCH version used is MODBRANCH 3.7. The source cod for MODBRANCH 3.7 could be downloaded from the Internet site address: *http://water.usgs.gov/software/modbrnch.html*. Several modifications to the MODBRANCH and BRC2 Package are necessary. These modifications are :

1- File "sstmlink.f" that represents the SSTMLINK Package is created. The file is linked and compiled with the rest of MODBRANCH source code. This program creates the MODBRANCH-SSTM Interface File. This file writes time steps information of each MODBRANCH and MODFLOW, MODBRANCH control variables, and result of hydraulic variables of stream network

List of "sstmlink.f" file

```
      SUBROUTINE BRNCHCGI
C Subroutine to get MODBRANCH control parameters and geometry
      INCLUDE 'comcon.cmn'
      INCLUDE 'dimens.cmn'
      INCLUDE 'branch.cmn'
      INCLUDE 'xsinit.cmn'
      COMMON /IUNITFI/lSSTFI

      WRITE (LSSTFI, 906) NSTEPS
      WRITE  (LSSTFI,910) NBCH, NJNC, NBND
      XSKT(1) = MAXS
```

List of "sstmlink.f" file - continued

```
      DO 800 I = 1, NBCH
      J=0
      WRITE (LSSTFI, 920) NSEC(I)
      IF (I.GT.1) XSKT(I) = XSKT(I-1) - NSEC(I-1)
      NS = NSEC(I)
       IJ = MAXS - XSKT(I)
      DO 700  J = 1, NS
      IJ = IJ + 1
      WRITE (LSSTFI, 930) DX(IJ),ISTRM(3,IJ), ISTRM(2,IJ),  &
      ISTRM(1,IJ)
700   CONTINUE
800   CONTINUE
      RETURN
906   FORMAT (I4)
910   FORMAT (3I2)
920   FORMAT (I2)
930   FORMAT (F10.4,3I3)
      END

      SUBROUTINE SSTMINIT
C This subroutine writes number of stress periods and the length
C of each stress period to a file
      REAL PERSS(10)
      INTEGER NSTPP1(10)
      INTEGER NRATTMM(40)
      INTEGER NSTEPSS, NPER
      COMMON /INITIAL/NPER,PERSS, NSTPP1,NRATTMM,KRAT
      COMMON /NSTU/ NSTEPSS
      COMMON /IUNITFI/lSSTFI

      IF (KRAT .EQ. 1 ) WRITE (lSSTFI,1030)NPER
      WRITE (lSSTFI,1020)  NRATTMM(KRAT)
      RETURN
      1020 FORMAT (2I3)
      1030 FORMAT (I3)
      END

      SUBROUTINE MODFLWTIME

C This subroutine writes time length of each stress period and
C its corresponding time steps to the MODBRANCHSSTM
C interface file

      REAL PERSS(10)
      INTEGER NSTPP1(10)
      INTEGER NRATTMM(40)
      INTEGER NSTEPSS, NPER
```

List of "sstmlink.f" file - continued

```
      COMMON /INITIAL/NPER,PERSS, NSTPP1,NRATTMM,KRAT
      COMMON /NSTU/ NSTEPSS
      COMMON /IUNITFI/lSSTF

      DO 300 KPER=1,NPER
      WRITE(lSSTFI,1050) PERSS(KPER), NSTPP1(KPER)
300   CONTINUE
      RETURN
1050  FORMAT (F10.2, I3)
      END

      SUBROUTINE BRANCHFLO

C   THIS SUBROUTINE OUTPUTS FLOW COMPUTATION RESULTS
C   TO MODBRANCH-SSTM INTERFACE FILE THAT WILL BE USED IN SSTM
      INCLUDE 'dimens.cmn'
      INCLUDE 'dtcomp.cmn'
      INCLUDE 'datime.cmn'
      INCLUDE 'branch.cmn'
      INCLUDE 'comcon.cmn'
      INCLUDE 'untmes.cmn'
      INCLUDE 'convt.cmn'
      INCLUDE 'lunums.cmn'
      INCLUDE 'modbrn.cmn'
      INCLUDE 'xsinit.cmn'
      COMMON /IUNITFI/lSSTF
      INTEGER lSSTFI, I, NS, IJ, J
      REAL ZBIJ,ZIJ, QIJ,AIJ,BIJ,BSIJ,ZBOTIJ,
     &QLIJ,DXIJ, VIJ, HYDEP,TIMEEL

C   ---OUTPUT FLOW RESULTS AT EACH TIME STEP
      TIMEEL =  (M-1)*DT
      WRITE (LSSTFI,2005)KYR, KMO, KDA, KHR, KMN,M,DT,TIMEEL
      DO 20 I = 1, NBCH
      NS = NSEC(I)
      IJ = MAXS - XSKT(I)
      DO 10 J = 1, NS
      IJ = IJ + 1
      ZBIJ= Z(IJ)
      ZIJ = Z(IJ) + ZDATUM
      QIJ = Q(IJ)
      AIJ = A(IJ)
      BIJ = B(IJ)
      BSIJ = BT(IJ) - B(IJ)
      ZBOTIJ = ZBOT(IJ)
      QLIJ = QLSUM(IJ)
      DXIJ = DX(IJ)
      IF (IUNIT.NE.OUNIT) THEN
```

List of "sstmlink.f" file - continued

```
C---CONVERT FROM ENGLISH TO METRIC OR FROM METRIC TO ENGLISH
      ZBIJ =  Z(IJ)*ZCONVT
      ZIJ = ZIJ*ZCONVT
      QIJ = QIJ*QCONVT
      AIJ = AIJ*ACONVT
      BIJ = BIJ*ZCONVT
      BSIJ = BSIJ*ZCONVT
      ZBOTIJ = ZBOTIJ*ZCONVT
      ENDIF
      IF (AIJ.NE.0.0) THEN
      VIJ = QIJ/AIJ
      ELSE
      VIJ = 0.0
      ENDIF
      IF (BIJ.NE.0.0) THEN
      HYDEP = AIJ/BIJ
      ELSE
      HYDEP = 0.0
      ENDIF
      WRITE (LSSTFI,2013)I,J,QIJ, AIJ, BIJ,QLIJ,DXIJ,VIJ,HYDEP
10    CONTINUE
20    CONTINUE
      RETURN
C---OUTPUT FORMAT STATEMENTS
2005 FORMAT (I3.2,'/',I2.2,'/',I2.2,I3.2,':',I2.2,2X,I3,F10.2,\
    &F15.2)
2013 FORMAT (I3,I3,7F10.2)
      END
```

2-In file "brc2.f" that represents the BRC2 Package, the following variable are declared starting from line 38:

```
      REAL PERSS(10)
      INTEGER NSTPP1(10)
      INTEGER NRATTMM(40)
      INTEGER NSTEPSS
      COMMON /INITIAL/PERSS, NSTPP1,NRATTMM
      COMMON /NSTU/ NSTEPSS
      COMMON /IUNITFI/lSSTFI
      INTEGER I, J, K, L, IJ, NS, IBCH, LSSTM,LSSTFI
      INTEGER NPER
      CHARACTER STTMFLN*80
```

3- line 346 of brinit.f that represent BRINIT subroutine in MOBBRANCH the following code lines are added:

```
 WRITE (*,*) 'CREATE LINK FILE TO SSTM, ENTER 1 FOR YES, 0
&FOR NO'
 READ (*,*)LSSTM
 IF (LSSTM .EQ. 1) THEN
 WRITE (*,*) 'ENTER FILE NAME'
 READ(*,'(A80)')STTMFLN
 LSSTFI = 175
 OPEN (UNIT=LSSTFI, FILE = STTMFLN
 END IF
```

4- In file "brc2.f" in BRC2RP subroutine, add the following line:

```
CALL BRANCHCGI
```

5- In file "solver.f" that represents SOLVER subroutine in MODBRANCH , after code line 170 add:

```
IF (Otfile.EQ.3) CALL BRANCHFLO
```

Table A1 List of variables appeared in MODFLOW-MODBRANCH modifications

Variable	Definition
PERSS	dimensional array of length of stress period
NSTPP1	dimensional array of number of time steps in stress period
NTSAQ1	ratio of MODFLOW time step to MODBRANCH time step
KRAT	NTSAQ1 counter
NRATTMM	dimensional array of ratio of time step between MODFLOW and MODBRANCH
PERLEN	length of stress period in MODFLOW
KPER	stress period counter
NSTP	number of modflow time steps in each stress period
IMT3D	MODFLOW-MT3D interface flag, if # 0 interface file created, otherwise not
IUSTR	index to save leakage of STREAM Package to MODFLOW-MT3D interface file, if > 0, save, otherwise not.
NBCH	number of branches in network
NJNC	number of junctions both internal and external
NBND	number of open boundaries
NSEC	number of cross sections input
MXBH	maximum number of branches in network
MAXS	maximum number of cross sections in network
DX	cross section length

Table A - continued

Variable	Definition
ISTRM	layer, column and row of aquifer model cell that corresponds to the channel cross-section
NSTEPS	number of time steps in MODBRANCH
LSSTFI	unit number on which MODBRANCH-SSTM output is written
KYR	saved value of year
KMO	saved value of month
KDA	saved value of day
KHR	saved value of hour
M	time step number in MODBRANCH
DT	Length of time step of MODBRANCH in seconds
TIMEEL	time elapsed since beginning of simulation in seconds
I	branch number
IJ	cross section number
Q	discharge in stream cross section
A	area of stream cross section
B	width of stream cross section
Q	leakage from stream cross section to or from the aquifer
V	velocity in stream cross section
HYDEP	mean depth in stream cross section
ZBOT	elevation of streamed
NROW	number of model rows
NCOL	number of model columns
NLAY	number of model layers
ZDATUM	elevation of MODBRANCH datum

Modification to MT3D code

The MT3D code used is version 1.11 developed by Zheng (1990). MT3D source code could be downloaded from the Internet site : ***http://www.epa.gov/ada/mt3d.html.*** MT3D code is composed of main file and secondary files. File "mt3d.f" represents the main file. Several modifications are taken to link this file to SSTM, These modifications are:

1. At the beginning of "mt3d.f" file the following variables are declared by adding the following code lines:

```
INTEGER ISEGMNS
REAL DTS
LOGICAL*4 TRNOPS(10)
INTEGER ICBND
REAL CONINT,SLOPESC
REAL CSOLD,CSNEW
DIMENSION ICBND(MAXS),CONINT(MAXS),SLOPESC(MAXS),CSNEW(MAXS)
DIMENSION CSOLD(MAXS)
```

2. In the process of read and prepare for the several packages, read and prepare for Stream Solute Transport Package is executed through calling subroutine SSL1RP, the following code is added in lines 197 and 198:

```
 IF(TRNOP(7)) CALL SSL1RP(NCOL,NROW,NLAY,DTS,ISEGMNS,TRNOPS,
&ICBND,CONINT,SLOPESC)
```

3. When solving the transport equation, subroutine SSL1SV is called after calling DSP1SV subroutine. This is accomplished by adding lines 305-308:

```
 IF (TRNOP(7)) CALL
 SSL1SV(MNN,NCOL,NROW,NLAY,IX(LCIB),X(LCH),
&X(LCPR),X(LCDELR),X(LCDELC),X(LCCOLD),MXSS,NTSS,NSS,X(LCSS),
&DTS,ISEGMNS,TRNOPS,ICBND,CONINT,SLOPESC,CSNEW,CSOLD)
```

4. Package SSL1 that link MT3D to SSTM is added as a secondary file like other secondary files of

MT3D. This package is represented by the file "ssl1.f". The code list of "ssl1.f" is shown below.

Listing of file "ssl1.f"

```
      SUBROUTINE SSL1RP(NCOL,NROW,NLAY,DT,ISEGMNS,TRNOPS,ICBND,
     &CONINT,SLOPESC)
      PARAMETER (MAXS = 200)
      PARAMETER (MAXTSTP = 400)
      IMPLICIT NONE
      INTEGER*4 NCOL,NROW,NLAY
      INTEGER IQ
      REAL QLCONC, SSR
      REAL DX, QL,A,Q,B,V,D
      REAL DT
      INTEGER ISTRM , IJUMP,
      ISEGMNS,NSTEPS,ISM,NUM,MTC,MXC,MTTC,MXXC
     &,K,I,J
      LOGICAL*4 TRNOPS(10)
      INTEGER ICBND
      REAL CONINT,SLOPESC
      DIMENSION ISTRM(3,MAXS)
      DIMENSION  DX(MAXS)
      DIMENSION QL(MAXS,MAXTSTP)
      DIMENSION SSR(6,MAXS)
      DIMENSION QLCONC(2,MAXS,MAXTSTP)
      DIMENSION Q(MAXS,MAXTSTP),A(MAXS,MAXTSTP),
     &B(MAXS,MAXTSTP),V(MAXS,MAXTSTP),D(MAXS,MAXTSTP)
      DIMENSION ICBND(MAXS),CONINT(MAXS),SLOPESC(MAXS)
      COMMON /REST/ DX,QL,Q,A,B,V,D,ISTRM
      COMMON /SSRS/ SSR, QLCONC
C     QLCONC LEAKAGE CONCENTRATION ARRAY IN TIME
           IJUMP = 0
      IQ = 4
      CALL SSTM(IJUMP,ISEGMNS,NSTEPS,ISM,DT,TRNOPS,ICBND,CONINT,
     &SLOPESC)
      DO 250 NUM=1,ISEGMNS
      SSR(1,NUM) = ISTRM(3,NUM)
      SSR(2,NUM) = ISTRM(2,NUM)
      SSR(3,NUM) = ISTRM(1,NUM)
      SSR(6,NUM) = IQ
      250  CONTINUE
      DO 270 MTC  = 1, ISM-1
      DO 290 MXC = 1,ISEGMNS
      QLCONC(1,MXC,MTC) = QL(MXC,MTC+1)
      QLCONC(2,MXC,MTC) = 630.
      290CONTINUE
      270   CONTINUE
      WRITE (*,*) 'SSTM OUTPUT '
      DO 350  MTTC = 1,ISM-1
      DO 300 MXXC=1,ISEGMNS
      K=SSR(1,MXXC)
```

Listing of file "ssl1.f" - continued I

```
      I=SSR(2,MXXC)
      J=SSR(3,MXXC)
300   CONTINUE
350   CONTINUE
      RETURN
      END

      SUBROUTINE SSL1SV (MNN,NCOL,NROW,NLAY,ICBUND,H,PRSITY,DELR,
     &DELC,COLD,
     &MXSS,NTSS,NSS,SS,DT,ISEGMNS,TRNOPS,ICBND,CONINT,SLOPESC,
     &CSNEW,CSOLD)
      PARAMETER (MAXS = 200)
      PARAMETER (MAXTSTP = 400)
      PARAMETER (INADVS = 26)
      IMPLICIT NONE
      INTEGER*4 NCOL,NROW,NLAY,MXSS,NTSS,NSS
      INTEGER ISEGMNS, MNN
      INTEGER K,I,J,IQ
      INTEGER KSSM,ISSM,JSSM
      INTEGER*4 ICBUND
      REAL CTMP, QSS
      REAL*4 SS,TM
      REAL SSR,DTSSM
      REAL TFCTR
      REAL*4     H,DELR,DELC,VOLAQU,PRSITY
      REAL QLCONC
      INTEGER MXXC , NUM,IJUMP,NSTEPS,ISM
      INTEGER ICBND
      REAL ST,ST1,ST2,DT,CONINT,CSOLD,SLOPESC,CSNEW
      LOGICAL*4 TRNOPS(10)
      INTEGER ISTRM
      REAL DX,QL,Q,A,B,V,D
      REAL*4 COLD
      DIMENSION SS(6,MXSS)
      DIMENSION SSR(6,MAXS)
      DIMENSION QLCONC(2,MAXS,MAXTSTP)
      DIMENSION ICBUND(NCOL,NROW,NLAY),H(NCOL,NROW,NLAY)
      DIMENSION DELR(NCOL),DELC(NROW),PRSITY(NCOL,NROW,NLAY)
      DIMENSION ISTRM(3,MAXS)
      DIMENSION  DX(MAXS)
      DIMENSION QL(MAXS,MAXTSTP)
      DIMENSION Q(MAXS,MAXTSTP),A(MAXS,MAXTSTP),
     &B(MAXS,MAXTSTP),V(MAXS,MAXTSTP),D(MAXS,MAXTSTP)
      DIMENSION CONINT (MAXS)
      DIMENSION CSOLD (MAXS)
      DIMENSION CSNEW (MAXS)
      DIMENSION SLOPESC(MAXS)
      DIMENSION ICBND(MAXS)
      DIMENSION COLD(NCOL,NROW,NLAY)
```

Listing of file "ssl1.f" - continued

```
      COMMON /REST/ DX,QL,Q,A,B,V,D,ISTRM
      COMMON /SSRS/ SSR, QLCONC
C TFCTR IS INTRODUCED TO CONVERT LEAKAGE TIME UNIT
      DO 600 MXXC=1,ISEGMNS
      K=SSR(1,MXXC)
      I=SSR(2,MXXC)
      J=SSR(3,MXXC)
      SS(1,MXXC)= SSR(1,MXXC)
      K = SS(1,MXXC)
      SS(2,MXXC) = SSR(2,MXXC)
      I = SS(2,MXXC)
      SS(3,MXXC) = SSR(3,MXXC)
      J= SS(3,MXXC)
      SS(4,MXXC) = QLCONC(2,MXXC,MNN)
      SS(5,MXXC) = QLCONC(1,MXXC,MNN)
      600   CONTINUE
      ST = 0.
      ST1=0.
      ST2=0.
      CALL BSC1AD(ST1,ST2,DT,ISEGMNS,CONINT,CSOLD,MNN,CSNEW)
      IF (TRNOPS(1))  CALL
      ADS1SV(INADVS,ST1,ST2,DT,NSTEPS,ISEGMNS,
     &ICBND,CONINT,SLOPESC,CSOLD,MNN,COLD,NCOL,NROW,NLAY,CSNEW)
96    FORMAT (I3,2F10.2)
      TFCTR = 86400.0
C DIVIDE BY AQUIFER VOLUME
C TO GET FLUXES OF SINKS/SOURCES PER UNIT AQUIFER VOLUME.
C--ALSO DETERMINE STEPSIZE WHICH MEETS STABILITY CRITERION
C--FOR SOLVING THE SINK/SOURCE TERM
      DTSSM=1.E30
      DO 610 NUM=1,ISEGMNS
      K=SS(1,NUM)
      I=SS(2,NUM)
      J=SS(3,NUM)
      VOLAQU=DELR(J)*DELC(I)*H(J,I,K)
      IF(ICBUND(J,I,K).EQ.0.OR.VOLAQU.LE.0) THEN
      SS(5,NUM)=0
      ELSE
      SS(5,NUM)=SS(5,NUM)*TFCTR/VOLAQU
      ENDIF
      IF(SS(5,NUM).LE.0 .OR. ICBUND(J,I,K).LT.0) GOTO 610
      TM=PRSITY(J,I,K)/SS(5,NUM)
      IF(ABS(TM).LT.DTSSM) THEN
      DTSSM=ABS(TM)
      KSSM=K
      ISSM=I
      JSSM=J
      ENDIF
610   CONTINUE
```

Listing of file "ssl1.f" - continued

```
      DO 70 NUM=1,NTSS
      K=SS(1,NUM)
      I=SS(2,NUM)
      J=SS(3,NUM)
      CTMP=SS(4,NUM)
      QSS=SS(5,NUM)
      IQ=SS(6,NUM)
70    CONTINUE
      WRITE (*,*) 'INSIDE SSL1SV ,ACCUMULATED TRANSPORT STEP  = ',
     &MNN
      RETURN
      END
```

Development of SSTM

The SSTM version 1.0 code is written in a similar structure to MODFLOW-96, MODBRANCH 3.7 and MT3D 1.1. The code is designed with a main program that performs primary tasks and secondary programs that simulate specific processes. The structure of the SSTM is explained in Chapter 5. The files of the SSTM are sstm.f, mbn1.f, bsc1.f, ads1.f, dds1.f, and utls.f. The 'sstm.f' represents the main program, mbn1.f and bsc1.f represent the SSTM-MODBRANCH interface package and basic stream transport package respectively. ads1.f and dds1.f represent advection and dispersion packages. utls.f is the utility package and is similar to the utility package in MT3D. The code of sstm.f, mbn1.f, bsc1.f, ads1.f, and dds1.f are listed below.

List of file "sstm.f" file

```
C*****************************************************************
C   MAIN CODE FOR STREAM SOLUTE TRANSPORT MODEL (SSTM)
C
C
C
C                              BY HASHEM FAIDI
C
C
C
C
C
C
C
C                              CIVIL ENGINEERING DEPARTMENT
C
C                              COLORADDO STATE UNIVERSITY
C
C                              FORT COLLINS, CO 80523
C
C      THIS MODEL IS DEVELOPED TO SIMULATE THE TRANSPORT OF
C      SOLUTE IN THE STREAM AND THE INTERCHANGE OF SOLUTE BETWEEN
C      THE STREAM AND THE AQUIFER. THIS MODEL IS PART OF THE
C      MODEL FOR STREAM-AQUIFER SOLUTE TRANSPORT (MSAST) WHICH
C      SIMULATES THE SOLUTE TRANSPORT IN A STREAM-AQUIFER
C      SYSTEM. OTHER PARTS OF THE MSAST ARE MODFLOW96, MT3D V1.1
C      AND MODBRANCH 3.7. ALL THESE MODELS ARE CONNECTED TO form
C      THE MSAST.
C
C*****************************************************************

      SUBROUTINE SSTM(IJUMP,ISEGMNS,NSTEPS,ISM,DT,TRNOPS,ICBND,
     &CONINT,SLOPESC)
      PARAMETER (LENXS=00700000,LENIXS=000700000)
      PARAMETER (INBTNS=25,INADVS=26,INDSPS=27,INSAIS=28)
      PARAMETER (IOUTS=36)
      PARAMETER (MAXS=200)
      PARAMETER (MAXTSTP = 400)
      IMPLICIT NONE
      INTEGER*4 ISUMS,ISUMS2,NCOL,NROW,NLAY,NPER,
     &ISTATS
      REAL  XS
      LOGICAL*4 TRNOPS(10)
      CHARACTER TUNITS*4,LUNITS*4,MUNITS*4,
     &FINDEXS*30, FLNAMES*50
      INTEGER ISEGMNS ,NSTEPS,I
      REAL DT, ST,ST1,ST2,CSOLD
      INTEGER IJUMP, J,IXS
      INTEGER ISTRM
      REAL DX, QL,A,Q,B,V,D
```

Listing of file "sstm.f" - continued

```
      INTEGER ISM
      REAL CONINT,SLOPESC
      INTEGER ICBND
      INTEGER N
      DIMENSION ISTRM(3,MAXS)
      DIMENSION DX(MAXS)
      DIMENSION QL(MAXS,MAXTSTP)
      DIMENSION A(MAXS,MAXTSTP),Q(MAXS,MAXTSTP),
     &B(MAXS,MAXTSTP),V(MAXS,MAXTSTP),D(MAXS,MAXTSTP)
      DIMENSION ICBND(MAXS), CONINT(MAXS),SLOPESC(MAXS)
      DIMENSION CSOLD(MAXS)
      COMMON /REST/ DX,QL,Q,A,B,V,D,ISTRM

C DEFINE PROBLEM DIMENSION AND SIMULATION OPTIONS
C INBTNS IS THE UNIT NUMBER FOR BASIC TRANSPORT
C INSAIS IS THE UNIT NUMBER FOR MODBRANCH OUTPUT
C INADVS IS THE UNIT NUMBER FOR ADVECTION
C INDSPS IS THE UNIT NUMBER FOR DISPERSION
C IOUTS  IS THE UNIT NUMBER FOR STANDARD OUTPUT FILE
C IJUMP IS A FLAG SO THAT WHEN SSTM IS CALLED IT WILL NOT OPEN
C FILES EACH TIME
      IF(IJUMP .NE. 0) GO TO 1000
C--WRITE AN IDENTIFIER TO SCREEN
      WRITE(*,101)
101   FORMAT(//,1X,'SSTM  - STREAM SOLUTE TRANSPORT MODEL  '
     &/1X,'(C) HASHEM FAIDI, COLORADO STATE UNIVERSITY  '/)
C--OPEN STANDARD OUTPUT AND BASIC INPUT FILES
      FINDEXS='STANDARD OUTPUT FILE: '
      ISTATS=0
      CALL OPENFLS(IOUTS,ISTATS,FLNAMES,0,FINDEXS)
      FINDEXS='BASIC TRANSPORT INPUT FILE: '
      ISTATS=1
      CALL OPENFLS(INBTNS,ISTATS,FLNAMES,0,FINDEXS)
      FINDEXS='MODBRANCH OUPUT FILE : '
      ISTATS=1
      CALL OPENFLS(INSAIS,ISTATS,FLNAMES,0,FINDEXS)
C-- WRITE PROGRAM TITLE TO OUTPUT FILE
      WRITE(IOUTS,11)
11    FORMAT(/30X,71('+')/30X,'+',69X,'+'
     &/30X,'+',40X,'S S T M ',21X,'+'
     &/30X,'+',25X,'A STREAM SOLUTE TRANSPORT MODEL',
     &13X,'+'
     &/30X,'+', 20X,'FOR SIMULATION OF ADVECTION, DISPERSION',
     &/10X,'+'
     &/30X,'+',20X, 'OF SOLUTE IN THE STREAM AND INTERCHANGE
     &',10X,'+'
     &/30X,'+',20X,'OF SOLUTE WITH THE AQUIFER ',22X,'+'
     &/30X,'+',30X,'(V.1.1)',31X,'+'/30X,'+',69X,'+'/30X,71('+')/)
```

Listing of file "sstm.f" - continued

```
      CALL BSC1DF(INBTNS,IOUTS,ISUMS,ISUMS2,NCOL,NROW,NLAY,NPER,
     &NSTEPS,ISEGMNS,TRNOPS,TUNITS,LUNITS,MUNITS)
      CALL MODBR(INSAIS,IOUTS,ISEGMNS,NSTEPS,ISM,DT)
 C--OPEN INPUT FILES FOR THE VARIOUS TRANSPORT OPTIONS
      IF(TRNOPS(1)) THEN
       FINDEXS='ADVECTION INPUT FILE: '
       ISTATS=1
       CALL OPENFLS(INADVS,ISTATS,FLNAMES,0,FINDEXS)
      ENDIF
      IF(TRNOPS(2)) THEN
      FINDEXS='DISPERSION INPUT FILE: '
      ISTATS=1
       CALL OPENFLS(INDSPS,ISTATS,FLNAMES,0,FINDEXS)
       ENDIF
      CALL BSC1AL(INBTNS,IOUTS,ISUMS,ISUMS2)
      IF(TRNOPS(1)) CALL ADS1AL
      IF(TRNOPS(2)) CALL DSS1AL
      READ AND PREPARE DATA RELEVANT TO THE ENTIRE SIMULATION
      CALL BSC1RP(INBTNS,IOUTS,ISEGMNS,ICBND,CONINT)
      IF(TRNOPS(1)) CALL ADS1RP
      IF(TRNOPS(2)) CALL DSS1RP(INDSPS,IOUTS,ISEGMNS,SLOPESC)
C--FOR EACH STREAM TIME STEP
1000    IJUMP = 1
      IF (IJUMP .EQ. 1 ) GO TO 2000
      WRITE (*,*) 'DT ',DT
      ST = 0.
      ST1=0.
      ST2=0.
      DO 500 N=1,1
C--ADVANCE ONE TRANSPORT STEP
CALL BSC1AD (ST1,ST2,DT,ISEGMNS,CONINT,CSOLD,N)
C--FORMULATE AND SOLVE
      CALL BSC1SV
      IF (TRNOPS(1))   CALL
      ADS1SV(INADVS,ST1,ST2,DT,NSTEPS,ISEGMNS,
     &ICBND,CONINT,SLOPESC,CSOLD,N)
IF    (TRNOPS(2))   CALL DSS1SV
500   CONTINUE
2000  RETURN
      END
```

Listing of file "mbn1.f"

```
C SUBROUTINE TO READ OUTPUT FILE OF MODBRANCH AND USE THAT IN
C SSTM THE OUTPUT FILE INCLUDE THE STREAM GEOMETRY AND HYDRAULIC
C SOLUTION PRODUCED BY MODBRANCH

      SUBROUTINE MBN1RP (INSAIS,IOUTS,ISEGMNS,NSTEPS,ISM,DT)
      PARAMETER (MAXTSTP = 400)
      PARAMETER (MXBH = 50,MAXS = 200)
      IMPLICIT NONE
      CHARACTER NETNAM*80
      INTEGER INSAIS
      INTEGER IOUTS
      INTEGER KYR,KMO,KDA,KHR,KMN,M,K
      INTEGER NSTEPS
      INTEGER NPER, NTSAQ(100),NSTP
      INTEGER NBCH,NJNC,NBND
      INTEGER ISEGMNS
      REAL DT,TIMEEL
      REAL DELT,IDTM, PERLEN
      INTEGER NSEC, XSKT, ISTRM
      INTEGER IS
      REAL DX
      REAL DXI,Q,A,B,QL,V,D
      REAL QIJ, AIJ, BIJ,QLIJ,DXIJ,VIJ,HYDEP
      INTEGER I, NS, IJ, J
      INTEGER ISUM, IV
      INTEGER ISM, L, IVV
      REAL DIFF,QLDIFF
      DIMENSION IS(MAXS)
      DIMENSION NSEC(MXBH),XSKT(MXBH), ISTRM(3,MAXS)
      DIMENSION  DX(MAXS)
      DIMENSION DXI(MAXS),Q(MAXS,MAXTSTP),A(MAXS,MAXTSTP),
     &B(MAXS,MAXTSTP),
     &QL(MAXS,MAXTSTP)   ,V(MAXS,MAXTSTP),D(MAXS,MAXTSTP),
     &QLDIFF(MAXS,MAXTSTP)
      COMMON /REST/ DX,QL,Q,A,B,V,D,ISTRM
      READ (INSAIS,402)NSTEPS
      WRITE (IOUTS,403)NSTEPS
      READ (INSAIS,406) NBCH, NJNC, NBND
C  NSEC NUMBER OF CROSS SECTIONS INPUT
C  BRNAME(I) NAME OF BRANCH
C  MXBH   MAXIMUM NUMBER OF BRANCHES IN NETWORK
C  MAXS  MAXIMUM NUMBER OF CROSS SECTIONS IN NETWORK
C  DX    SEGMENT LENGTH
C  ISTRM LAYER, COLUMN AND ROW OF AQUIFER MODEL CELL THAT
C  CORRESPONDS TO THE CHANNEL SEGMENT
      XSKT(1) = MAXS
      DO 105 I = 1, NBCH
      J=0
      READ (INSAIS, 407) NSEC(I)
```

Listing of file "mbn1.f" - continued

```
      IF (I.GT.1) XSKT(I) = XSKT(I-1) - NSEC(I-1)
      NS = NSEC(I)
      IJ = MAXS - XSKT(I)
      DO 10 J = 1, NS
      IJ = IJ + 1
      READ (INSAIS,408) DX(IJ),ISTRM(3,IJ), ISTRM(2,IJ),
      ISTRM(1,IJ)
10    CONTINUE
105   CONTINUE
      READ (INSAIS,404)NPER
C I         BRANCH NUMBER
C J         SEGMENT NUMBER
C QIJ       DISCHARGE
C AIJ       AREA
C BIJ       WIDTH
C QLIJ      LEAKAGE TO AQUIFER
C DXIJ      LENGTH OF SEGMENT
C VIJ       VELOCITY
C HYDEP     MEAN DEPTH
      ISM = 1
C MSTPS NUMBER OF TIME STEPS IN ALL MODFLOW SIMULATION

      DO 120 L=1, 2
      READ (INSAIS,506)NTSAQ(L)
      WRITE (IOUTS,*) 'L = ', L
      WRITE (IOUTS,*) 'NTSAQ(L) =', NTSAQ(L)
      IVV = NTSAQ(L)
      ISM = ISM +IVV
C READ INITIAL VALUES OF HYDRAULIC SOLUTION OF MODBRANCH
      READ (INSAIS,500) KYR, KMO, KDA, KHR, KMN,M,DT,TIMEEL
      DO 106 I=1,NBCH
      NS = NSEC(I)
      IJ = MAXS - XSKT(I)
      DO 20 J = 1, NS
      IJ = IJ + 1
      READ (INSAIS,409)I,J,QIJ, AIJ, BIJ,QLIJ,DXIJ,VIJ,HYDEP
20    CONTINUE
106   CONTINUE
      DO110  K = 1 , IVV
      READ (INSAIS,500) KYR, KMO, KDA, KHR, KMN,M,DT,TIMEEL
      WRITE(IOUTS,500)KYR, KMO, KDA, KHR, KMN,M,DT,TIMEEL
      DO 107 I=1,NBCH
      NS = NSEC(I)
      IJ = MAXS - XSKT(I)
      DO 30 J = 1, NS
      IJ = IJ + 1
      READ (INSAIS,409)I,J,QIJ, AIJ, BIJ,QLIJ,DXIJ,VIJ,HYDEP
      IS (IJ) =0
      IS (IJ) = IJ
```

Listing of file "mbn1.f" - continued

```
      DXI(IJ) = 0.0
      DXI(IJ) = DXIJ
      Q(IJ,M-1) = 0.0
      Q(IJ,M-1) =  QIJ
      A(IJ,M-1) = 0.0
      A(IJ,M-1) = AIJ
      B(IJ,M-1)=0.0
      B(IJ,M-1) = BIJ
      QL(IJ,M-1)=0.0
      QL(IJ,M-1)= QLIJ
      V(IJ,M-1)=0
      V(IJ,M-1) = VIJ
      D(IJ,M-1)=0.0
      D(IJ,M-1) = HYDEP
      WRITE(IOUTS,410)I,J,IJ,QIJ, AIJ, BIJ,QLIJ,DXIJ,VIJ,HYDEP
30    CONTINUE
107   CONTINUE
110      CONTINUE
      IF (M .EQ. NSTEPS ) GO TO 109
120   CONTINUE
109   CONTINUE
C NUMBER OF SEGMENTS IN ALL BRANCHES
      ISEGMNS = IJ
C ASSIGN VALUES OF TWO DIMENSIONAL ARRAYS OF FLOW, AREA
C IN SECTION AND TIME
      DO 55 I =1,30
      DO 58 J = 1,ISEGMNS
      IF (I .EQ. 1) THEN
      DIFF = QL(J,I)
      QLDIFF (J,I) = DIFF
      ELSE
      DIFF= QL(J,I)-QL(J,I-1)
      QLDIFF (J,I) = DIFF
      ENDIF
58    CONTINUE
55         CONTINUE
      DO 45 I = 31,60
      DO 48 J = 1,ISEGMNS
      IF (I .EQ. 31) THEN
      DIFF = QL(J,I)
      QLDIFF (J,I) = DIFF
      ELSE
      DIFF = QL(J,I)-QL(J,I-1)
      QLDIFF (J,I) = DIFF
      ENDIF
48    CONTINUE
45         CONTINUE
      DO 111 I = 1,NSTEPS
      DO 101 J = 1,ISEGMNS
```

Listing of file "mbn1.f" - continued

```
      QL(J,I)=QLDIFF(J,I)
101   CONTINUE
111      CONTINUE
      DO 60 J=1,NSTEPS
      WRITE (IOUTS,416) J
      DO 50 I=1,IJ
      WRITE (IOUTS,415) IS(I),DXI(I),Q(I,J),A(I,J),B(I,J),
     &QLDIFF(I,J),V(I,J),D(I,J)
50    CONTINUE
60    CONTINUE
      RETURN
402   FORMAT (I4)
403   FORMAT('NUMBER OF MODBRANCH TIME STEPS=',I4)
404   FORMAT(I4)
406   FORMAT (3I2)
407   FORMAT (I2)
408   FORMAT (F10.4,3I3)
409   FORMAT (I3,I3,7F10.2)
410   FORMAT(3I3,7F10.2)
415   FORMAT(I3,7F10.2)
416   FORMAT (I3)
500   FORMAT (I3.2,'/',I2.2,'/',I2.2,I3.2,':',I2.2,2X,I3,F10.2,
      F15.2)
506   FORMAT (I3)
      END
```

Listing of file "bsc1.f"

```
      SUBROUTINE BSC1DF(INBTNS,IOUTS,ISUMS,ISUMS2,NCOL,NROW,NLAY,
     &NPER,TRNOPS,TUNITS,LUNITS,MUNITS)

C ***************************************************
C       THIS SUBROUTINE READS PROBLEM DIMENSIONS AND
C        TRANSPORT OPTIONS.
C***************************************************
      IMPLICIT NONE
      INTEGER*4 INBTNS,IOUTS,ISUMS,ISUMS2,NCOL,NROW,NLAY,NPER,I,
     &ITUSEDS
      LOGICAL*4 TRNOPS(10)
      CHARACTER HEADNGS(2)*80,TUNITS*4,LUNITS*4,MUNITS*4
C--READ AND PRINT HEADING
C HEADNGS(1) THE FIRST LINE OF ANY TITLE OR HEADING FOR THE
C SIMULATION RUN. THE LINE SHOULD NOT BE LONGER THAN 80
C CHARACTERS
C HEADNGS(2) IS THE SECOND LINE OF ANY TITLE OR HEADING FOR THE
C SIMULATION RUN

      READ(INBTNS,'(A80)') (HEADNGS(I),I=1,2)
```

Listing of file "bsc1.f" - continued

```
      WRITE(IOUTS,300)
      WRITE(IOUTS,301) (HEADNGS(I),I=1,2)
      WRITE(IOUTS,300)
300   FORMAT(1X,' ----- ')
301   FORMAT(1X,'| SSTM | ',A80/1X,'| 3 D | ',A80)
C  READ AND PRINT NO. OF LAYERS, ROWS, COLUMNS, AND STRESS
      READ(INBTNS,'(4I10)') NLAY,NROW,NCOL,NPER
      WRITE(IOUTS,302) NLAY,NROW,NCOL,NPER
302   FORMAT(1X,'THE STREAM TRANSPORT CONSISTS OF ',I5,'
      LAYER(S)',I5,
     &' ROW(S)',I5,' COLUMN(S)',
     &/1X,'NUMBER OF STRESS PERIOD(S) IN SIMULATION =',I5)
C--READ AND PRINT UNITS FOR TIME, LENGTH AND MASS TO BE USED
      READ(INBTNS,'(3A4)') TUNITS,LUNITS,MUNITS
      WRITE(IOUTS,303) TUNITS,LUNITS,MUNITS
303   FORMAT(1X,'UNIT FOR TIME IS ',A4,';',2X,'UNIT FOR LENGTH IS
      ',
     &A4,';',2X,'UNIT FOR MASS IS ',A4)

C TRNOPS : ARRAY CONTAINS MAJOR FLAGS FOR MAJOR TRANSPORT OPTIONS
C--READ AND PRINT MAJOR TRANSPORT OPTIONS USED IN THE SIMULATION
      ITUSEDS=3
      READ(INBTNS,'(10L2)') (TRNOPS(I),I=1,ITUSEDS)
      WRITE(IOUTS,304)
      I=0
      IF(TRNOPS(1)) THEN
      I=I+1
      WRITE(IOUTS,305) I
      ENDIF
      IF(TRNOPS(2)) THEN
      I=I+1
      WRITE(IOUTS,306) I
      ENDIF
      IF(TRNOPS(3)) THEN
      WRITE(IOUTS,'(1X)')
 304  FORMAT(1X,'MAJOR TRANSPORT COMPONENTS TO BE SIMULATED:')
 305  FORMAT(1X,I2,2X,'ADVECTION')
 306  FORMAT(1X,I2,2X,'DISPERSION')
C 307     FORMAT(1X,I2,2X,'STREAM AQUIFER INTERCHANGE')
C--INITIALIZE ARRAY POINTERS FOR ALLOCATING MEMORY
      ISUMS=1
      ISUMS2=1
       RETURN
      END
```

Listing of file "bsc1.f" - continued

```
 SUBROUTINE BSC1AL (INBTNS ,IOUTS,ISUMS,ISUMS2)

C*************************************************************************
*****
C THIS SUBROUTINE ALLOCATES SPACE FOR ARRAYS NEEDED BY THE ENTIRE
MODEL.
C*************************************************************************

      IMPLICIT NONE
      INTEGER*4 INBTNS,IOUTS,ISUMS,ISUMS2,ISOLD,ISOLD2
C--PRINT PACKAGE NAME AND VERSION NUMBER
      WRITE(IOUTS,308) INBTNS
308   FORMAT(1X,'BTN1 -- BASIC STREAM TRANSPORT PACKAGE,',
     &' VER 1.0, 1999, INPUT READ FROM UNIT',I3)
C ALLOCATE SPACE FOR ARRAYS
      ISOLD = ISUMS
      ISOLD2 = ISUMS2
      RETURN
      END

      SUBROUTINE BSC1RP (INBTNS,IOUTS,ISEGMNS,ICBND,CONINT)

C*****************************************************
C THIS SUBROUTINE READS AND PREPARES INPUT DATA RELEVANT TO THE
C ENTIRE SIMULATION
C*****************************************************
      PARAMETER (MAXS = 200)
      PARAMETER (MAXTSTP = 400)
      IMPLICIT NONE
      INTEGER ISEGMNS,INBTNS , IOUTS
      INTEGER  ICBND,I
      REAL CONINT
      DIMENSION ICBND(MAXS)
      DIMENSION CONINT (MAXS)
      CHARACTER ANAME*24
C     CALL IARRAY TO READ IN CONCENTRATION BOUNDARY ARRAY
      ANAME = 'BOUNDARY C'
      CALL IARRAYS (ICBND(1), ANAME,1,ISEGMNS,0,INBTNS,IOUTS)
C CALL RARRAY TO READ IN INITIAL CONCENTRATION IN EACH CROSS
C SECTION'
      ANAME = 'INITIAL CONCENT'
      CALL RARRAYS (CONINT(1),ANAME,1,ISEGMNS,0,INBTNS,IOUTS)
      RETURN
      END
```

Listing of file "bsc1.f" - continued

```
      SUBROUTINE BSC1AD(ST1,ST2,DT,ISEGMNS,CONINT,CSOLD,N,CSNEW)


C*********************************************************************
C THIS SUBROUTINE ADVANCES THE TRANSPORT SIMULATION ONE STEP,
C DETERMINING THE STEPSIZE TO BE USED AND WHETHER PRINTOUT IS
C REQUIRED FOR NEXT TRANSPORT STEP.
C*********************************************************************

      PARAMETER (MAXS = 200)
      IMPLICIT NONE
      REAL ST1,ST2,DT,CSOLD,CONINT,CSNEW,CSOLD1
      INTEGER ISEGMNS,I
      INTEGER N
      DIMENSION CONINT (MAXS)
      DIMENSION CSOLD (MAXS),CSOLD1(MAXS)
      DIMENSION CSNEW (MAXS)
      ST1 = ST2
      ST2=ST1+DT
      IF (N.EQ. 1 ) THEN
      DO 9 I =1,ISEGMNS
      CSOLD(I) = CONINT(I)
      CSOLD1(I) = CSOLD(I)
      CSNEW(I) = 0.0
9     CONTINUE
      ELSE
      DO 19 I =1,ISEGMNS
      CSOLD1(I) = CSOLD(I)
      CSOLD(I) = CSNEW(I)
19    CONTINUE
      ENDIF

      DO 29 I =1,ISEGMNS
      WRITE (*,*) I,CSOLD1(I),CSNEW(I)
29    CONTINUE

      WRITE (*,*) ' INSIDE BSC1AD  N= ', N
      RETURN
      END

      SUBROUTINE BSC1SV
      RETURN
      END
```

List of file "ads1.f"

```
      SUBROUTINE ADS1SV(INADVS,ST1,ST2,DT,NSTEPS,ISEGMNS,
     &ICBND,
     &CONINT,SLOPESC,CSOLD,N,CAOLD,NCOL,NROW,NLAY,CSNEW)
      PARAMETER (MAXS = 200)
      PARAMETER (MAXTSTP = 400)
      IMPLICIT NONE
      INTEGER  INADVS,NSTEPS,ISEGMNS
      REAL ST1,ST2,DT
      REAL CONINT,SLOPESC,CSOLD
      INTEGER ICBND,I,J,NUM
      INTEGER II,KK,JJ
      INTEGER ISTRM
      INTEGER N
      REAL DX, QL,A,Q,B,V,D
      REAL GRAVITY, SHEARV
      REAL E,F,G,R,DSPL
      REAL*4 CAOLD
      REAL CAQ
      REAL GW, WW
      INTEGER*4 NCOL,NROW,NLAY
      INTEGER NSEC
      REAL CSNEW
      INTEGER ICOUNTBD
      DIMENSION ICBND(MAXS)
      DIMENSION CONINT (MAXS)
      DIMENSION SLOPESC (MAXS)
      DIMENSION CSOLD (MAXS)
      DIMENSION DX(MAXS)
      DIMENSION A(MAXS,MAXTSTP),Q(MAXS,MAXTSTP),
    &B(MAXS,MAXTSTP),V(MAXS,MAXTSTP),D(MAXS,MAXTSTP)
      DIMENSION ISTRM(3,MAXS)
      DIMENSION QL(MAXS,MAXTSTP)
      DIMENSION E(MAXS), F(MAXS), G(MAXS),R(MAXS)
      DIMENSION DSPL(MAXS,MAXTSTP)
      DIMENSION CAOLD(NCOL,NROW,NLAY)
      DIMENSION CAQ(MAXS)
      DIMENSION GW(MAXS),WW(MAXS)
      DIMENSION CSNEW(MAXS)
      COMMON /REST/ DX,QL,Q,A,B,V,D,ISTRM
C ESTIMATE LONGITUDINAL DISPERSION IN THE STREAM
      GRAVITY= 32.2
      DO 240 J = 1,ISEGMNS
      IF ( D(J,N) .EQ. 0. ) D(J,N) = .0001
      SHEARV = SQRT(GRAVITY*D(J,N)*SLOPESC(J))
      DSPL(J,N) = (.011* V(J,N)**2)*(0.093*B(J,N)**2)*0.093/
     &(D(J,N)*SHEARV*.093)
240   CONTINUE

C ESTIMATE F COEFFICIENTS
```

Listing of file "ads1.f" - continued

```
C IN CASE OF INFLOW
      DO 250 J = 1,ISEGMNS
      IF (QL(J,N) .LT. 0. ) THEN
      IF (J .EQ. 1) THEN
      F(J) = 1.+ Q(J,N)*DT/(DX(J)*A(J,N))+
     &A(J,N)*DSPL(J,N)*DT/(A(J,N)*DX(J)**2.)
      ELSE
      F(J) = 1.+ Q(J,N)*DT/(DX(J)*A(J,N))+
     &A(J,N)*DSPL(J,N)*DT/(A(J,N)*DX(J)**2.) +
     &A(J-1,N)*DSPL(J-1,N)*DT/(A(J,N)*DX(J)**2.)
      END IF
C IN CASE OF OUTFLOW
      ELSE
      IF (J .EQ. 1) THEN
      F(J) = 1.+ Q(J,N)*DT/(DX(J)*A(J,N))+
    &A(J,N)*DSPL(J,N)*DT/(A(J,N)*DX(J)**2.)+QL(J,N)/(A(J,N)*DX(J))
      ELSE
      F(J) = 1.+ Q(J,N)*DT/(DX(J)*A(J,N))+
     &A(J,N)*DSPL(J,N)*DT/(A(J,N)*DX(J)**2.) +
     &A(J-1,N)*DSPL(J-1,N)*DT/(A(J,N)*DX(J)**2.)+
     &QL(J,N)/(A(J,N)*DX(J))
      ENDIF
      ENDIF
250   CONTINUE
C    ESTIMATE E COEFFICIENTS
      DO 270 J = 2, ISEGMNS
      E(J) = -Q(J-1,N)*DT/(A(J,N)*DX(J))-(A(J-1,N)*DSPL(J-1,N))
270   CONTINUE

C    ESTIMATE G COEFFICIENTS
      DO 290 J = 1,ISEGMNS
      G(J) = -A(J,N)*DSPL(J,N)*DT/(A(J,N)*DX(J)**2.)
290   CONTINUE

C   ESTIMATE R COEFFICIENTS
      DO 295 J = 1,ISEGMNS
C FIRST ESTIMATE CAQ: CONCENTRATION IN AQUIFER CELL
      KK= ISTRM(3,J)
      II= ISTRM(2,J)
      JJ= ISTRM(1,J)
      CAQ(J)= CAOLD(JJ,II,KK)
C IN CASE OF INFLOW
      IF (QL(J,N) .LT. 0. ) THEN
      QL(J,N)= -QL(J,N)
      IF (N .EQ. 1) THEN
      IF (J .EQ. 1 ) THEN
      R(J) = CSOLD(J)*A(J,N)/A(J,N)+
      CAQ(J)*QL(J,N)*DT/(A(J,N)*DX(J))
      ELSE
```

Listing of file "ads1.f" - continued

```
      R(J) = CSOLD(J)*A(J,N)/A(J,N)+
      CAQ(J)*QL(J,N)*DT/(A(J,N)*DX(J))
      ENDIF
      ELSE
      IF (J .EQ. 1 ) THEN
      R(J) = CSOLD(J)*A(J,N-1)/A(J,N)+ CAQ(J)*QL(J,N)*DT/
     &(A(J,N)*DX(J))
      ELSE
      R(J) = CSOLD(J)*A(J,N-1)/A(J,N)+ CAQ(J)*QL(J,N)*DT/
     &(A(J,N)*DX(J))
      ENDIF
      ENDIF
C IN CASE OF OUTFLOW
      ELSE
      IF (N .EQ. 1) THEN
      IF (J .EQ. 1 ) THEN
      R(J) = CSOLD(J)*A(J,N)/A(J,N)
      ELSE
      R(J) = CSOLD(J)*A(J,N)/A(J,N)
      ENDIF
      ELSE
      R(J) = CSOLD(J)*A(J,N-1)/A(J,N)
      END IF
      ENDIF
 295  CONTINUE
 C       SET BOUNDARY VALUE
      ICOUNTBD = 0
      IF (ICBND(J) .LT. 0 ) THEN
      ICOUNTBD = ICOUNTBD +1
      ENDIF
289   CONTINUE
      DO 301 J =2, ISEGMNS-1
      IF (J .EQ. 2) THEN
      WW(J) = G(J)/F(J)
      GW(J) = (R(J)-E(J)*600.)/F(J)
      ELSEIF (J .EQ. ISEGMNS-1) THEN
      GW(J) = (R(J)-E(J)*GW(J-1)-G(J-1)*600.)/(F(J)-E(J)*WW(J-1))
      WW(J) = G(J)/(F(J)-E(J)*WW(J-1))
      ELSE
      WW(J) = G(J)/(F(J)-E(J)*WW(J-1))
      GW(J) = (R(J)-E(J)*GW(J-1))/(F(J)-E(J)*WW(J-1))
      ENDIF
301   CONTINUE
      DO 310 J= 2,ISEGMNS-1
      NSEC = ISEGMNS-J+1
      IF (J.EQ.2 ) THEN
      CSNEW(NSEC) = GW(NSEC)
      ELSE
      CSNEW(NSEC) = GW(NSEC) - WW(NSEC)*CSNEW(NSEC+1)
```

Listing of file "ads1.f" - continued

```
      ENDIF
310   CONTINUE

56    FORMAT (I3,7F10.2)
      RETURN
      END
```

Listing of file "dss1.f"

```
      SUBROUTINE  DSS1RP(INDSPS,IOUTS,ISEGMNS,SLOPESC)

C*****************************************************************
C THIS SUBROUTINE READS AND PREPARES INPUT DATA NEEDED BY THE
C DISPERSION (DSP) PACKAGE.
C*****************************************************************

      PARAMETER (MAXS = 200)
      PARAMETER (MAXTSTP = 400)
      IMPLICIT NONE
      INTEGER ISEGMNS,INDSPS, IOUTS,I
      DIMENSION SLOPESC(MAXS)
      REAL SLOPESC

      CHARACTER ANAME*24
C     CALL RARRAY TO READ IN STREAM SLOPE IN EACH CROSS SECTION

      ANAME = 'STREAM SLOPE'
      CALL RARRAYS(SLOPESC(1), ANAME,1,ISEGMNS,0,INDSPS,IOUTS)
      RETURN
      END
```

Table A2 List of variables appeared in MT3D modifications and SSTM development

Variable	Definition
ISEGMNS	number of stream cross sections
DTS	time step length in seconds
TRNOPS	array contains flags for major transport options in SSTM
ICBND	array contains index values for stream boundary conditions in stream sections icbnd < 0, concentration boundary cross section, otherwise variable Concentration cross section

Table A2 - continued

Variable	Definition
CONINT	array contains initial concentration for each cross section
SLOPESC	array contains streamed slope for each cross section
CSOLD	stream solute concentration in the old time step
CSNEW	stream solute concentration in the new time step
TRNOP	array contains flags for major transport options in MT3D
Q	discharge in stream cross section
A	area of stream cross section
B	width of stream cross section
QL	leakage from stream cross section to or from the aquifer
V	velocity in stream cross section
D	mean depth in stream cross section
ISTRM	layer, column and row of aquifer model cell that corresponds to the stream cross-section
SSR	
INBTNS	unit number of stream basic solute transport input file
INADVS	unit number of stream solute advection input file
INDSPS	unit number of stream solute dispersion input file
INSAIS	unit number of MODBANCH-SSTM interface file
IOUTS	unit number of SSTM output file
MAXS	maximum number of stream cross sections allowed in simulation
MAXTSTP	maximum number of time steps allowed in simulation
TUNITS	character variable represents units of time , T English, F Metric
LUNITS	character variable represents units of length , T English, F Metric
MUNITS	character variable represents units of mass , T English, F Metric
NSTEPS	number of time steps in SSTM
IJUMP	integer flag if not equal to zero the SSTM solution subroutines will be called
DSPL	Longitudinal dispersion coefficient in the stream